

Modern Physics

About the Authors



Gurbinder Kaur obtained her B.Sc. (Hons. Physics) and M.Sc. (Hons. Physics) from Guru Nanak Dev University, Amritsar. She then began her teaching career at DAV College, Amritsar, where she taught from 2004 to 2005. Her second academic appointment was at R R Bawa DAV College, Batala, where she served as Head of the Physics Department from 2005–2009. She then moved to Thapar University, Patiala, to pursue her research work in the field of solid oxide fuel cells (SOFC) and received her doctorate in 2012. She has published more than 25 research papers in the field of Materials Science. She has also carried on research in Biomedical Engineering and Bioglasses. She is the recipient of fellowship under the Research Fellowship in Sciences for Meritorious Students (RFSMS) scheme of University Grants Commission (UGC), including a fellowship under Women-Scientist Scheme, DST, New Delhi, from 2010–2012. After completing her doctorate, she moved to Virginia Tech, USA, to work as a post-doctoral fellow with Dr Gary R Pickrell. She is working on various materials and their applications including high-temperature energy materials, bioactive materials and optical materials.



Gary R Pickrell is Professor in the Department of Materials Science and Engineering. He is also the Director of the Nano-Bio Materials Laboratory at Virginia Tech, and the Associate Director of the Center for Photonics Technology in the Electrical and Computer Engineering Department, the largest academic fiber optic sensor research group dedicated to applications of sensors in harsh industrial environments. He also serves as the VT Director of Surface Engineering for the Commonwealth Center for Advanced Manufacturing, a partnership including Rolls Royce, Siemens, Canon, Sulzer Metco, Aerojet, Chromalloy, Newport News Shipbuilding, Virginia Tech, UVA, VSU, and the State of Virginia, among others. He has been a principal investigator on over 10 million dollars in funded research. His industrial experience includes positions as process engineer, research scientist, technical director, and member of the Board of Directors in various organizations. He was named a Faculty Fellow (2007–2010), Outstanding Assistant Professor (2005), and an R&D 100 Award winner (2004). He serves on the Editorial Boards of the *International Journal of Lean Six Sigma*, the *Journal of Nanotechnology and Energy*, the *New Journal of Glass and Ceramics*, and the *Journal Sensors*. He has authored or coauthored over 150 publications including 14 issued patents. His current research is focused on surface engineering, plasma spray coatings, random-hole optical fibers and optical fiber sensors, nanomedicine, nanotechnology, nanobiotechnology, glass, ceramic, and various other aspects of Materials Science and Engineering. Industrially, he has worked on the development of ceramic matrix and metal matrix porous infiltration preforms for 3–3 composite manufacturing.

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Gurbinder Kaur

*Materials Science and Engineering Department
Virginia Polytechnic Institute and State University,
Blacksburg, Virginia, USA*

Gary R Pickrell

*Professor, Materials Science and Engineering Department,
Director of Surface Engineering, Commonwealth Center for Advance Manufacturing
Director, Nano Bio Materials Laboratory
Associate Director, Center for Photonics Technology, Electrical and Computer Engineering
Virginia Polytechnic Institute and State University, Blacksburg, Virginia, USA*



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For my loving grandmother
Late Smt. Tripta Devi

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“An understanding of physics, and in particular modern physics, provides the best conceptual framework for graduate level work in any applied science or engineering field. As we design and structure materials and devices at ever decreasing dimensions, the effects of modern physics become inescapable.. Kaur and Pickrell provide an excellent text that in each chapter first outline objectives, then intertwine experimental physics history with clear concept explanations, equations, derivations, and example problems. Students engaged in internalizing the material will no doubt be better prepared to someday make their own contributions to human kind's advancement in science and technology.”

David Sherrer, President, Nuvotronics, LLC, USA

“The book with the title “Modern Physics” is truly modern in every sense and is an essential source of latest information to material scientists. It is a wonderfully written book and is structured extremely well with all nuances of latest principles and details of physics, which can be of immense use to beginners as well as experts. This book is a treasure chest of information, and stands as a testimony of the depth of authors' knowledge in varied technical fields and their dexterity in handling difficult subjects and making the same simple. Each chapter is conceived thoughtfully and interlaced with short descriptions of elite scientists who contributed immensely to research in physics. The system of providing questions and answers corresponding to each section of the chapter along with different categories of questions is highly innovative and unique. All these elements contributed towards a book that is easily readable and understandable. The authors succeeded in generating interest in the reader as he turns each page of the book making it captivating.”

Dr. Suresh M R, Scientist, ISRO, Thiruvananthapuram, India

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Preface

This book has emerged out of the notes made during our teaching of graduation and postgraduation classes, and from question papers of *UGC examinations*. We have prepared this text with the sole aim of providing a suitable book covering many topics common to various degree and postgraduate courses. Atomic physics is an indispensable study material for such courses, as it encompasses almost every aspect of physics, starting from classical to quantum mechanics. Irrespective of the areas in which the students plan to specialize, this subject helps in providing an insight and basic understanding into diverse branches of physics from which the authors conceived the idea of writing *Modern Physics*.

Target Audience

At the time of preparing this manuscript, the most important things taken into consideration were language and the main dictum, “a good book is one which can be read by a student with minimum guidance from his/her instructor.” Great care has been taken to keep the text as simple as possible. Every derivation step has been solved and analyzed rationally along with supplementing illustrations and diagrams. The manuscript begins with a thorough analysis of the subject in an easy-to-read style. It analyzes the basic concepts systematically and logically so that students can comprehend the subject with ease. Efforts have been made to present the subject matter in a simple and lucid style. This manuscript is designed creatively to serve as a textbook for undergraduate science and engineering students. Basically, it is a student-friendly book written in very simple language with step-by-step solutions of mathematical derivations.

Salient Features

The salient features of the book are the following:

- Comprehensive coverage to Quantum Mechanics, Nuclear and Particle Physics, Thermal Properties, Semiconductors, Electrostatics and Electronics, Optics and Lasers
- Clear exposition of background concepts
- Lucid, explanatory, and student-friendly language
- Interesting and innovative pedagogical features that inculcate interest in the subject:
 - Key terms—*list of significant words and abbreviations*
 - 85 interesting facts—*engaging and exciting facts within each chapter*
 - 500 solved examples—*fully worked problems following stepwise methodologies*
 - 350 micro-assessment questions—*topic-wise microquestions to assess conceptual understanding*
 - 360 critical thinking questions—*questions honing skills to think critically about a situation*
 - 420 graded chapterwise questions—*categorized into remember, understand, apply, and analyze*
 - 200 objective questions

Chapter Organization

Divided into eighteen chapters, this book gives a clear and concise understanding of the relationship between macro- and microlevels of physical phenomena.

Chapter 1 gives Einstein's theory of relativity, and its after-effects like length contraction and time dilation. **Chapters 2 to 4** describe the origin of quantum mechanics and its applications to the hydrogen-atom problem and different potential wells. **Chapter 5** deals with many of the successful and unsuccessful atomic models that describe the atomic and molecular structure of atoms, whereas **Chapters 6 to 9** demonstrate nuclear structure and nuclear models, detectors, elementary particles, and particle accelerators.

Chapter 10 emphasizes on charge and its properties along with fundamental description of electric field for different geometrical structures, electric potential, and the concept of polarization. The thermodynamic variables as well as the formalism of classical and quantum approach for different states are given in **Chapter 11**. **Chapters 12 and 13** cover the properties and theory of superconductors, basic structure of semiconductors and electronic devices made by different semiconductors.

Chapter 14 deals with lasers and their fundamental principle, whereas **Chapter 15** emphasizes on optoelectronic devices such as semiconductor laser diodes. Lattice structure and their types along with the packing of different atoms in crystals have been described in **Chapter 16**. **Chapter 17** describes the properties of monoatomic and diatomic lattice, free-electron theory and Sommerfeld theory. Finally, **Chapter 18** covers nanophysics and characterization techniques used to analyze the nanoparticles.

Hence, all the chapters are connected in such a way that the flow of contents is maintained. For example, before understanding of fiber optics and various optoelectronic devices (Chapter 15), the authors have demonstrated the basic principles of electronics (Chapters 12 and 13) and optics (Chapter 14). This flow is required to understand every physical phenomenon along with their gradual emergence in the form of various theories and their significance in day-to-day applications.

Every chapter is endowed with learning objectives, solved examples, summary, micro-assessment questions, critical thinking questions and graded questions, which are very helpful while preparing for competitive or professional examinations. Several interesting facts are embedded in each chapter, so that students can know some facts, not described as part of the text.

Online Learning Center

PowerPoint slides and overview of brief tutorials for every chapter have been provided on the Online Learning Center (OLC). In addition to this, some important brief lectures from Authors on their subject expertise have been given on the OLC. The OLC also has the model question papers, university pattern questions and links for additional resources

The facility can be availed by logging on to the following <http://www.mhhe.com/kaur/mp1> or by accessing the code given on the cover of the book.

Acknowledgements

A big *thank you* goes to McGraw Hill Education (India) for the time, promptness, perfection, and cordiality they provide to their authors. We thank all the reviewers for their useful comments and suggestions, which helped significantly in improving the manuscript. They deserve a special mention for sending us their feedback and suggestions.

Nataraj Sarma	<i>Bhaba Atomic Research Centre, Mumbai, Maharashtra</i>
Surjit Mukherjee	<i>The M S University of Baroda, Vadodara, Gujarat</i>
Hema Kanitkar	<i>University of Pune, Pune, Maharashtra</i>
K S Ramakrishnan	<i>Tamil Nadu Open University (TNOU), Chennai, Tamil Nadu</i>
Dr. Ravneet Kaur	<i>Guru Nanak Dev University, Amritsar</i>
Dr. Harpreet Kaur	<i>Guru Nanak Dev University, Amritsar</i>
Dr. Poonam Sharma	<i>Khalsa College, Jalandhar.</i>

Dr Gurbinder Kaur says thus: “Book writing has encompassed a wonderful time of my life during my stay in USA. During this journey, there have been many people who have knowingly and unknowingly helped me in successfully completing this project. At this overwhelming moment of accomplishment, first of all, I am indebted to two wonderful persons—Dr O P Pandey and Dr Kulvir Singh—whose understanding, encouragement, and personal attention have always provided decisive and energetic support. Dr Pandey was the one who stood by me during my struggling days (*thanks for believing in me more than I do*), whereas Dr Singh always invested extra hours in my work to churn the best out of it (*thanks for making me what I am*). I am short of adjectives for both of them as both have been an indispensable part of my journey.

“I would like to thank my mentor and co-author **Dr Gary R Pickrell**, who provided the most conducive and comfortable environment to me. He is one of the most wonderful persons and a superb scientist. All the faculties and staff members of the Physics Department (Guru Nanak Dev University), SPMS, (Thapar University) and MSE (Virginia Tech, USA) are acknowledged—who never turned me down whenever I approached them for any help. I cannot forget the support provided by Dr S S Sekhon during the toughest phase of my life. His motivation and zeal for hard work has enlightened my path always.

“This book gradually emerged among the friendships that provided their most lasting lessons. It is a pleasure to mention my good friends Gourav Singla, Dr Ravi Shukla, Paramjyot Kumar Jha, Jagdeep, Suresh Kumar, Dr Ranvir Panwar, Shalu Panwar, and Sunil Arya for always providing a fun-filled and supportive environment. I thank my unforgettable dear friends Samuel Jones, Hannah Beach, Nataynah, Shaumaya, Lynn Hagy, Shawn Martin, Heather Allbee, Eunice Ofori, Chrystal Akers, Yujie Cheng, Brian Scott, Daniel Homa, Edward Liang, Christopher Winkler, Amy Hill, Cindy Perdue, Susan Fleming Cook, Kim Grandstaff, Steve McCartney, and Andre Stevenson, all of whom made my working atmosphere very conducive.

“Finally, my most personal source of gratitude is my husband, my true soulmate, Dr Vishal Kumar, who is my enduring strength. During every downhill phase of my life, it was he who lifted up my spirits and helped me in innumerable ways. It is only and only due to him that I could put in many work hours tirelessly. Honestly, he sheltered me through every thick and thin and took the entire burden of responsibilities off my shoulders. He was very concerned about me sticking to my work schedule and kept reminding me about it along with my diet chart!

“I am highly thankful to my parents-in-law and parents for their support, encouragement, care, understanding and creation of a pleasant atmosphere for me. A special thanks to my father-in-law, Shri Surinder Kumar, and my father, Shri Harbhajan Singh, the strong pillars of my career, who have always motivated

me to fly high and change my dreams into reality. I am very lucky to have wonderful in-laws for whom I am more of a daughter than a daughter-in-law. I doubt if I will ever be able to convey my appreciation fully, but I owe them my eternal gratitude.

Besides this, above all, thanks to the Almighty beneath the blue sky for bestowing me with his precious blessings”

Dr Gary R Pickrell says thus: “I would like to acknowledge Dr Gurbinder Kaur for her diligence, persistence and vitality, for without these traits, this book would not have been possible. I feel honored to be able to coauthor this book with such a talented scientist. I would also like to acknowledge my wife, Claire, daughter, Lydia, and son, Alex, for their patience and support during the time when my work schedule became too hectic.”

Feedback Request

For further improvement of the book, readers are requested to post their comments and suggestions at the publisher’s email given below.

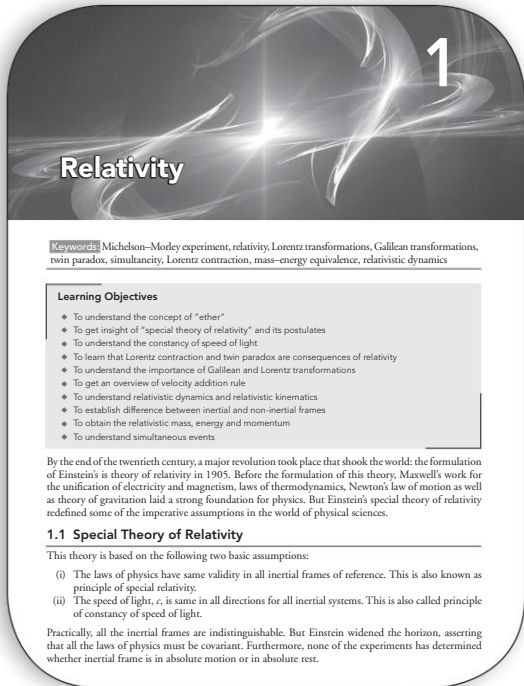
Gurbinder Kaur

Gary R Pickrell

Publisher’s Note

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Guided Tour



1

Relativity

Keywords: Michelson–Morley experiment, relativity, Lorentz transformations, Galilean transformations, twin paradox, simultaneity, Lorentz contraction, mass–energy equivalence, relativistic dynamics

Learning Objectives

- To understand the concept of “ether”
- To get insight of “special theory of relativity” and its postulates
- To understand the constancy of speed of light
- To learn that Lorentz contraction and twin paradox are consequences of relativity
- To understand the importance of Galilean and Lorentz transformations
- To get an overview of velocity addition rule
- To understand relativistic dynamics and relativistic kinematics
- To establish difference between inertial and non-inertial frames
- To obtain the relativistic mass, energy and momentum
- To understand simultaneous events

By the end of the twentieth century, a major revolution took place that shook the world: the formulation of Einstein’s theory of relativity in 1905. Before the formulation of this theory, Maxwell’s work for the unification of electricity and magnetism, laws of thermodynamics, Newton’s law of motion as well as theory of gravitation laid a strong foundation for physics. But Einstein’s special theory of relativity redefined some of the imperative assumptions in the world of physical sciences.

1.1 Special Theory of Relativity

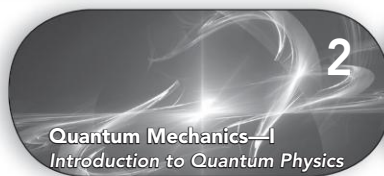
This theory is based on the following two basic assumptions:

- (i) The laws of physics have same validity in all inertial frames of reference. This is also known as principle of special relativity.
- (ii) The speed of light, c , is same in all directions for all inertial systems. This is also called principle of constancy of speed of light.

Practically, all the inertial frames are indistinguishable. But Einstein widened the horizon, asserting that all the laws of physics must be covariant. Furthermore, none of the experiments has determined whether inertial frame is in absolute motion or in absolute rest.

Each chapter begins with a set of **Keywords** and **Learning Objectives** to guide and motivate the student about the significant words, abbreviations and important topics discussed in the chapter.

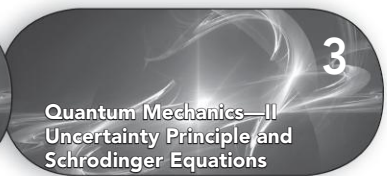
The text focuses on a detailed coverage of Quantum mechanics, Thermal Properties, Semiconductors, Electronics, Optics and Lasers with clear exposition of background concepts



2

Quantum Mechanics—I

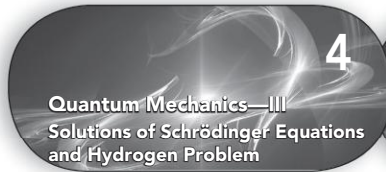
Introduction to Quantum Physics



3

Quantum Mechanics—II

Uncertainty Principle and Schrödinger Equations



4

Quantum Mechanics—III

Solutions of Schrödinger Equations and Hydrogen Problem



12

Superconductors and Semiconductors



13

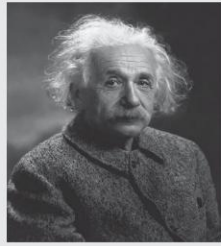
Electronic Devices



14

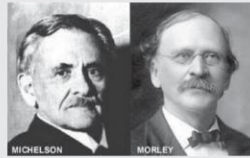
Lasers

Albert Einstein was born on March 14, 1879 in Ulm, Germany. He was one of the most renowned physicists and a Nobel laureate who gained worldwide fame due to his extraordinary theories of relativity. He was the backbone and pillar of physics. He lived with his family in Munich and had an electronic equipment store. Einstein did not talk much till the age of 3 years. As he grew up, he developed an interest in nature and complicated theories of arithmetic. At the age of 12 years, Einstein was aware of geometry. When Einstein was 15 years old, he left Germany due to a constant failure in their business. He and his family settled in Milan where Einstein spent a year with them. To survive, he had to make his own living. He did his secondary school from Switzerland and afterwards joined Swiss National Polytechnic, which was located in Zurich. Einstein used to bunk the classes and play violin, as he did not like the teaching method. He cleared his exams with the help of his classmate and graduated in 1900.



ALBERT EINSTEIN

Albert Abraham Michelson was born on December 19, 1852 Strzelino, Provinz Posen, in the Kingdom of Prussia, to a Jewish family. Michelson's childhood was in the rough mining towns of Murphy's Camp, California and Virginia City, Nevada. His father worked as a trader. After completing his high school education in San Francisco, he went to Annapolis as an appointee of President U.S. Grant.



A.A. MICHELSON & E.W. MORLEY

Albert Abraham Michelson was the first American who was awarded a Nobel Prize in Physics for his optical precision instruments and the spectroscopic and metrological investigations carried out with their aid. He stepped up his career and did teaching as well as got research positions at the Case School of Applied Science, the Naval Academy, Clark University and University of Chicago. Michelson executed his most successful experiment with the chemist Edward W. Morley at Cleveland. Light waves were considered to travel in ether medium. The speed of light would have been different in each direction, if light source would have been moving through ether. In contrast, the Michelson-Morley experiment demonstrated equal time taken by two beams of light, which passed out and reflected back at right angles to each other. Hence, the concept of stationary ether had to be discarded. He established the speed of light to be a fundamental constant using spectroscopic and metrological investigations along with Morley. Michelson with his colleague Francis G. Pease measured the diameter of super-giant star, Betelgeuse, using astronomical interferometer. Michelson won the Copley Medal, the Henry Draper Medal in 1916, and the Gold Medal of the Royal Astronomical Society in 1923. In addition, a crater on the Moon is also named after him. While working on a more refined measurement of the velocity of light in Pasadena, California, on May 9, 1931, Michelson left this world.

85 Engaging and Exciting Facts are spread out in the text to enable students get a glimpse of the history of certain inventions and discoveries, and the biographies of pioneering scientists.

Over 450 illustrations help clarify the concepts.

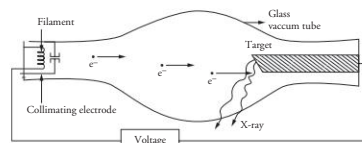


Figure 2.10 X-ray tube.

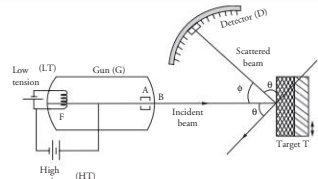


Figure 3.1 The Davison-Germer experimental setup.

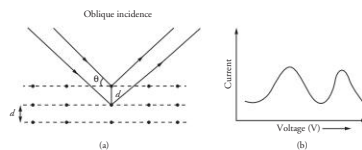


Figure 3.2 (a) Bragg's Reflection and (b) current versus voltage for oblique incidence.

SOLVED PROBLEMS

Q. 1: The de-Broglie wavelength of an electron is 4 \AA . Calculate its momentum.

Ans: $\lambda = 4 \text{ \AA}$

According to de-Broglie hypothesis,

$$\lambda = \frac{h}{mv}$$
$$mv = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34}}{4 \times 10^{-10}}$$
$$p = 1.65 \times 10^{-24} \text{ kg m/s}$$

Q. 2: The speed of a proton is 10^5 m/s . Calculate its de-Broglie wavelength.

Ans:

Velocity of proton = 10^5 m/s

Mass of proton = $1.67 \times 10^{-27} \text{ kg}$

According to de Broglie relation

$$\lambda = \frac{h}{mv}$$
$$\lambda = \frac{6.63 \times 10^{-34}}{1.67 \times 10^{-27} \times 10^5}$$
$$\lambda = \frac{6.63 \times 10^{-2}}{1.67} = 3.97 \times 10^{-2} \text{ m.}$$

500 fully worked-out Solved Examples with stepwise methodologies are given in the text to help reinforce the understanding of concepts and illustrate the way for solving problems.

A Summary at the end of each chapter helps reinforce the learning objectives and summarize the concepts.

SUMMARY

The chapter deals with the Heisenberg's uncertainty principle, de-Broglie hypothesis and Schrödinger formulation of wave equations. de-Broglie hypothesis states that the moving particles always have matter waves associated with them. These matter waves are also known as de-Broglie waves. Davisson and Germer performed the experiments to prove the presence of matter waves associated with electron. But, then it was found that waves do not travel as a single wave, rather as a wave packet. Many waves interfere with each other to form a wave packet. Wave packet travels with group velocity (v_g) and every individual wave travels with a phase velocity (v_p). Furthermore, the relation of equivalence of group and phase velocity is established. But, it was well demonstrated by Heisenberg that the position and momentum cannot be measured accurately simultaneously, that is, if position is measured with greater accuracy, then the momentum remains uncertain and vice versa. The product of uncertainties of position and momentum are greater than or equal to Planck's constant. The need of differential equations was there, as exact location and momentum of particle could not be determined. Hence, the probabilistic approach is required. Hence, differential equation describes the motion of particles. Schrödinger used wave functions for the formulation of Schrödinger's equation. Wave functions are continuous, single-valued, and finite at every point in the space. The expectation values have been used to obtain uncertainty principle. The product of two wave functions satisfying Schwarz inequality has also been demonstrated. The bridge between classical and quantum mechanics is demonstrated by Ehrenfest theorem. Eigen values and Eigen value equations have also been explained for different operators.

Micro-Assessment Questions

1. What is radioactivity?
2. Which nuclei are considered as radioactive nuclides?
3. What are α -particles?
4. Give the description of radioactive particles.
5. How does penetration power vary for α -, β -, and γ particles?
6. Which radioactive particle exhibits highest ionizing power?
7. γ -rays are not deflected by electric or magnetic field. Explain.
8. Which radioactive particles are deflected toward positive plate?
9. What are β -particles?
10. When is the atomic number of a nuclide increased by one unit?
11. Give the units of radioactivity.
12. Which properties are conserved during α -decay?
13. What is disintegration energy?
14. Write down the relation between range and energy of particle.
15. Define the disintegration constant.
16. Write down the relation between disintegration constant and number of atoms in substance.
17. Give the relation between disintegration constant and range of particle.

350 Micro-Assessment Questions, distributed over the chapters, enable the student to assess conceptual understanding through topicwise microquestions.

Graded Questions

1. Write in detail the principle, working, and construction for Van de Graaff generator. Which type of particles can be accelerated using Van de Graaff generator?
2. Explain in detail the principle construction and working of cyclotron.
3. Describe the principle, working, and construction of Cockcroft–Walton machine.
4. Write in detail the principle, working, and construction for the betatron. How is the problem of “loss of resonance” resolved?
5. Explain in detail the working of electron synchrotron. How does its working differ from proton synchrotron?
6. Describe the principle, working, and construction for synchrocyclotron. What is the frequency of particle revolution?

420 Graded Questions test the student's understanding of the key concepts.

200 Objective Questions (with Answers) are given in the book to help students have a quick recap of important terms and concepts.

OBJECTIVE QUESTIONS

1. Which is the electrostatic accelerator?
(a) Van de Graaff generator
(b) Cockcroft–Walton machine
(c) Both (a) and (b)
(d) none of these
2. Which of the following is cyclic accelerator?
(a) betatron
(b) synchrocyclotron
(c) synchrotron
(d) all of these
3. Van de Graaff Generator could accelerate particles up to.
(a) 10 MeV
(b) 5 MeV
(c) 20 MeV
(d) 50 MeV

Critical Thinking Questions

1. Give any two laws of probability.
2. Calculate the percentage error in Sterling formula when $n = 3$.
3. What do you understand by phase space?
4. What should be the minimum size for a phase space cell according to quantum and mechanics?
5. Give the various microstates and macrostates for system with two distinguishable particles.
6. Describe briefly the two main classifications for statistics.
7. What are the assumptions for Bose–Einstein statistics?
8. Explain how Fermi–Dirac statistics could be applied to electron gas?
9. Give the derivation for Maxwell–Boltzmann statistics.
10. What do you understand by photon gas?
11. The identical gas molecules are treated distinguishable classically. Explain.
12. Define cells for a compartment.
13. What is the meaning and importance of “a priori probability”?

360 Critical Thinking Questions help students develop skills to critically analyze a situation and reach a solution.

Remember and Understand section at the end of each chapter further helps drill in the concepts.

Remember and Understand

1. The macroscopic behavior of a system is identified by the compartments. Each compartment has definite energy, momentum, velocity, and specific volume.
2. Thermodynamic probability depends upon nature of particles. In other words, it treats particles to be distinguishable or indistinguishable.
3. All the distinct arrangements of particles are termed macrostates for the particles.
4. When the particle is at rest, only three position coordinates are required to define the state that is, x , y , z . But when the particle is moving, then momentum coordinates are

Relativity

Keywords: Michelson–Morley experiment, relativity, Lorentz transformations, Galilean transformations, twin paradox, simultaneity, Lorentz contraction, mass–energy equivalence, relativistic dynamics

Learning Objectives

- ◆ To understand the concept of “ether”
- ◆ To get insight of “special theory of relativity” and its postulates
- ◆ To understand the constancy of speed of light
- ◆ To learn that Lorentz contraction and twin paradox are consequences of relativity
- ◆ To understand the importance of Galilean and Lorentz transformations
- ◆ To get an overview of velocity addition rule
- ◆ To understand relativistic dynamics and relativistic kinematics
- ◆ To establish difference between inertial and non-inertial frames
- ◆ To obtain the relativistic mass, energy and momentum
- ◆ To understand simultaneous events

By the end of the twentieth century, a major revolution took place that shook the world: the formulation of Einstein’s theory of relativity in 1905. Before the formulation of this theory, Maxwell’s work for the unification of electricity and magnetism, laws of thermodynamics, Newton’s law of motion as well as theory of gravitation laid a strong foundation for physics. But Einstein’s special theory of relativity redefined some of the imperative assumptions in the world of physical sciences.

1.1 Special Theory of Relativity

This theory is based on the following two basic assumptions:

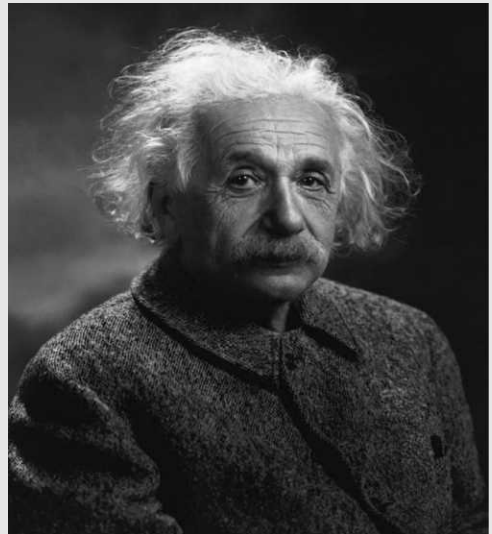
- (i) The laws of physics have same validity in all inertial frames of reference. This is also known as principle of special relativity.
- (ii) The speed of light, c , is same in all directions for all inertial systems. This is also called principle of constancy of speed of light.

Practically, all the inertial frames are indistinguishable. But Einstein widened the horizon, asserting that all the laws of physics must be covariant. Furthermore, none of the experiments has determined whether inertial frame is in absolute motion or in absolute rest.

All the electromagnetic waves travel with a velocity, $c = 3 \times 10^8$ m/s, and have both electric and magnetic field vectors perpendicular to each other as well as to the direction of propagation of wave. This speed of light is the zenith or upper limit for all waves and material particles as well as for transmission. The Newtonian mechanics basically deals with low speeds, but it cannot describe the particles moving approximately with the speed of light. Although Newtonian mechanics can describe other important phenomena, it reveals that the velocity of a particle becomes $1.98c$ when accelerated by a potential four times greater than its original value. But, at the same time, it has been experimentally proven that the velocity of any particle in universe cannot exceed the velocity of light and is independent of voltage applied. Hence, we can conclude that Newtonian approach is a limiting factor to Einstein's approach. To support this notion, CERN particle-physics laboratory conducted an experiment in 1964. They measured the velocity of γ -rays emitted from unstable short-lived neutral pions to be 2.9977×10^8 m/s which is acceptable compared to velocity of light. Although the research used high-velocity source of neutral pions with a velocity of $0.99975c$, it did not affect the velocity of γ -rays.

This chapter basically deals with the transformations that occur when a particle moves from one frame to another in a specific coordinate system. This chapter is an attempt to collect the intellectual contribution made by Albert Einstein to the world of physics.

Albert Einstein was born on March 14, 1879 in Ulm, Germany. He was one of the most renowned physicists and a Nobel laureate who gained worldwide fame due to his extraordinary theories of relativity. He was the backbone and pillar of physics. He lived with his family in Munich and had an electronic equipment store. Einstein did not talk much till the age of 3 years. As he grew up, he developed an interest in nature and complicated theories of arithmetic. At the age of 12 years, Einstein was aware of geometry. When Einstein was 15 years old, he left Germany due to a constant failure in their business. He and his family settled in Milan where Einstein spent a year with them. To survive, he had to make his own living. He did his secondary school from Switzerland and afterwards joined Swiss National Polytechnic, which was located in Zurich. Einstein used to bunk the classes and play violin, as he did not like the teaching method. He cleared his exams with the help of his classmate and graduated in 1900. His teachers did not consider Einstein a good student. Einstein married his classmate Mileva Maric in 1903. He had two sons with her but they later divorced. He was awarded doctorate in 1905 University of Zurich. His thesis was based on the different sizes and extent of molecules. In 1905, Einstein's paper was published on dynamics of bodies in motion. Later on, this was known as the theory of relativity. Einstein was capable of explaining physical actions and measures for varying inertial positions without assuming about the matter or radiation's nature, or their interaction. But practically, Einstein's argument was not understood by any one and his work was not appreciated by others. The innovation in Einstein's postulates made it difficult for his colleagues to understand his work. Einstein was supported by Max Planck during his work.



ALBERT EINSTEIN

In 1907, Einstein left his job at patent office and started working on the theory of relativity. Einstein explained changes in the orbital movement of planets on the grounds on general theory of relativity. In 1919, Einstein got worldwide fame when his theory was confirmed throughout the eclipse of the sun. In 1921, Einstein received Nobel Prize in physics. Einstein supported pacifism and Zionism movement, and many a times, he was attacked by Germans because of his continuous support for Zionists and pacifists. When Hitler gained power, Einstein left Germany and moved to the United States. He joined the Institute of



Advanced Study at Princeton, New Jersey. Einstein left Princeton on 18 April 18 18, 1955. The whole scientific community mourned over the death of this genius.

1.2 Michelson–Morley Experiment

In 1887, American physicist A.A. Michelson and E.W. Morley conducted a famous experiment for detecting changes in speed of light due to ether medium.

When an observer moves towards a stationary light source, it should measure velocity greater than c . Similarly, if a light source or observer moves away then the velocity should be less than c . If c is the velocity of light and u is the velocity of the observer, then for the former case, it is $c + u$ and for the latter it is $c - u$. For an observer, if light propagates at right angle, then the relative speed of the observer is $\sqrt{c^2 - u^2}$.

The validity of these assumptions was investigated by Michelson and Morley. The experimental tool used by them was Michelson interferometer as shown in Figure 1.1. M_1 and M_2 are two mirrors aligned perpendicular to each other, whereas mirror M_0 splits the beams

This interferometer is based on interference patterns produced by visible light. Monochromatic light splits into two coherent beams. These split beams produce interference pattern after traveling through different paths and then recombining. The interference pattern constitutes alternative bright and dark fringes due to constructive or destructive interference, respectively. The formation of these beams is highly phase dependent, as any change in phase difference will cause a shift in the position of the interference fringes. The Michelson apparatus was mounted on retractable heavy base in order to make observations at different orientations.

Details of the Experiment

Let us assume that both the arms of interferometer have equal length, L . If we consider the beam moving parallel to ether wind, then the speed of beam is $c - u$, according to Newtonian mechanics. During its return journey, the velocity of beam should be $c + u$. Thus, if a beam moves from left to

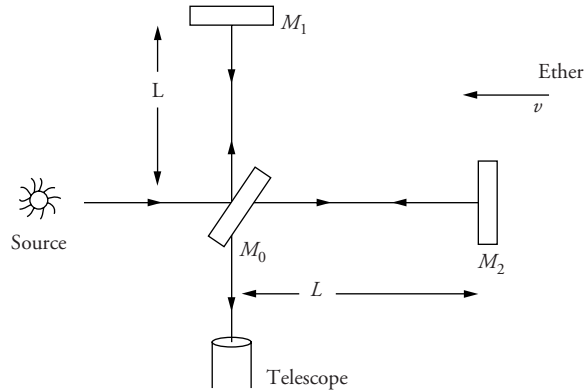


Figure 1.1 The Michelson interferometer used by Michelson–Morley.

right, that is, in a direction opposite to ether wind, then the time of travel is $\frac{L}{c-u}$, and accordingly, the time of travel from right to left is $\frac{L}{c+u}$. The total time for a round trip is

$$t_1 = \frac{L}{c-u} + \frac{L}{c+u} \quad (1)$$

$$t_1 = \frac{c+u+c-u}{c^2-u^2} = \frac{2cL}{c^2-u^2} = \frac{2L}{c} \left(1 - \frac{u^2}{c^2}\right)^{-1}$$

Consider the second case when the beam moves in perpendicular direction as shown in Figure 1.1.

The speed of beam relative to earth is $(c^2 - u^2)^{1/2}$ and the total time for a round trip is $\frac{2L}{(c^2 - u^2)^{1/2}}$:

$$t_2 = \frac{2L}{c} \left(1 - \frac{u^2}{c^2}\right)^{-1/2} \quad (2)$$

The time difference between a horizontally and perpendicularly traveling beam is

$$\Delta t = t_2 - t_1 = \frac{2L}{c} \left(1 - \frac{u^2}{c^2}\right)^{-1/2} - \frac{2L}{c} \left(1 - \frac{u^2}{c^2}\right)^{-1} \quad (3)$$

We can solve the expression using binomial expansion.

$$\text{That is, } (1-x)^n = 1 - nx - nx^2 \dots$$

$$\text{and for } x \ll 1 \quad (1-x)^n = 1 - nx$$

In this case, $x = \frac{u^2}{c^2} \ll 1$, therefore

$$\Delta t = t_2 - t_1 = \frac{2L}{c} \left[1 + \frac{u^2}{c^2} - 1 - \frac{u^2}{2c^2} \right]$$

$$\Delta t = t_2 - t_1 = \frac{2L}{c} \left(\frac{u^2}{2c^2} \right) = \frac{Lu^2}{c^3}$$

$$\Delta t = \frac{Lu^2}{c^3}$$

Hence, the corresponding path difference before rotation is

$$\Delta = c\Delta t = \frac{Lu^2}{c^2}$$

and after rotation is also $\frac{Lu^2}{c^2}$. Therefore, the total path difference is $\frac{2Lu^2}{c^2}$ and the corresponding fringe shift can be obtained by dividing by wavelength of light, λ .

i.e. Shift of 1 fringe = change in path of 1 wavelength

$$\text{Shift } (n) = \frac{2Lu^2}{\lambda c^2} \quad (4)$$

For Michelson experiment, $L = 11 \text{ m}$, $u = 3 \times 10^4 \text{ m/s}$ and $\lambda = 500 \text{ nm}$

$$\text{Shift } n = 0.44 \quad (5)$$

The sensitivity of Michelson interferometer was $n = 0.01$. These pioneer scientists repeated the experiments many times but did not find any fringe shift even after setting the apparatus in different orientations relative to the orbital motion of earth. Hence, the conclusion was that no luminiferous ether exists. A lot of efforts were made to prove these results, especially by Lorentz and Fitz Gerald. They assumed that the length of an object moving with speed u will contract along the direction of travel.

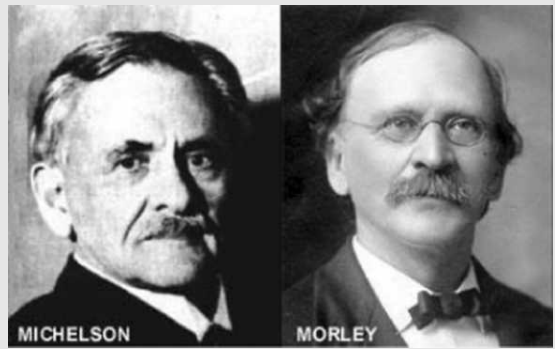
The factor of contraction was $\sqrt{1 - \frac{u^2}{c^2}}$. This contraction would further lead to contraction of one arm of the interferometer and hence result in no path difference. But, the following many new set of questions also need to be answered:

1. If ether does not exist, what is the reference frame for velocity as they are relative quantities?
2. How do Galilean transformations not reconcile with measurement of velocity of light? Even if flaw exists in them, the transformations are valid in everyday experience.
3. What are the alternative correct transformations if Galilean transformations have flaws?
4. How can we understand light waves? Sound waves always require material medium for their propagation unlike light waves. How can light waves carry energy without any medium?

Many of these questions were answered by A. Einstein when he set a special stage with his special theory of relativity.

Albert Abraham Michelson was born on December 19, 1852 Strzelno, Provinz Posen, in the Kingdom of Prussia, to a Jewish family. Michelson's childhood was in the rough mining towns of Murphy's Camp, California and Virginia City, Nevada. His father worked as a trader. After completing his high school education in San Francisco, he went to Annapolis as an appointee of President U.S. Grant.

Albert Abraham Michelson was the first American who was awarded a Nobel Prize in Physics for his optical precision instruments and the spectroscopic and metrological investigations carried out with their aid. He stepped up his career and did teaching as well as got research positions at the Case School of Applied Science, the Naval Academy, Clark University and University of Chicago. Michelson executed his most successful experiment with the chemist Edward W. Morley at Cleveland. Light waves were considered to travel in ether medium. The speed of light would have been different in each direction, if light source would have been moving through ether. In contrast, the Michelson–Morley experiment demonstrated equal time taken by two beams of light, which passed out and reflected back at right angles to each other. Hence, the concept of stationary ether had to be discarded. He established the speed of light to be a fundamental constant using spectroscopic and metrological investigations along with Morley. Michelson with his colleague Francis G. Pease measured the diameter of super-giant star, Betelgeuse, using astronomical interferometer. Michelson won the Copley Medal, the Henry Draper Medal in 1916, and the Gold Medal of the Royal Astronomical Society in 1923. In addition, a crater on the Moon is also named after him. While working on a more refined measurement of the velocity of light in Pasadena, California, on May 9, 1931, Michelson left this world.



A.A. MICHELSON & E.W. MORLEY

1.3 Galilean Transformations

To describe the position of an object in space, a coordinate system is required that defines every position for particles using its unique set of coordinates. The coordinate space system defines the reference frame. The reference frames without acceleration are called inertial frames of reference.

All laws of physics are valid in every inertial frame of reference according to the special theory of relativity. But depending on reference frame of the observer, they can see things differently, that is, the sequence of events can be different (Figure 1.2).

An event is something that happens independently w.r.t. reference frame. Suppose there are two reference frames, S and S' . Both frames are inertial and an event P has (x, y, z, t) set of coordinates w.r.t. S frame, whereas it has (x', y', z', t') set of coordinates w.r.t. reference frame S' . Frame S' moves with speed u w.r.t. frame S (Figure 1.3).

It is important to establish the equivalence of a set of observations made in different reference frames. Such a procedure is called transformation. If the transformation of formulation made by an observer gives the same result as made by another observer, then the laws are invariant. The transformations that are in agreement with Newtonian conception of motion are called Galilean transformations. That

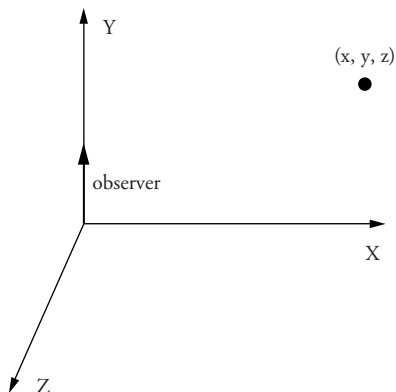


Figure 1.2 An observer in a reference frame, which describes position as (x, y, z) .

is the reason why a relation between (x, y, z, t) and (x', y', z', t') is required. The main concern is time. Time is an invariant quantity according to Newtonian mechanics. Hence, if both the observers in frame S and S' used synchronized watches and recorded an event at the same instant, then

$$t = t' \quad (6)$$

Now for position coordinates, we have to find a relation. As x -coordinate is recorded to be greater for S frame than S' frame, that is, the difference is ut . Hence,

$$x = x' + ut \quad (7)$$

No relative motion is observed for y and z . Hence

$$y = y' \quad (8)$$

$$z = z' \quad (9)$$

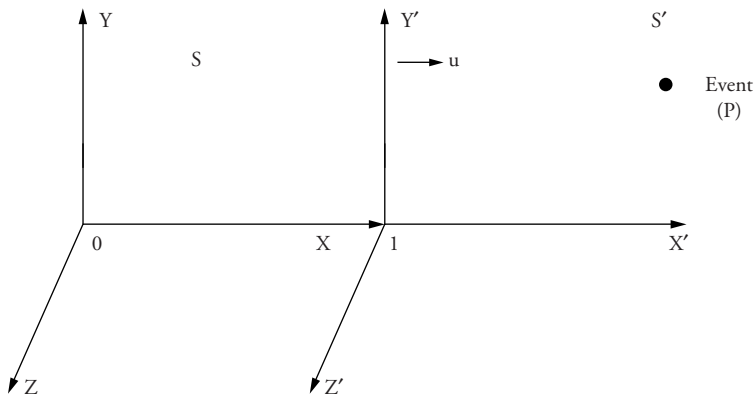


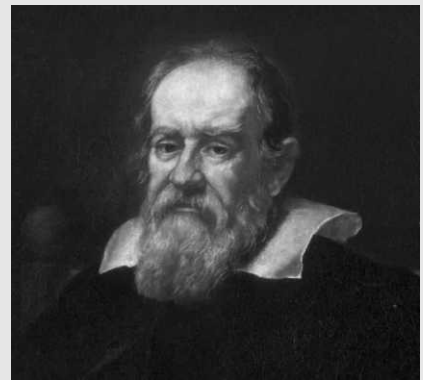
Figure 1.3 Observer in S' frame is moving with velocity u .

These four equations constitute inverse Galilean transformations. Hence, we obtain systematic conversion of position–time coordinates from one reference frame to other. Therefore, the Galilean transformations can be summarized as

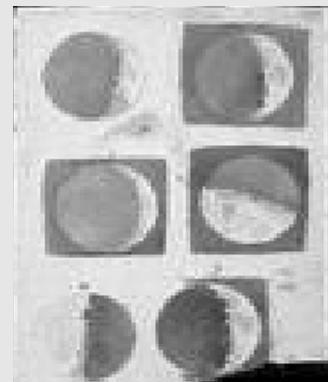
$$\left. \begin{aligned} x' &= x - ut \\ y' &= y \\ z' &= z \\ t' &= t \end{aligned} \right\} \quad (10)$$

Born on February 15, 1564 in Pisa, Galileo was an Italian physicist, astronomer, mathematician and philosopher. He used refracting telescope for the first time and supported Copernicanism. Galileo has been called the “father of modern observational astronomy”, “father of modern physics”. Sir Isaac Newton used Galileo’s mathematical descriptions, “The Law of Inertia”, as the foundation for his “First Law of Motion”. Galileo studied motion of uniformly accelerated objects and kinematics. He was a professor of astronomy at University of Pisa and taught conventional theory that the sun and all other planets revolved around the Earth. Later on, at the University of Padua, he was influenced by the theory of Nicolaus Copernicus that the Earth and all the other planets revolved around the sun; in other words, he agreed with Copernicus’s sun-centered or heliocentric theory. In 1615, Galileo was in big trouble with the Roman Catholic Church for the support of heliocentric theory.

In February 1616, he was cleared of any offence and Galileo was warned to abandon his support for heliocentric theory. But his views were published in 1632 in *Dialogue Concerning the Two Chief World Systems*, and he was found “vehemently suspect of heresy” and forced him to publicly withdraw his support for Copernicus. He was sentenced to life imprisonment, but due to his old age, he was allowed to serve his term at his house. Galileo became blind at the age of 72 years due to damage done to his eyes by constant telescopic observations. Actually, he was blinded by cataract and glaucoma. In 1642, Galileo died at Arcetri and the same year Isaac Newton was born to continue his findings.



GALILEO



Moon phase drawing by Galileo

1.4 Galileo Velocity Addition Rule

According to Galilean transformation, the event was considered to be at rest. But if the event is also moving, then we have to evaluate the relations. According to Newtonian physics, $v = dx/dt$, hence differentiating Equations (10)

$$\frac{dx'}{dt} = \frac{dx}{dt} - u$$

$$v'_x = v_x - u \quad (11a)$$

$$\frac{dy'}{dt} = \frac{dy}{dt}$$

$$v'_y = v_y \quad (11b)$$

$$\frac{dz'}{dt} = \frac{dz}{dt}$$

$$v'_z = v_z \quad (11c)$$

If Eqn. 11(a)–(c) are combined, then

$$v' = v - u \quad (12)$$

These results are known as classical velocity addition theorem, and it summarizes the transformations of velocities between the Galilean reference frames. Hence, like position, velocity is also relative and depends on the reference frame. If $u = 0$, then $v = v'$; similarly, we can obtain the relation between accelerations from the two reference frames S and S'.

Differentiate Equations 11(a)–(c) w.r.t. time

$$\frac{dv'_x}{dt} = \frac{dv_x}{dt} - \frac{du}{dt} \quad (u \text{ is constant})$$

$$a'_x = a_x \quad (12a)$$

$$\frac{dv'_y}{dt} = \frac{dv_y}{dt}$$

$$a'_y = a_y \quad (12b)$$

$$\frac{dv'_z}{dt} = \frac{dv_z}{dt}$$

$$a'_z = a_z \quad (12c)$$

Hence, according to Galilean transformations, acceleration is an invariant quantity. Mass is also invariant and the invariance of force automatically follows, that is, $F = ma$. If the velocity of an event is equal to the velocity of a reference frame, then $v' = 0$. Hence, we can summarize this concept as follows:

1. Position and velocity are relative measures, hence measurements in S and S' will differ. Whereas measurements for time, mass and acceleration are same in all reference frames and these quantities are invariant.
2. To convert (x, y, z, t) to (x', y', z', t') , we need transformation equations.

Newton wrote in his work Principia in 1687, "All motions may be accelerated and retarded, but the flowing of absolute time is not liable to any change ... the existence of things remain the same, whether the motions are swift or slow, or none at all".

1.5 Lorentz Transformations

In 1890, a Dutch physicist Lorentz worked on Maxwell's equations to make them covariant. He gave an approach for inertial frames whether stationary or moving, so that the equations are equivalent and undistinguishable.

At higher velocities, Galilean velocities were no longer valid, that is, the accurate coordinate equations should be derived for the particles moving in the range $0 \leq v \leq c$. Hence, Lorentz coordinate transformations describe only such set of equations in the best way. Lorentz transformation relates the space–time coordinates for observers moving with relative speed v . Lorentz velocity transformation is the set of equations relating velocity of particle in reference frame S, that is, (u_x, u_y, u_z) , to velocity in S' frame (u'_x, u'_y, u'_z) (moving with speed v) (see Figure 1.3 for deriving). x' and x can be related as

$$x' = x - vt$$

But if the coordinates are at $t = t' = 0$, then dependence can be given by (Figure 1.4)

$$x' = G(x - vt) \quad (13)$$

where G is a dimensionless factor depending on v/c such that $G \rightarrow 1$ as $v/c \rightarrow 0$.

The inverse Lorentz transformation can be written as

$$x = G(x' + vt') \quad (14)$$

This is in accordance with Einstein's first postulate of relativity, which requires the criteria of fulfillment of the same form of laws of physics in all reference frames. (Only the sign of v has changed)

By substituting Eqn. (13) in (14), we obtain

$$t' = G \left[t + \left(\frac{1}{G^2} - 1 \right) \frac{x}{v} \right] \quad (15)$$

Differentiating Eqs (13) and (15), we obtain

$$dx' = G(dx - vdt) \quad (16)$$

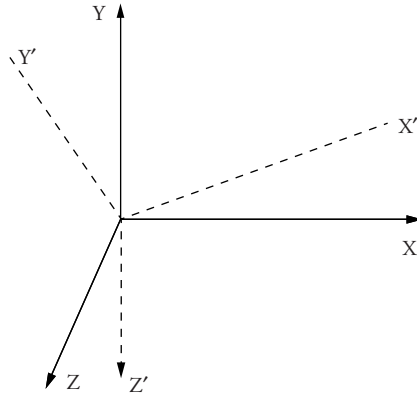


Figure 1.4 Orientation of S and S'.

$$dt' = G \left[dt + \left(\frac{1}{G^2} - 1 \right) \frac{dx}{v} \right] \quad (17)$$

As $u'_x = \frac{dx'}{dt'}$, dividing Eqn. (16) by (17)

$$u'_x = \frac{dx'}{dt'} = \frac{(dx - vdt)}{\left(dt + \left(\frac{1}{G^2} - 1 \right) \frac{dx}{v} \right)} \quad (18)$$

$$u'_x = \frac{dx'}{dt'} = \frac{\left(\frac{dx}{dt} - v \right)}{\left(\frac{dt}{dt} + \left(\frac{1}{G^2} - 1 \right) \frac{dx}{vdt} \right)} \quad (19)$$

$$u'_x = \frac{dx'}{dt'} = \frac{(u_x - v)}{\left(1 + \left(\frac{1}{G^2} - 1 \right) \frac{u_x}{v} \right)} \quad (20)$$

According to Einstein's second postulate, the velocity of light is the constant and c for any observer i.e. $u_x = c$ and $u'_x = c$.

This substitution in eqn. 20, leads to

$$c = \frac{c - v}{1 + \left(\frac{1}{G^2} - 1 \right) \left(\frac{c}{v} \right)} \quad (21)$$

$$\text{i.e. } G = \frac{1}{\sqrt{1 - \left(\frac{v^2}{c^2}\right)}} = \gamma \quad (22)$$

Hence, Eqn. (17) is transformed as

$$x' = \gamma(x - vt) \quad (23)$$

and similarly Eqn. (18) is transformed as

$$x = \gamma(x' + vt') \quad (24)$$

For obtaining the transformation equation for time, substituting G to Eqn. (19)

$$t' = \gamma \left[t - \frac{vx}{c^2} \right] \quad (25)$$

No motion is along y and z direction.

Hence, we can write:

$$\left. \begin{array}{l} y' = y \\ z' = z \end{array} \right\} \quad (26)$$

Summarizing all the equations:

$$\left. \begin{array}{l} x' = \gamma(x - vt) \\ y' = y \\ z' = z \\ t' = \gamma \left[t - \frac{vx}{c^2} \right] \end{array} \right\} \quad (27)$$

Inverse transformation of an event happening in S' frame can be obtained by replacing v with $-v$ and changing prime to unprime or vice versa. This leads to

$$\left. \begin{array}{l} x = \gamma(x' + vt') \\ y = y' \\ z = z' \\ t = \gamma \left[t' + \frac{vx'}{c^2} \right] \end{array} \right\} \quad (28)$$

If we observe Eqs (27) and (28), we find that t and t' are dependent on x and x' unlike Galilean transformation in which $t = t'$. At low speeds, that is, $v \ll c$, the Lorentz transformations reduce to Galilean transformations.

For velocity transformations, substitute the value of G in Eqn. (20):

$$u'_x = \frac{u_x - v}{\left[1 - \frac{u_x v}{c^2}\right]} \quad (29)$$

Similarly, if the object possesses velocity along y and z directions, then the components in S' are obtained as

$$u'_y = \frac{dy'}{dt'} = \frac{u_y}{\gamma \left[1 - \frac{u_x v}{c^2}\right]} \quad (30)$$

$$\text{and} \quad u'_z = \frac{dz'}{dt'} = \frac{u_z}{\gamma \left[1 - \frac{u_x v}{c^2}\right]} \quad (31)$$

If u_x and v are small, then for the non-relativistic case, we obtain Galilean velocity transformation equations as $u'_x = u_x - v$. If $u_x = c$, then u'_x also becomes c . Hence, we conclude that an object moving with speed c w.r.t. frame S also possesses the same velocity w.r.t. frame S' . In addition, the velocity of any object can never exceed velocity of light.

The inverse velocity transformations can be summarized as

$$\left. \begin{aligned} u_x &= \frac{(u'_x + v)}{\left(1 + \frac{u'_x v}{c^2}\right)} \\ u_y &= \frac{u'_y}{\gamma \left[1 + \frac{u'_x v}{c^2}\right]} \\ u_z &= \frac{u'_z}{\gamma \left[1 + \frac{u'_x v}{c^2}\right]} \end{aligned} \right\} \quad (32)$$

Hendrik Antoon Lorentz was born on July 18, 1853 in Arnhem, Gelderland, to a Dutch family. He was the son of Gerrit Frederik Lorentz, who was a well-off nurseryman, and Geertruida van Ginkel (mother). In 1862, his father married Luberta Hupkes after his mother's death. He was a freethinker in religious matters despite being raised as a Protestant. He attended the Hogere Burger School in Arnhem from 1866 to 1869. He excelled in sciences, English, French and German. The theory of electromagnetism was the prime interest of Lorentz. This explained the relationship of electricity, magnetism as well as light. He broadened the spectrum of his research, although his main focus was theoretical physics, hydrodynamics and general relativity. He shared the 1902 Nobel Prize in Physics with Pieter Zeeman for the discovery and theoretical explanation of the Zeeman effect. He worked on the transformation equations, which were used by Albert Einstein to describe space and time.

Einstein wrote for Lorentz:

The enormous significance of his work consisted therein, that it forms the basis for the theory of atoms and for the general and special theories of relativity. The special theory was a more detailed expose of those concepts which are found in Lorentz's research of 1895. For me personally he meant more than all the others I have met on my life's journey.

In January 1928, Lorentz became seriously ill and died shortly after on February 4.



**H.A. LORENTZ (RIGHT)
WITH A. EINSTEIN**

1.6 Relativity of Simultaneity and Time Dilation

Newtonian mechanics describes a universal time scale for all observers. Newton described the time to flow equally without relation to anything external. But, Einstein justified that the time interval measurement is dependent on the reference frame in which measurement is made. Einstein ensured that in order to compare events at two places, time should be common, that is, synchronize time. For example, if one wants to compare two events occurring at A and B points, then the clocks at A and B should read the same time. This will confirm whether the events at A and B occurred at the same time. Now, the question arises whether clocks situated in different inertial frames are synchronized. In other words, we need to define a common time for clocks in reference frames S and S'.

Einstein devised the thought experiment to elaborate this point in Figure 1.5. A boxcar moves with uniform velocity, and two lightning bolts strike the end of the boxcar as shown in Figure 1.5. The marks on the ground are labeled A and B, whereas those in the boxcar are labeled A' and B'. Observer O is in between A and B, O' is in between A' and B'. Light signals are events recorded by both the observers.

For observer O, both the light signals arrive at the same time, that is, A and B occur simultaneously. But for observer O', the events happen at different times. They can be explained in detail. If light reaches O, observer O' already moves as illustrated in Figure 1.5(b), then the light signal from B' has already swept past O'; but the light signal from A' has not yet reached. Hence, observer O' must find that lightning struck B' first and then A'. Hence, this experiment demonstrates that for O, the events appear to be simultaneous and for O' they are not.

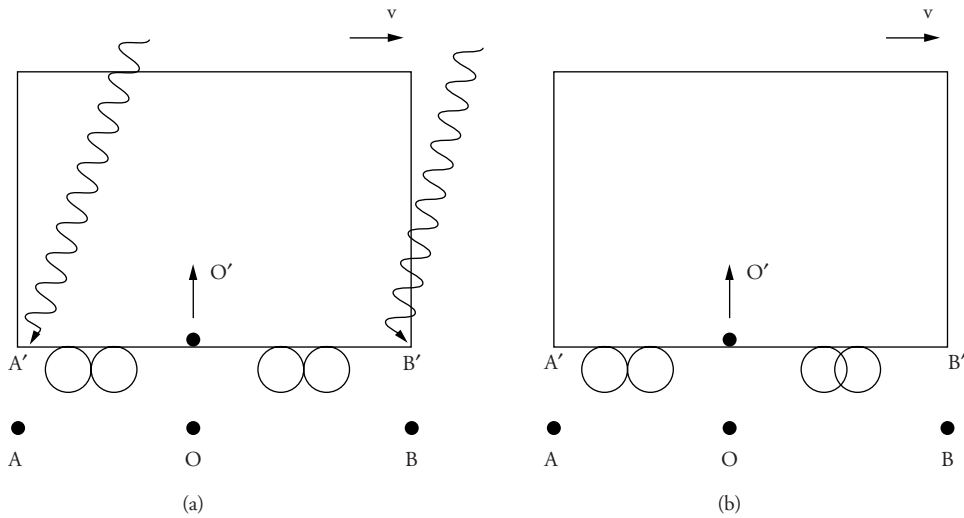


Figure 1.5 Lighting bolts striking both ends. (a) Events appear simultaneous to stationary observer at O; (b) events do not appear to be simultaneous for observer at O'.

Hence, the question arises in our mind, which observer is right? The answer is both are right in their own reference frames. Here, we can also say the principle of simultaneity is not absolute and depends on the observer’s state of motion. Hence, observers in different inertial systems measure different time intervals on their respective clocks. Because of such differences, at large distances, an observer standing on earth can have different set of events in “current moment”. We can explain this effect with the help of “Andromeda Paradox”, commonly known as “Rietdijk–Potnam–Penrose” argument. The description given by Penrose is as follows:

Two people pass each other on street, and according to one of the two people, an Andromedan space fleet has already set off on its journey while to the other, the decision as to whether or not the journey will actually take place or has not been yet made. How can there still be some uncertainty as to outcome of that decision? If to either person the decision has already been made, then surely there cannot be any uncertainty. The launching of the space fleet is an inevitability Penrose 1989.

For a moment, if we think that simultaneity of events occurring in different reference frames cannot be presumed, then Newton’s third law also cannot be applied. We can also illustrate the time difference between a pair of events in different inertial frames as follows:

Let us suppose that observers in reference frames S and S' exhibit identical clocks for measuring an event occurring in S' frame, that is, with x', y', z' coordinates as shown in Figure 1.6. $\Delta t_0'$ is a difference of t_2' and t_1' and is called proper time interval because an observer at rest can measure the sequences with a single clock. But for frames S, to measure both the events, two clocks are required. Hence, the observer O finds the coordinates to be (x_1, y, z) and (x_2, y, z) . Thus, observer O requires two synchronized clocks.

Hence,
$$\Delta t_0 = t_2 - t_1, \text{ for frame S} \tag{33a}$$

$$\Delta t_0' = t_2' - t_1', \text{ for frame S'} \tag{33b}$$

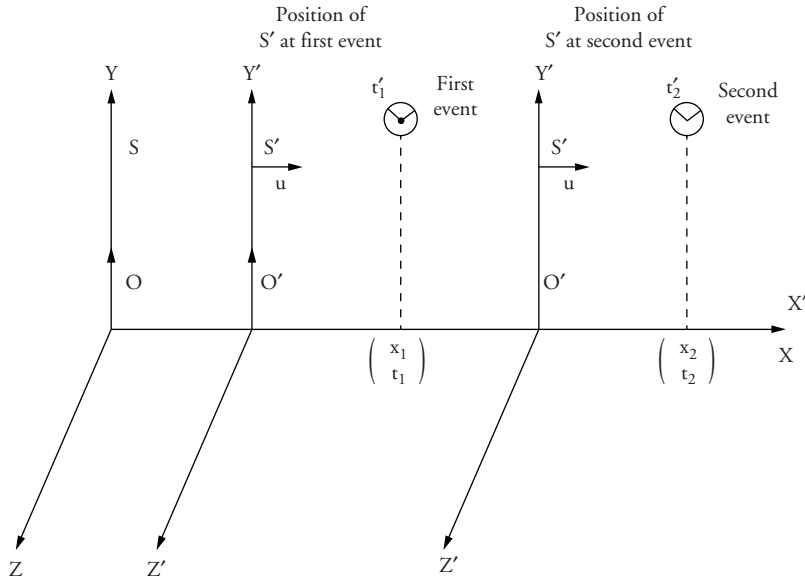


Figure 1.6 Both the events occur at same coordinate for observer O' , but for O they occur at (x_1, y, z) and (x_2, y, z) . Observer O in S needs two clocks to measure time difference, that is, $\Delta t_0 = t_2 - t_1$. But for S' , the events occurring at same point can be measured as $\Delta t'_0 = t'_2 - t'_1$ with a single clock.

From Lorentz transformations

$$\begin{aligned}
 \Delta t_0 &= \gamma \left[t'_2 + \frac{ux'_1}{c^2} \right] - \gamma \left[t'_1 + \frac{ux'_1}{c^2} \right] \\
 &= \gamma [t'_2 - t'_1] = \gamma \Delta t'_0 \\
 \Delta t_0 &= \gamma \Delta t'_0 \\
 \gamma &\geq 1 \\
 \text{Hence, } \Delta t_0 &\geq \Delta t'_0
 \end{aligned} \tag{34}$$

Hence, the time interval for the observer moving w.r.t. clock is greater than the time interval for the observer at rest w.r.t. clock. This effect is called time dilation. In other words, a moving clock runs slower than a clock at rest by a factor of γ . The phenomena of time dilation has been verified through various experiments. For example, muons have charge equal to that of electron and mass 207 times that of electron. These unstable particles are produced at a height of several thousand metres above the surface of earth by the collision of cosmic radiations. Their average lifetime is $2.2 \mu\text{s}$ (proper time), and their speed is approximately close to the speed of light; then it is expected that these particles should travel a distance of 650 m before coming to the surface of earth. This implies that no particle should reach the surface of earth, but experiments have shown quite a large number of muons reaching the surface of earth. This can be explained using time dilation. For an observer on earth, the time appears to be $2.2 \mu\text{s}$, if $v = 0.99c$, $\gamma \approx 7.1$, then the time appears to be

16 μs . Hence, the average distance travelled by a muon is 4,700 m and these are able to reach the surface of earth. Thus, the results of time dilation are in agreement with the experimental results.

CERN in Geneva conducted an experiment in 1976, in which muons were injected into large storage rings reaching speeds of about $0.9994c$. Electrons were produced by decaying of muons. The decay lifetime of muons was measured. The lifetime of moving muons was found to be 30 times higher than that of stationary muons, in perfect agreement with the theory of relativity.

1.7 Lorentz Contraction (Length Contraction)

In the previous sections, we have discussed that time is not absolute. In other words, we can say that the time interval between two events depend on the reference frame. In the same way, the measured distance also depends on the reference frame.

If we consider Galilean transformations, then the measured size for an object remains unaffected by the relative motion of observers. But for Lorentz transformation, length varies as time interval varies. To understand this concept, we consider a stick AB at rest w.r.t. frame S and moving w.r.t. frame S' as shown in Figure 1.7.

The rod is parallel to X-axis and difference between AB gives actual length, L_0 .

According to reference frame S

$$L_0 = x_2 - x_1 \quad (35)$$

and from reference frame S'

$$L'_0 = x'_2 - x'_1 \quad (36)$$

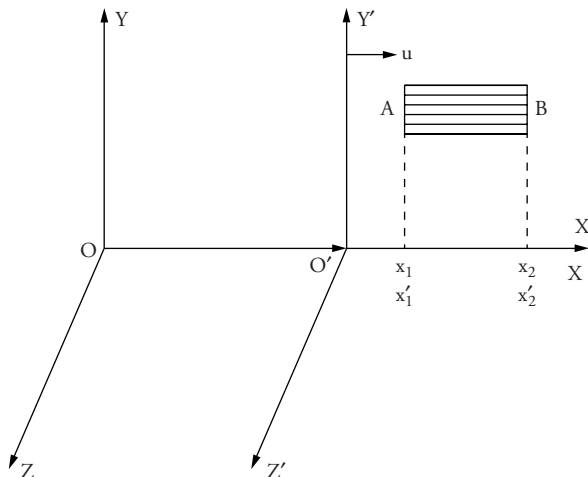


Figure 1.7 The length of rod for S = $x_2 - x_1$ and for S' = $x'_2 - x'_1$.

Substitute $x_2' = \gamma(x_2 - ut)$

$$\left. \begin{aligned} \text{or } x_2 &= \gamma(x_2' + ut') \\ \text{and } x_1 &= \gamma(x_1' + ut') \end{aligned} \right\} \text{in Eqn. (35)}$$

$$L_o = \gamma[x_2' + ut' - x_1' - ut']$$

$$L_o = \gamma(x_2' - x_1') \quad (37)$$

$$L_o = \gamma L_o'$$

$$\text{As } \gamma > 1 \quad L_o \geq L_o' \quad (38)$$

The dimensions of the rod are same in y and z directions because there is no motion along these directions. L_o is the proper length of the object. The proper length (like proper time) of an object is always measured by someone who is at rest w.r.t. the object. Hence, if the length of an object is measured from some moving reference frame, then the length appears to be small. This phenomena is called length contraction.

Although muons are formed at a proper height of 6,000 m, the muons move towards earth at $U = 0.998c$, and hence the length appears to be contracted for them as $L_o' = \frac{L_o}{\gamma}$ with a value of $\gamma = 15.82$. The height becomes $L_o' = \frac{6,000}{15.82} = 379.2$ m.

1.8 Concept of Space–time (Minkowski Space)

Einstein proposed the special theory of relativity, but the modern approach to the theory depends on the concept of four-dimensional universe as proposed by Hermann Minkowski in 1908. He proposed that if things could be arranged in time, then universe becomes four dimensional. He also emphasized that Einstein's discovery is a consequence of a four-dimensional universe. He used Pythagoras' theorem to relate space and time in four-dimensional space i.e.

$$S^2 = x^2 + y^2 + z^2 + (ict)^2 \quad (39)$$

where x , y and z are displacements, c is constant and t is time spanned by space–time interval S . If we do a dimensional analysis, then it becomes

$$\text{Meters} = (\text{Conversion constant}) \times \text{Time}$$

c has a value of 3×10^8 m/s. This transforms Eqn. (39) as

$$S^2 = x^2 + y^2 + z^2 - (ct)^2 \quad (40)$$

If universe is four dimensional, then the space–time interval will be invariant. The constancy of velocity is also its consequence, as explained:

(i) If an object is travelling at velocity c , then the space–time interval is 0.

$$S^2 = x^2 + y^2 + z^2 - (ct)^2 \tag{41a}$$

(ii) If an object moves along x -direction for t seconds with velocity v , then

$$S^2 = (vt)^2 - (ct)^2 \tag{41b}$$

If $v = c$, then

$$S^2 = 0 \tag{42}$$

Hence, we can say that if an object is traveling at c m/s, then all observers will measure the same velocity for it, no matter how fast the observers are moving. This universal constant “ c ” is the velocity of light. The second consequence of space–time demonstrates that clocks will appear to go slower on objects moving relative to observer.

To illustrate this, we can take the example of Jack and Jill. Let us assume that Jack and Jill are on separate planets moving away from each other. Jack draws a graph for Jill’s motion through space and time as demonstrated below (Figure 1.8): Jack and Jill are on planets and they think they are stationary and moving through time only. Both think the same way for each other.

Jack calculates Jill’s space–time as

$$S^2 = (vt)^2 - (ct)^2 \tag{43}$$

whereas Jill calculates his space–time as

$$S^2 = (0t)^2 - (cT)^2 \tag{44}$$

But as the space–time interval is invariant, that is,

$$-(cT)^2 = (vt)^2 - (ct)^2$$

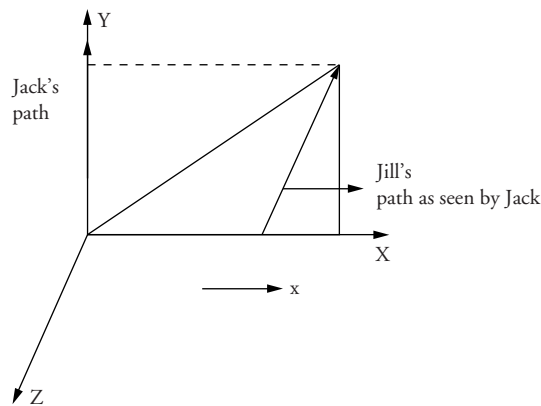


Figure 1.8 Jill thinks he is moving through time only, but Jack thinks he is moving through both space and time.

$$t = \frac{T}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (45)$$

Hence, $T = 1$ between two ticks of clocks that are in rest in Jill's reference frame.

Great care must be taken while interpreting space–time diagrams. The general space–time diagram is shown in Figure 1.9. Time is plotted on a vertical axis and space coordinates on a horizontal axis. World line represents the plot of position of an object w.r.t. time. Hence, an event is a point in space–time and world line indicates a line of space–time. Line of simultaneity is the line parallel to x -axis, and it makes a difference in Galilean relativity and special relativity. In Galilean relativity, all events occur simultaneously on line of simultaneity.

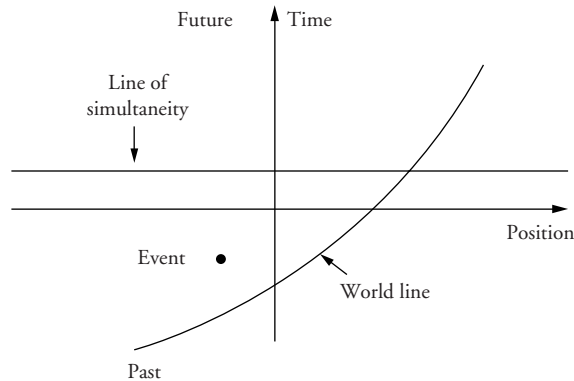


Figure 1.9 Space–time diagram.

The slope of world line has significant meaning.

$$\text{Velocity} = \frac{1}{\text{Slope of world line}} \quad (46)$$

This is valid for “+ve” and “-ve” slopes. If an object changes its velocity, then the world line is curved and velocity is represented by tangent to curve.

In conclusion, the space time as interpreted by minkowski is:

The views of space and time which I wish to lay before you have spring from the soil of experimental physics, and therein lies their strength. They are radical. Henceforth time by itself and space by itself are doomed to fade away in mere shadows and only a union of two will preserve an independent reality. (Herman Minkowski, 1908, Assembly of German Natural Scientists and Physicians)

The motion of objects was provided by earth itself: from astronomical calculations, it was predicted to be 30,000 m/s. As this speed is 4 orders smaller than the velocity of light, the maximum difference expected in terrestrial measurements was 0.0002c.

1.9 Twin Paradox: Doppler's Relativistic Effect

Twin paradox was a consequence of time dilation. Suppose Jack and Jill are twins of 20 years of age; both carry identical clocks that have been synchronized. Suppose Jack starts his journey to planet A, which is 10 light years away from earth [1 light year = 9.46×10^{15} m]. The spaceship of Jack is moving with a velocity of $0.5c$ relative to Jill's inertial frame. But then Jack decided to come back home. But during his journey, he found that many things have changed. Above all, he found the most astonishing fact that his brother Jill was 40 years old and he was only 34.6 years. Hence, the most interesting question is, which twin is younger and which one develops the sign of ageing? As Jack is traveling in spaceship, his motion may not be uniform. Therefore, his reference frame may not be regarded as an inertial frame of reference. Hence, we cannot apply the time dilation on Jack. But because Jill is in an inertial frame, he can apply the time dilation formula. Hence, he finds the age of Jack to be 34.6 years. But Jack spends 17.3 years going to other planets and then coming back. Another important consequence is the shift in frequency for light emitted by atoms in motion. It is also known as Doppler effect, as we are familiar with the fact that the whistle of a train gets high pitched as it approaches the observer and vice versa. But Doppler effect is different for light waves. Light waves do not require any material medium for their propagation and it is hard to find out its relative motion w.r.t. an observer.

Let us consider a source of light wave at rest in frame S, emitting waves with wavelength λ and frequency f (Figure 1.10).

The main objective is to determine the wavelength λ' and frequency f' of wave as observed by an observer in frame S' . Frame S' is approaching with speed v towards a light source. If they approach each other, then we expect f' to be greater than f . Mathematically, we can explain it as

Between the wavefronts, the time of emission is T' as measured by S' .

The distance travelled by wave front is vT' and light source will advance with cT' .

The distance between successive wavefronts is

$$\lambda' = cT' - vT' \quad (47)$$

$$\frac{c}{f'} = (c - v)T' \quad (48)$$

$$f' = \frac{c}{(c - v)T'} \quad (49a)$$

According to the time dilation $T_0 = \gamma T'_0$

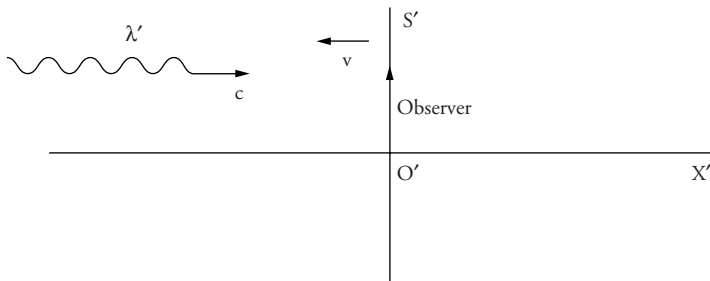


Figure 1.10 Observer S' measures the wavelength to be λ' .

$$\text{Here, } T = \gamma T' \quad (49b)$$

$$T' = \frac{T}{\gamma}$$

$$f' = \frac{c(\gamma)}{(c-v)T}$$

$$f' = \frac{\sqrt{1-(v/c)^2}}{1-(v/c)} f$$

$$f' = \frac{\sqrt{1+(v/c)}}{\sqrt{1-(v/c)}} f$$

$$f_{\text{obs}} = \frac{\sqrt{1+(v/c)}}{\sqrt{1-(v/c)}} f_{\text{source}} \quad (50)$$

This is relativistic Doppler shift formula, and it depends on the velocity v of inertial frame S' . If the objects recede from each other, then replace v by $-v$ and hence Eqn. (50) becomes

$$f_{\text{obs}} = \frac{\sqrt{1-(v/c)}}{\sqrt{1+(v/c)}} f_{\text{source}} \quad (51)$$

The red shift and blue shift of stars can be explained using Doppler shift. When shift of absorption lines occurs towards long wavelength, that is, towards red end of the spectrum, it is called red shift. Blue shift occurs when lines move toward short wavelength. Blue shift indicates that stars are approaching and red shift indicates that stars are receding. Edward Hubble explained that universe is expanding in accordance with Doppler effect.

1.10 Relativistic Mechanics

Like the relativistic kinematics, relativistic dynamics also propagated its roots. Einstein's equivalence of mass and energy brought a revolution to dynamic world. We will discuss linear momentum, energy, mass and force independently in the following sections.

1.10.1 Linear Momentum

The classical definition of momentum is $p = mv$, where m is mass and v velocity of object. In relativistic approach, where the speed of particles is approachable to velocity of light, the conservation of momentum does not follow. That is because in the inertial frames of reference, velocity differs according to Lorentz transformations.

But the laws of physics must be valid in all reference frames. Hence, there is a need of modification for the classical definition of momentum. In classical definition, the particle velocity is defined as the rate of change of displacement.

$$u = \frac{\Delta x}{\Delta t_0} \quad (52a)$$

Hence, Newtonian momentum can be written as

$$p_{\text{Newton}} = m \frac{\Delta x}{\Delta t_0} \quad (52b)$$

Equation (52b) does not take relativistic time; it just takes Δt_0 to be the time measured by the other observer. If we want to calculate relativistic momentum, then we have to take relativistic time into account as follows:

$$p_{\text{relativistic}} = m \frac{\Delta x}{\Delta t_0'} \quad (53)$$

According to time dilation, proper time and relativistic time are related as

$$\begin{aligned} \Delta t_0 &= \gamma \Delta t_0' \\ \Delta t_0' &= \frac{\Delta t_0}{\gamma} \end{aligned}$$

Substituting in Eqn. (53), we obtain

$$\begin{aligned} p_{\text{relativistic}} &= m \gamma \frac{\Delta x}{\Delta t_0} = \gamma p_{\text{Newtonian}} \\ p_{\text{relativistic}} &= \gamma p_{\text{classical}} \end{aligned} \quad (54)$$

Here, γ also has the same functional form of $\left(\frac{1}{\sqrt{1 - u^2/c^2}} \right)$ as that of Lorentz transformations except for the fact that in this case it contains u instead of v . Equation (54) implies the conservation of momentum irrespective of motion of inertial frames of reference.

1.10.2 Mass

If we rewrite Eqn. (54) as

$$p_{\text{rel}} = m_{\text{rel}} u \quad (55)$$

where $m_{\text{rel}} = \gamma m$, m is the mass of particle and u be the velocity
as $\gamma \geq 1$; hence, $m_{\text{rel}} \geq m$ (56)

Therefore,

$$m_{\text{rel}} = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}}$$

Thus, mass varies according to the velocity of particle. Hence, for relativistic mechanics, mass is not an invariant quantity unlike momentum. As the velocity of the particle approaches velocity of light, the mass of particle rises asymptotically to infinity.

1.10.3 Force

According to Newton's second law, force is defined as the rate of change of momentum.

$$F = \frac{dp}{dt} \quad (57a)$$

$$F = \frac{d(\gamma mu)}{dt} = (\gamma ma)$$

$F = \gamma ma$ seems to be the expression, but both γ and u are functions of time.

$$F = mu \frac{d\gamma}{dt} + m\gamma \frac{du}{dt} \quad (57b)$$

$$F = mu \frac{d\gamma}{dt} + m\gamma a \quad (57c)$$

If the particle moves at a constant speed u , then Eqn. (57c) becomes

$$F = mu \frac{d\gamma}{dt} \quad (58)$$

In other words, deriving acceleration directly from Newton's second law is as follows:

$$F = m_{\text{rel}} a$$

$$a = \frac{F}{m_{\text{rel}}} = \frac{F \sqrt{1 - \frac{u^2}{c^2}}}{m} \quad (\text{using 56}) \quad (59)$$

Hence, acceleration decreases as the velocity of the particle approaches velocity of light. In other words, we can also say that it is almost impossible to raise a particle from rest to speed of light.

1.10.4 Energy

In classical mechanics, the kinetic energy is described as follows:

$$K = \frac{1}{2} mu^2 \quad (60)$$

In relativistic regime, this equation also needs to be modified by taking relativistic effects into consideration. Hence, we proceed as follows: kinetic energy can also be defined as work done by an internal force in increasing the speed of the particle:

$$W = \int_{x_1}^{x_2} F dx = \int_{x_1}^{x_2} \frac{dp}{dt} dx \quad (61)$$

Now evaluating $\frac{dp}{dt}$

$$\begin{aligned} \frac{dp}{dt} &= \frac{d}{dt}(m\gamma u) \\ \frac{dp}{dt} &= \frac{m du/dt}{\sqrt{1-u^2/c^2}} \frac{1}{(1-u^2/c^2)} \end{aligned} \quad (62)$$

Substituting (62) in (61)

$$\begin{aligned} W &= \int_0^u \frac{m \left(\frac{du}{dt} \right) u dt}{\left(1 - \frac{u^2}{c^2}\right)^{3/2}} \quad \left[\frac{dx}{dt} = u \right] \\ W &= m \int_0^u \frac{u du}{\left(1 - \frac{u^2}{c^2}\right)^{3/2}} \end{aligned} \quad (63)$$

$$W = \frac{mc^2}{\sqrt{1-u^2/c^2}} - mc^2 = K \quad (64)$$

Equation (64) is obtained if we accelerate a particle from rest to some final velocity c . It is known that work done by the forces acting on a particle equals the change in kinetic energy of the particle. At $u \ll c$, Eqn. (64) becomes

$$\begin{aligned} K &= mc^2 \left(1 - \frac{u^2}{c^2}\right)^{-1/2} - mc^2 \\ K &= mc^2 \left(1 + \frac{1}{2} \frac{u^2}{c^2}\right) - mc^2 \quad (\text{expanding using binomial expansion}) \end{aligned}$$

$$K = \frac{1}{2} mu^2$$

which is a classical result. The term mc^2 is called rest mass energy of particle. From Eqn. (64),

$$K = \frac{mc^2}{\sqrt{1-u^2/c^2}} - mc^2$$

$$K = \gamma mc^2 - mc^2$$

$$K + mc^2 = \gamma mc^2$$

$$K + mc^2 = E \quad (65)$$

where

$$E = \gamma mc^2 \quad (66)$$

Equation (66) is the famous Einstein's mass energy equivalence. We have two relations: $E = \gamma mc^2$ and $p = \gamma mu$; squaring and subtracting these equations lead to the following equation:

$$E^2 = p^2 c^2 + (mc^2)^2 \quad (67)$$

When the particle is at rest, that is, $p = 0$

$$E = mc^2$$

which clearly implies that total energy is equal to rest mass energy. For particles with zero mass such as photons, $m = 0$,

$$E = pc \quad (68)$$

Equation (68) implies the relation between energy and momentum for photons traveling at a speed of light. The energy of electrons or other subatomic particles is eV , as the particles are accelerated using a potential difference

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

Using this, we can calculate rest mass energy of electron as

$$\begin{aligned} m_e c^2 &= (9.11 \times 10^{-31} \text{ kg})(3 \times 10^8 \text{ m/s})^2 \\ &= 8.2 \times 10^{-14} \text{ J} \end{aligned}$$

In eV , it becomes 0.511 MeV, which is the rest mass energy of electrons.

At the age of 26 years, Albert Einstein in his theory of relativity wrote:

The relativity arose from necessity, from serious and deep contradictions in old theory from which there seemed no escape. The strength of the new theory lies in the consistency and simplicity with which it solves all these difficulties, using only a few very convincing assumptions.

1.11 Velocity Addition in Special Relativity

Consider an object moving relative to two observers S and S'. Then the components of velocity in S frame are

$$v_x = \frac{dx}{dt}, \quad v_y = \frac{dy}{dt}, \quad v_z = \frac{dz}{dt} \quad (69)$$

and for observer in S' the components are

$$v'_x = \frac{dx'}{dt'}, \quad v'_y = \frac{dy'}{dt'}, \quad v'_z = \frac{dz'}{dt'} \quad (70)$$

We have to obtain expressions for dx , dy , dz and dt . The Lorentz transformations are

$$\begin{aligned}x' &= \gamma(x - ut) & x &= \gamma(x' + ut') \\y' &= y & y &= y' \\z' &= z & z &= z' \\t' &= \gamma\left(t - \frac{ux}{c^2}\right) & t &= \gamma\left(t' + \frac{ux'}{c^2}\right)\end{aligned}$$

Differentiating them, we obtain

$$\begin{aligned}dx' &= \gamma(dx - udt) & dx &= \gamma(dx' + udt') \\dy' &= dy & dy &= dy' \\dz' &= dz & dz &= dz' \\dt' &= \gamma\left(dt - \frac{udx}{c^2}\right) & dt &= \gamma\left(dt' + \frac{udx'}{c^2}\right)\end{aligned}$$

Now, substitute this set of differentials to obtain values of velocities:

$$\begin{aligned}v_x' &= \frac{dx'}{dt'} = \frac{\gamma(dx - udt)}{\gamma\left(dt - \frac{udx}{c^2}\right)} \\v_x' &= \frac{\left(\frac{dx}{dt} - u\right)}{\left(1 - \frac{u}{c^2} \frac{dx}{dt}\right)} = \frac{v_x - v}{\left(1 - \frac{u}{c^2} v_x\right)}\end{aligned}\tag{71}$$

Similarly, the components v_y' and v_z' are obtained as follows:

$$\begin{aligned}v_y' &= \frac{dy'}{dt'} \\&= \frac{dy}{\gamma\left(dt - \frac{udx}{c^2}\right)} = \frac{v_y}{\gamma\left(1 - \frac{uv_x}{c^2}\right)}\end{aligned}\tag{72}$$

and

$$v_z' = \frac{v_z}{\gamma\left(1 - \frac{uv_x}{c^2}\right)}\tag{73}$$

Corresponding equations relative to observer S in terms of S' are

$$v_x = \frac{v'_x + u}{1 + uv'_x / c^2} \quad (74)$$

$$v_y = \frac{v'_y}{\gamma(1 + uv'_x / c^2)} \quad (75)$$

$$v_z = \frac{v'_z}{\gamma(1 + uv'_x / c^2)} \quad (76)$$

Equations (71)–(76) are velocity addition rules.

Mass shows two interesting properties: gravitational attraction and inertia. Gravitational force is given by Gmm/R^2 and inertial property is given by $F = ma$, where G is a constant. Newton gave the general theory of relativity to describe gravitational mass and inertial mass. He gave the following two postulates:

- (i) The laws of nature have same form for observers in all reference frames whether accelerated or not.
- (ii) For any point near its vicinity, the gravitational field is equivalent to an accelerated reference frame in the absence of gravitational fields. This is also known as principle of equivalence.

SUMMARY

The chapter deals with the frames of reference and relative motion of objects. The frames can be inertial and non-inertial. The concept of “relativity” and “special theory of relativity” by Einstein is explained. The set of “Galilean Transformation equation” and “Lorentz transformation equations” have been derived. Michelson–Morley experiment demonstrated the absence of any material medium such as ether. Lorentz and Fitzgerald explained the negative results obtained from Michelson–Morley experiment. Einstein also explained the Michelson–Morley results and further he said that the light has constant velocity c in all frames of reference. The concept of “simultaneity” demonstrated that the two events occurring at the same time appear simultaneously to the observer. During relative motion,

the length of object appears to be contracted by a factor of $\sqrt{1 - \left(\frac{u^2}{c^2}\right)}$, where u is the velocity of the object.

The chapter deals with the transformations when the particle moves from one frame of reference to other. Lorentz contractions and time dilations are explained under the relativistic motion of particle. The twin paradox, which is a consequence of time dilation, is explained according to which one of the twin is younger than the other. This further establishes the slow motion for moving frames. As a consequence of relativity, the relativistic dynamics and kinematics are also explained, which gave rise to relativistic energy, momentum and mass.

SOLVED PROBLEMS

Q. 1: The length of paths in 11 m for two beams in Michelson–Morley experiment. The wavelength is $6,000\text{\AA}$. Calculate the velocity of earth w.r.t. other planet, if the expected fringe shift is 0.4 fringe.

Ans: The fringe shift is given by

$$S = \frac{2Lu^2}{c^2\lambda}$$

$$L = 11 \text{ m}, \quad \lambda = 6 \times 10^{-7} \text{ m}, \quad S = 0.4, \quad c = 3 \times 10^8 \text{ m/s}$$

$$u = (3 \times 10^8) \sqrt{\frac{6 \times 10^{-7} \times 0.4}{2 \times 11}} = 3.13 \times 10^4 \text{ m/s}$$

Q. 2: Show by Lorentz transformations that

$$x'^2 - c^2 t'^2 = x^2 - c^2 t^2$$

Ans: (x, y, z, t) are space–time coordinates in the inertial frame S and (x', y', z', t') are space–time coordinates for S' frame of reference. S' is moving with uniform velocity \vec{u} w.r.t. S. According to Lorentz transformation equations

$$x' = \frac{x - ut}{\sqrt{1 - v^2/c^2}} \quad \text{and} \quad y' = y, \quad z' = z$$

and
$$t' = \frac{t - \frac{u}{c^2}x}{\sqrt{1 - u^2/c^2}}$$

Squaring
$$x' = \frac{x - ut}{\sqrt{1 - u^2/c^2}} \quad \text{and} \quad t' = \frac{t - (u/c^2)x}{\sqrt{1 - u^2/c^2}}$$

we get
$$x'^2 = \frac{x^2 + u^2 t^2 - 2xut}{(1 - u^2/c^2)} \tag{a}$$

and
$$t'^2 = \frac{t^2 + \frac{u^2}{c^4}x^2 - \frac{2tu}{c^2}x}{1 - u^2/c^2}$$

Hence,
$$c^2 t'^2 = \frac{c^2 t^2 + \frac{u^2}{c^2}x^2 - 2tux}{1 - u^2/c^2} \tag{b}$$

Subtracting (b) from (a), we obtain

$$x'^2 - c^2 t'^2 = \frac{x^2 \left[1 - \frac{u^2}{c^2} \right] - c^2 t^2 \left[1 - \frac{u^2}{c^2} \right]}{1 - u^2/c^2}$$

$$x'^2 - c^2 t'^2 = x^2 - c^2 t^2 \quad (c)$$

Hence, $x'^2 - c^2 t'^2$ is Lorentz invariant.

Q. 3: An observer A observes the separation between events to be 1,000 m and 6×10^{-7} s. What should be the velocity of observer B moving w.r.t. A, so that the events appear to be simultaneous?

Ans: Let t be the time event in frame S for observer A and t'_1 be the time of event in frame S' . Let t_2 be the time of event in frame S for observer B and t'_2 for frame S' .

Then

$$t'_2 = \frac{t_2 - \frac{u}{c^2} x_2}{\sqrt{1 - u^2/c^2}} \quad \text{and} \quad t'_1 = \frac{t_1 - \frac{u}{c^2} x_1}{\sqrt{1 - u^2/c^2}}$$

$$t'_2 - t'_1 = \frac{(t_2 - t_1) - \frac{u}{c^2} (x_2 - x_1)}{\sqrt{1 - u^2/c^2}}$$

$$t'_2 - t'_1 = \frac{6 \times 10^{-7} - \frac{u}{c^2} (1000)}{\sqrt{1 - u^2/c^2}} = 0$$

$$6 \times 10^{-7} - \frac{u}{c} \left[\frac{1000}{3 \times 10^8} \right] = 0$$

$$6 \times 10^{-7} = \frac{u}{c} \left[\frac{1000}{3 \times 10^8} \right]$$

$$\frac{u}{c} = 6 \times 10^{-7} \times \frac{3 \times 10^8}{1000} = \frac{180}{1000} = 0.18$$

$$\frac{u}{c} = 0.18.$$

Q. 4: How fast should a rocket be moving such that its length appears to be 90 percent of its original length?

Ans: According to length contraction

$$L_0 = \frac{L}{\sqrt{1 - u^2/c^2}}$$

$$u = c \sqrt{1 - \left(\frac{L}{L_0}\right)^2} \quad \left[\frac{L}{L_0} = \frac{90}{100} = 0.9 \right]$$

$$u = c \sqrt{1 - 0.9} = \sqrt{0.1}c = .316c$$

$$u = .316c.$$

Q. 5: What is the observed length for a rod measured by an observer at rest. When the rod moves along its length with velocity $\sqrt{\frac{5}{3}}c$?

Ans:

$$L = L_0 \sqrt{1 - u^2/c^2}$$

$$u^2/c^2 = \frac{5}{9}$$

$$L = L_0 \sqrt{1 - \frac{5}{9}} = \frac{2}{3}L_0$$

Hence,

$$L = \frac{2}{3}L_0$$

Q. 6: Brian goes to another planet on a rocket moving with velocity $\frac{3}{4}c$. The distance between the planet and earth is 40 years. Brian's twin brother Adam is on planet earth. What will be the age difference between Brian and Adam when he comes back to earth.

Ans: For Adam, the journey appears to be

$$= 2 \times 40 \times \frac{3}{4} = 60 \text{ years}$$

For Brian, the time interval is

$$t' = t \sqrt{1 - u^2/c^2} = 60 \sqrt{1 - \left(\frac{3}{4}\right)^2}$$

$$t' = 60\sqrt{1 - \frac{9}{16}} = \frac{60}{4}\sqrt{7} = 15\sqrt{7}$$

$$t' = 39.68 \text{ years}$$

Hence, Brian is younger to Adams.

Q. 7: The rest length of rod is 40 cm. Obtain the length of rod observed by an observer moving with velocity $0.1c$.

Ans:

$$L = L_0 \sqrt{1 - \frac{u^2}{c^2}}$$

$$L = 40\sqrt{1 - 0.1}$$

$$L = 40\sqrt{0.9} = 37.94 \text{ cm}$$

Q. 8: A particle at rest has half-life of 19 ns. Obtain its half-life when it moves with speed $0.6c$?

Ans:

$$t' = 19 \times 10^{-9} \text{ s}$$

$$t = \frac{t'}{\sqrt{1 - \frac{u^2}{c^2}}} = \frac{19 \times 10^{-9}}{\sqrt{1 - (0.6)^2}} \quad (u = 0.6c)$$

$$t = \frac{19 \times 10^{-9}}{\sqrt{1 - 0.36}} = \frac{19 \times 10^{-9}}{0.8}$$

$$t = 23.75 \times 10^{-9} = 2.375 \times 10^{-8} \text{ s}$$

Hence $t > t'$

Q. 9: A clock gives accurate time. At what speed it should be moved relative to an observer so that it loses 2 minutes in 24 hours?

Ans: The time is given to be $24 \text{ h} = 24 \times 60$

$$t' = 1440 \text{ m}$$

After losing 2 minutes, it becomes

$$t = 1440 + 2 = 1442 \text{ m}$$

$$t = \frac{t'}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$1442 = \frac{1440}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$\frac{u^2}{c^2} = 1 + \left(\frac{1440}{1442}\right)^2$$

$$u = 0.0527c$$

Q. 10: Two photons are traveling in opposite directions. Obtain the relative velocity between them.

Ans: The $u_x = c$ and the velocity of second photon is $-c$. Hence, the speed of photon is

$$u'_x = \frac{u_x - v}{1 - \frac{vu_x}{c^2}}$$

$$u'_x = \frac{c - (-c)}{1 - \frac{(c)(-c)}{c^2}} = \frac{2c}{2} = c$$

Hence, the two photons move with relative velocity c .

Q. 11: Two electrons are moving opposite to each other with velocity $0.5c$ and $0.75c$. Calculate their relative speed.

Ans: Here $u_x = 0.5c$ and $v = -0.75c$

Now, the relative speed is given by

$$u'_x = \frac{u_x - v}{1 - \frac{u_x v}{c^2}} = \frac{0.5c - (-0.75c)}{1 - \frac{(0.5c)(-0.75c)}{c^2}}$$

$$u'_x = \frac{1.25c}{1 + 0.375}$$

$$u'_x = \frac{1.25c}{1.375}$$

$$u'_x = 0.909c$$

Q. 12: An electron has kinetic energy 1.02 MeV. Find out its speed, provided the rest mass energy of electron is 0.51 MeV.

Ans:

$$\text{Total energy (E)} = \text{KE} + mc^2$$

$$m_{\text{rel}}c^2 = 1.02 + 0.51 \text{ MeV}$$

$$m_{\text{rel}}c^2 = 1.53 \text{ MeV} \quad (\text{a})$$

$$\text{Rest mass energy} = mc^2 = 0.51 \text{ MeV} \quad (\text{b})$$

Dividing Eqs (a) and (b), we obtain

$$m_{\text{rel}} = 3m$$

According to relativistic equation:

$$m_{\text{rel}} = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$3m = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$\frac{u^2}{c^2} = \frac{8}{9}$$

$$u = 0.94c.$$

Q. 13: What will be the ratio of mass to its rest mass when a particle moves with velocity $0.9c$?

Ans:

$$m_{\text{rel}} = \frac{m}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$\frac{m_{\text{rel}}}{m} = \frac{1}{\sqrt{1 - (0.9)^2}}$$

$$\frac{m_{\text{rel}}}{m} = \frac{1}{\sqrt{1 - 0.81}} = \frac{1}{0.4358}$$

$$\frac{m_{\text{rel}}}{m} = 2.29.$$

Q. 14: Find out the mean life of π^+ mesons traveling with velocity 2.8×10^8 m/s. The proper life time of mesons is 2.5×10^{-8} m/s.

Ans:

$$t = \frac{t'}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$t = \frac{2.5 \times 10^{-8}}{\sqrt{1 - \left(\frac{2.5 \times 10^8}{3 \times 10^8}\right)^2}}$$

$$t = \frac{2.5 \times 10^{-8}}{\sqrt{1 - 0.333}} = 6.12 \times 10^{-8} \text{ s}$$

Q. 15: The life-time for μ -meson is 2×10^{-6} s. If it travels with velocity $0.8c$, then find out the distance which it will travel before decaying.

Ans: $t = \frac{t'}{\sqrt{1 - \frac{u^2}{c^2}}}$

The distance travelled will be $x = t' u$, $u = 0.8c$ and $t = 2 \times 10^{-6}$ s

$$x = \frac{2 \times 10^{-6} \times 0.8c}{\sqrt{1 - 0.64}}$$

$$x = \frac{2 \times 10^{-6} \times 0.8 \times 3 \times 10^8}{0.6} = 800 \text{ m}$$

Q. 16: Find out the total energy of proton at (a) rest and (b) when it is moving with velocity 2.8×10^8 m/s.

Ans: (a) At rest, the total energy

$$E = mc^2 \quad (\text{in non-relativistic regime})$$

$$E = (1.673 \times 10^{-27} \text{ kg}) \times (3.0 \times 10^8 \text{ m/s})^2$$

$$E = 1.673 \times 10^{-27} \times 9 \times 10^{16} \text{ kg m/s}^2$$

$$E = \frac{1.673 \times 10^{-11} \times 9}{1.6 \times 10^{-19}} \text{ eV}$$

$$E = 9.41 \times 10^{+8} \text{ eV}$$

$$E = 941 \text{ MeV}$$

(b) When it moves with velocity 2.8×10^8 m/s

$$u = 2.8 \times 10^8 \text{ m/s}$$

$$m_{\text{rel}} = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}} = \frac{1.673 \times 10^{-27} \text{ kg}}{\sqrt{1 - \left(\frac{2.8 \times 10^8}{3 \times 10^8}\right)^2}}$$

$$m_{\text{rel}} = \frac{1.673 \times 10^{-27} \text{ kg}}{\sqrt{1 - 0.87108}}$$

$$m_{\text{rel}} = \frac{1.673 \times 10^{-27} \text{ kg}}{0.35905}$$

$$m_{\text{rel}} = 4.66 \times 10^{-27} \text{ kg}$$

Total energy = $m_{\text{rel}} c^2$

$$E = \frac{4.66 \times 10^{-27} \times (3 \times 10^8)^2}{1.6 \times 10^{-19}} \text{ eV}$$

$$E = 26.21 \times 10^8 \text{ eV}$$

$$E = 2621 \text{ MeV}$$

Q. 17: The total energy of particle is thrice its rest energy. Obtain the speed of particle.

Ans: The total energy of particle is the sum of kinetic energy and rest energy E_0

$$\text{Total } E = \text{Kinetic energy} + mc^2 \quad [m \text{ is rest mass}]$$

Here

$$E = 3mc^2$$

$$3mc^2 = \text{KE} + mc^2$$

$$3mc^2 = (m_{\text{rel}} - m)c^2 + mc^2$$

$$3mc^2 = m_{\text{rel}}c^2$$

$$3m = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$3\left(1 - \frac{u^2}{c^2}\right)^{1/2} = 1$$

$$9\left(1 - \frac{u^2}{c^2}\right)^{1/2} = 1$$

$$1 - \frac{u^2}{c^2} = \frac{1}{9}$$

$$u^2/c^2 = 1 - \frac{1}{9} = \frac{8}{9}$$

$$u = \sqrt{8/9}c = 0.942c$$

Q. 18: Prove that three-dimensional volume element $dx dy dz$ is not invariant for Lorentz transformations, but the space–time volume $dx dy dz dt$ is invariant under the Lorentz transformation.

Ans: Under Lorentz transformation, the proper length is given by

$$x' = \frac{x}{\sqrt{1 - \frac{u^2}{c^2}}}$$

Hence, $dx' = \frac{dx}{\sqrt{1 - \frac{u^2}{c^2}}}$; whereas $dy' = dy$ and $dz' = dz$

Hence, $dx' dy' dz' \neq dx dy dz$, which indicates the non-invariance of volume element under Lorentz transformation.

Now the transformation for time is given by

$$t = \frac{t'}{\sqrt{1 - u^2/c^2}}$$

$$dt' = dt \left[1 - u^2/c^2 \right]^{1/2}$$

Now

$$dx' dy' dz' dt' = \frac{dx}{\sqrt{1 - v^2/c^2}} dy dz dt \left(1 - v^2/c^2 \right)^{1/2}$$

$$dx' dy' dz' dt' = dx dy dz dt$$

Hence, the four-dimensional volume element is invariant under Lorentz transformations.

Q. 19: Prove the invariance of $\left(p^2 - \frac{E^2}{c^2} \right)$ under Lorentz transformation.

Ans:

$$p = m_{rel} u = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}} . u$$

E is given by

$$p^2 = \frac{m^2 u^2}{\left(1 - \frac{u^2}{c^2}\right)} \quad (\text{a})$$

$$E = m_{\text{rel}} c^2 = \frac{m c^2}{\sqrt{1 - \frac{u^2}{c^2}}}$$

$$E^2 = \frac{m^2 c^4}{\left(1 - \frac{u^2}{c^2}\right)}$$

$$\frac{E^2}{c^2} = \frac{m^2 c^2}{\left(1 - \frac{u^2}{c^2}\right)} \quad (\text{b})$$

Subtracting Eqn. (b) from (a)

$$p^2 - \frac{E^2}{c^2} = \frac{m^2}{\left(1 - \frac{u^2}{c^2}\right)} (u^2 - c^2)$$

$$p^2 - \frac{E^2}{c^2} = \frac{m^2 c^2 \left(1 - \frac{u^2}{c^2}\right)}{\left(1 - \frac{u^2}{c^2}\right)}$$

$$p^2 - \frac{E^2}{c^2} = -m^2 c^2 = \text{constant}$$

Hence, $\left(p^2 - \frac{E^2}{c^2}\right)$ is invariant under Lorentz transformations.

Q. 20: Obtain the relation $E = \sqrt{p^2 c^2 + m^2 c^4}$ under the Lorentz invariance of scalar product of momentum vectors $\left[p_x, p_y, p_z, \frac{iE}{c}\right]$.

Ans: We have obtained $p^2 - \frac{E^2}{c^2} = \text{constant}$

Where constant $= -m^2 c^2$

$$p^2 - \frac{E^2}{c^2} = -m^2 c^2$$

$$p^2 c^2 - E^2 = -m^2 c^4$$

$$E^2 = p^2 c^2 + m^2 c^4$$

$$E = \sqrt{p^2 c^2 + m^2 c^4}$$

Q. 21: Give the increase in the mass of proton, when it is accelerated to KE of 400 MeV?

Ans: The kinetic energy for moving photon is

$$K = (m_{rel} - m)c^2$$

$$K = mc^2 \left[\frac{1}{\sqrt{1 - \frac{u^2}{c^2}}} - 1 \right]$$

$$m = \text{mass of proton} = 1.67 \times 10^{-27} \text{ kg}$$

Gain in mass is $(m_{rel} - m)$

$$(m_{rel} - m) = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}} - m$$

$$= m \left[\frac{1}{\sqrt{1 - \frac{u^2}{c^2}}} - 1 \right]$$

$$m_{rel} - m = m \times \frac{K}{mc^2}$$

$$m_{rel} - m = \frac{400 \times 10^6 \times 1.6 \times 10^{-19}}{(3 \times 10^8)^2}$$

$$m_{rel} - m = \frac{640 \times 10^{-13}}{9 \times 10^{16}} = 71.11 \times 10^{-29} \text{ kg}$$

$$m_{rel} - m = .711 \times 10^{-31} \text{ kg}$$

Q. 22: At what speed an electron should move so that its mass becomes equal to the rest mass of proton?

Ans:

$$m_{rel} = \frac{m}{\sqrt{1 - \frac{u^2}{c^2}}}$$

According to statement

Mass of electron = rest mass of proton

$$\frac{\text{Rest mass of electron}}{\sqrt{1 - \frac{u^2}{c^2}}} = \text{Rest mass of proton}$$

$$\frac{9.1 \times 10^{-31}}{\sqrt{1 - \frac{u^2}{c^2}}} = 1.6 \times 10^{-27}$$

$$\sqrt{1 - \frac{u^2}{c^2}} = \frac{9.1 \times 10^{-31}}{16 \times 10^{-27}} = 5.43 \times 10^{-4}$$

$$1 - \frac{u^2}{c^2} = 69 \times 10^{-8}$$

$$1 - 29.69 \times 10^{-8} = \frac{u^2}{c^2}$$

$$1 \approx \frac{u^2}{c^2}$$

$$u \approx c$$

Hence, the electron should be moving with velocity of light.

Q. 23: No signal can travel faster than light. Prove it.

Ans:

$$v_x = \frac{v_x' + v}{1 + \frac{v v_x'}{c^2}}$$

If $v_x' = v = c$, then

$$v_x = \frac{c + c}{1 + \frac{c \cdot c}{c^2}} = c.$$

Hence, the velocity of light can be added to any velocity to obtain the velocity of light.

OBJECTIVE QUESTIONS

- An inertial frame is
 - moving with uniform velocity or at rest
 - decelerated
 - accelerated
 - none of the above
- The presence/absence of ether using Michelson interferometer works on the principle of
 - interference
 - polarization
 - diffraction
 - dispersion
- The momentum for a photon of energy E is given by
 - E/c^2
 - E/c^4
 - E/c
 - E/c^3
- If the speed of light is c in all the directions for a given frame, then the frame is said to be
 - accelerated
 - decelerated
 - inertial
 - non-inertial
- Special theory of relativity states that
 - mass and time are relative
 - Newton's laws are valid in all the inertial frames of reference
 - correspondence of laws hold good
 - none of the above
- The increase in kinetic energy is given by
 - $(m - m_0)/c^2$
 - $(m_0 - m)c^2$
 - m_0c^2
 - $(m - m_0)c^2$
- If two velocities v and c are added such that they are inclined at angle θ , then the velocity after addition is
 - $v + c/v - c$
 - c
 - $vc \cos \theta$
 - $\sqrt{v^2 + c^2 + 2vc \cos \theta}$
- Pair production phenomena requires minimum energy of
 - 13.6 MeV
 - 1.02 MeV
 - 15.4 MeV
 - 10.2 MeV
- The postulates of special theory of relativity are valid for
 - inertial frame
 - non-inertial frame
 - both Inertial and non-inertial frame
 - neither inertial, nor non-inertial

10. The rest mass of photon is
- (a) infinite (b) $2m_0$
(c) 0 (d) p/c
11. Two photons approaching each other will have relative velocity of
- (a) c (b) c^2
(c) $\frac{c}{2}$ (d) $2c$
12. The kinetic energy of particle is equal to rest mass energy at a velocity of
- (a) $\sqrt{3}c$ (b) $4c$
(c) $2c$ (d) $\frac{\sqrt{3}}{2}c$
13. If a body moves with velocity of light, then its mass becomes
- (a) zero (b) twice
(c) infinite (d) does not change
14. The motion and velocity of starts is best explained by
- (a) Minkowski space (b) Lorentz transformation
(c) Doppler effect (d) Galilean transformation
15. A clock runs slow in
- (a) rest frame (b) inertial frame
(c) moving frame (d) accelerated frame
16. μ -meson decay provides an evidence for
- (a) energy relativity (b) Lorentz contraction
(c) momentum relativity (d) time dilation
17. Relativistic energy is given by
- (a) $\sqrt{p^3 c^2 + m_0^2}$ (b) pc
(c) $mv^2 + pc$ (d) $\sqrt{p^2 c^2 + m_0^2 c^4}$
18. Maxwell's equations are not invariant for
- (a) Lorentz transformation (b) Galilean transformation
(c) both of them (d) none of them
19. When one sibling among twins goes to moon and comes back (with relativistic velocities), then he will be
- (a) of the same age as his other sibling (b) become younger
(c) get older (d) none of the above

20. Relativistic time is given by

(a) $\frac{t'}{\sqrt{1-u^2/c^2}}$

(b) $t'(\sqrt{1-u^2/c^2})$

(c) $\frac{t' + \frac{ux'}{c^2}}{\sqrt{1-u^2/c^2}}$

(d) t'

ANSWERS

1. (c)

8. (b)

15. (c)

2. (a)

9. (a)

16. (d)

3. (c)

10. (c)

17. (d)

4. (c)

11. (a)

18. (a)

5. (b)

12. (d)

19. (b)

6. (d)

13. (c)

20. (c)

7. (b)

14. (c)

Micro-Assessment Questions

1. Describe the postulates of special theory of relativity.
2. Explain time dilation and length contraction.
3. What do you understand by twin paradox?
4. Why the compensating glass plate is used in Michelson–Morley Experiment?
5. Explain the space–time or Minkowski space.
6. How does the mass vary with velocity? Explain.
7. What do you understand by simultaneity?
8. Show that the motion of body is identical in all inertial frames of reference.
9. Why the compensating mirror is used in Michelson–Morley experiment?
10. No signal can travel faster than velocity of light. Explain.

Critical Thinking Questions

1. For an inertial system S , an event is observed to take place at point A on the x -axis and 10^{-6} s later another event takes place at point B , 600 m further down. Find the magnitude and direction of the velocity of S' w.r.t. S in which these two events appear simultaneous.
2. Show that Maxwell's equations for the propagation of electromagnetic waves are Lorentz invariant.
3. A neutral K meson decays in flight via $K^0 \rightarrow \pi^+ + \pi^-$. If the negative pion is produced at rest, calculate the kinetic energy of the positive pion. [mass of K^0 is $498 \text{ MeV}/c^2$ and that of π^0 is $140 \text{ MeV}/c^2$].
4. A particle decays into two particles of mass M_1 and M_2 with a release of energy Q . Calculate relativistically the energy carried by the decay products in the rest frame of the decaying particle.
5. If a rod is to appear shrunk by half along its direction of motion, at what speed should it travel?
6. A biker is moving with a speed of $0.600c$ past a stationary observer. If the rider tosses a coin in the forward direction with a speed of $0.400c$ with respect to himself, what is the speed of the coin as obtained by the stationary observer?
7. The radius of earth is 6,400 km and its orbital speed about the sun is 30 km^{-1} . How much does earth's diameter appear to be shortened to an observer on the sun, due to earth's orbital motion?
8. Establish Einstein's mass–energy equivalence.
9. Derive the relativistic velocity addition theorem and show its consistency with Einstein's second postulate.
10. How can photons have momentum when they are massless particles?
11. Describe Michelson–Morley experiment in detail along with the results.
12. Obtain kinetic energy of particle in relativistic terms. Show that at smaller velocities relativistic kinetic energy reduces to classical energy.
13. For relativistic particles, obtain the relation between energy and momentum.

14. Obtain the total energy for 4 MeV electron.
15. Obtain the kinetic energy for electron moving with 0.96 times the velocity of light.
16. What is the total energy of proton and electron both with momentum $3 \text{ MeV}/c$?

Graded Questions

1. Ionized calcium atoms (in ionosphere) produce very strong absorption at 394 nm for a galaxy at rest with respect to the earth. For the galaxy Hydra, which is 200 million light years away, this absorption is shifted to 475 nm. Obtain the speed of Hydra with respect to earth?
2. A 130-MeV electron moves along the axis of an evacuated tube of length 4.5 m fixed to the laboratory frame. What length of the tube would be measured by the observer moving with the electron?
3. A man has a mass of 110 kg on earth. When he is in the space craft, an observer from the earth registers his mass as 118 kg. Obtain the speed of the space craft.
4. An observer on earth sees a spaceship at an altitude of 250 m moving downward toward the earth at $0.960c$. What is the altitude of the spaceship as measured by an observer in the spaceship?
5. A spaceship moves with speed $u = 0.6c$ and sends a radio signal from the station to earth. This signal is received on earth 1,800 s later. How long does the spaceship take to reach the earth according to the observers on earth?
6. The mean lifetime of muons at rest is 2.2×10^{-6} s. The observed mean lifetime of muons as measured in the laboratory is 6.6×10^{-6} s. Find
 - (a) the effective mass of a muon at this speed when its rest mass is $207 \text{ MeV}/c^2$
 - (b) its kinetic energy
 - (c) its momentum
7. Calculate the energy that can be obtained from complete annihilation of 2.5 g of mass.
8. What is the speed of a proton whose kinetic energy equals its rest energy? Does the result depend on the mass of proton?
9. What is the speed of a particle when accelerated to 4.0 GeV when the particle is (a) proton (b) electron.
10. What potential difference is required to accelerate an electron from rest to velocity $0.5c$?
11. The period of a pendulum is measured to be 8.0 s in the rest frame of the pendulum. What is the period of the pendulum when measured by an observer moving at a speed of $0.99c$ with respect to the pendulum?
12. At what velocity does the relativistic kinetic energy differ from the classical energy by (a) 5% and (b) 10%?
13. Prove that if $u/c < 1$, the kinetic energy of a particle will be much less than its rest energy. Further, show that the relativistic expression reduces to the classical one for small velocities.
14. An electron has kinetic energy equal to its rest energy. Show that the energy of a photon that has the same momentum as this electron is given by $E\gamma = \sqrt{3E}$, where $E = mc^2$.
15. Find the Doppler shift in wavelength of H line at $6,563 \text{ \AA}$ emitted by a star receding with a relative velocity equal to velocity of light.
16. A neutrino of energy 3.5 GeV collides with an electron. Calculate the maximum momentum transfer to the electron.

17. A particle of mass M_1 collides elastically with a target particle of mass M_2 at relativistic energy. Show that the maximum angle at which M_1 is scattered in the laboratory system is dependent only on the masses of particles provided $M_1 > M_2$.
18. Find the wavelength shift in the Doppler effect for the sodium line 589 nm emitted by a source moving in a circle with a constant speed $0.7c$ observed by a stationary person.

Remember and Understand

- (i) The laws of physics have same validity in all inertial frames of reference. This is also known as principle of special relativity.
- (ii) The speed of light, c , is same in all directions for all inertial system. This is also called principle of constancy of speed of light.

Summarizing all the equations:

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$t' = \gamma \left[t - \frac{vx}{c^2} \right]$$

the inverse velocity transformations, can be summarized as

$$\left. \begin{aligned} u_x &= \frac{(u'_x + v)}{\left(1 + \frac{u'_x v}{c^2}\right)} \\ u_y &= \frac{u'_y}{\gamma \left[1 + \frac{u'_x v}{c^2}\right]} \\ u_z &= \frac{u'_z}{\gamma \left[1 + \frac{u'_x v}{c^2}\right]} \end{aligned} \right\}$$

- (iii) Mass varies as the velocity of particle. Thus, for relativistic mechanics, mass is not an invariant quantity unlike momentum. As the velocity of the particle approaches velocity of light, the mass of particle rises asymptotically to infinity.

Corresponding equations relative to observer S in terms of S' are

$$v_x = \frac{v'_x + u}{(1 + uv'_x / c^2)}$$

$$v_y = \frac{v_y}{\gamma(1 + uv'_x / c^2)}$$

$$v_z = \frac{v_z}{\gamma(1 + uv'_x / c^2)}$$

These are the velocity addition rules.

Quantum Mechanics—I

Introduction to Quantum Physics

Keywords: quantum mechanics, thermal radiations, blackbody radiations, Planck's hypothesis, photoelectric effect, Rayleigh–Jeans law, ultraviolet catastrophe, Compton effect

Learning Objectives

- ◆ To understand the thermal radiations and distribution of frequencies in continuous spectrum
- ◆ To understand Prevost theory of exchanges
- ◆ To get insight into blackbody radiations and blackbody spectrum
- ◆ To obtain Stefan's law and Wien's law
- ◆ To understand the distribution of intensity for blackbody radiations corresponding to different temperatures
- ◆ To understand Planck's hypothesis of discrete energy in terms of "photons"
- ◆ To learn the Rayleigh–Jeans law and occurrence of ultraviolet catastrophe
- ◆ To learn and understand photoelectric effect
- ◆ To understand threshold frequency and work function for surface and deeper electrons
- ◆ To get insight into photoelectric effect and Millikan's experiment
- ◆ To learn about stopping potential and its variation with frequency f
- ◆ To learn about photon mass
- ◆ To obtain the change in wavelength upon incidence of radiations on free electrons (Compton effect)
- ◆ To understand the characteristic X-rays and continuous X-rays
- ◆ To learn Moseley's law
- ◆ To understand X-ray crystallography in terms of Bragg's reflection planes

Newton and Maxwell are the pillars of mechanics and electromagnetism, respectively. Classical mechanics was established by many great personalities such as Gibbs, Stefan, Boltzmann, Helmholtz, Lord Kelvin, Carnot, and Clausius. The following four Maxwell's equations formed a strong base for the physics:

$$\oint E \cdot ds = \frac{q}{\epsilon_0} \quad (1)$$

$$\oint E \cdot dl = \frac{-d\phi_B}{dt} \quad (2)$$

$$\oint B \cdot ds = 0 \quad (3)$$

$$\oint B \cdot dl = \mu_0 I + \epsilon_0 \mu_0 \frac{d\phi_E}{dt} \quad (4)$$

But the Maxwell's equations and Newton's laws could not be applied to an atom. In addition to this, the intensity of radiations that come out from the closed cavity could not be calculated using the Maxwell's or Newton's approach. Later on, Max Planck discovered a solution to this problem in 1900.

Further more, the efforts of Planck and Einstein led to the formulation of the quantum mechanics. Einstein explained photoelectric effect along with the quantization of energy. In the sections that follow, the main aim is to discuss the quantum theory of light and formulation of the quantum mechanics.

2.1 Thermal Radiations

Any object emits radiation at the cost of its energy, and if any object absorbs energy, then the energy of the object increases. Whenever an object emits radiation, two kinds of spectra arise: continuous and discrete. In continuous spectrum, the distribution of frequencies or wavelengths is continuous. The discrete spectrum consists of a discrete group of energies. The characteristics of an object and its temperature determine the electromagnetic radiations emitted or absorbed. Whenever a body emits or absorbs electromagnetic radiations by virtue of its temperature, then those electromagnetic radiations are termed as thermal/heat radiation.

Thomas Wedgewood noted the features of all heated objects. In 1792, he observed that all objects became red at the same temperature irrespective of their size/shape and chemical nature. In the same year, Pierre Prevost, a Swiss physicist, proposed that all the bodies emit heat at all times; at higher temperature, the rate of emission is fast, whereas at lower temperature, the rate is small. Hence, the object will try to be in thermal equilibrium with all the surrounding objects, that is, the rate of absorption is equal to the rate of emission of radiations.

Prevost gave the theory of exchanges from which it can be concluded that good absorbers are good emitters and vice versa. This condition is very important to maintain thermal equilibrium. If an object does not lose energy (in the form of heat radiation), then it will continue to warm up even more than the surrounding temperature. But, usually in everyday experience, it is observed that the objects are neither lower nor higher than the surrounding temperatures.

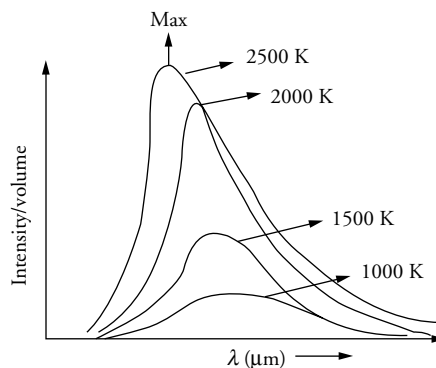


Figure 2.1 Emission spectra for an object at different temperatures.

Figure 2.1 shows the emission spectra for glowing solids. It is observed that as the temperature of object increases, the wavelength shifts to lower wavelength side. Below 1,000 K, the wavelengths of emitted radiations fall in invisible infrared region. Radiations of lower wavelength start appearing in the spectrum with a rise in temperature. Moreover, with the rise in temperature, the color of objects also changes, that is, red \rightarrow orange \rightarrow yellow \rightarrow white.

2.2 Blackbody Radiation

An object that absorbs all electromagnetic radiations falling on it and consequently appears black is called a blackbody. In general, everyday objects do not absorb all the light incident on them. Hence, it is difficult to find a perfect absorber or emitter of light. According to Gustav Kirchhoff, for any body in thermal equilibrium with radiation, the power absorbed is proportional to the power emitted as follows:

$$E = J(f, T)A \quad (5)$$

where E is the power emitted per unit area per frequency for heated object, $J(f, T)$ is a universal function dependent on frequency f and absolute temperature T of the object, and A is the absorption power. For blackbody radiation, the absorption power is 1 at all the frequencies. Hence, Eqn. (5) becomes

$$E = J(f, T) \quad (6)$$

Therefore, we can say that if a blackbody is considered a perfect absorber, then it should also be a perfect emitter. Figure 2.2 shows the blackbody as a heated cavity with a small opening. If radiation falls on this hollow cavity, then it will be trapped inside. This cavity will also act as a perfect emitter of radiation. If radiation is generated inside this cavity, then it will escape out of it.

If the hollow object with cavity is at constant temperature, then every point within the cavity is in thermal equilibrium with each other. The cavity will exhibit electromagnetic radiations with all wavelengths particular to that temperature irrespective of the material from which the cavity is made up of. In addition, the hollow cavity will be blackbody when viewed from outside.

After the understanding of blackbody radiation, the next important concept was proposed by the Austrian Physicist Josef Stefan in 1879. He postulated that the energy radiated per second per unit area of surface of the blackbody is directly proportional to the fourth power of absolute temperature of body, that is,

$$E = \sigma T^4 \quad (7)$$

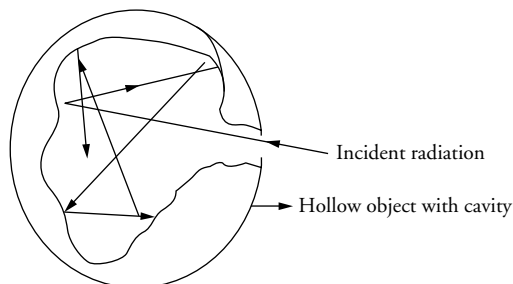


Figure 2.2 Blackbody as a hollow object with small cavity.

where E is energy per second per unit area of body, T is absolute temperature of body, and σ is proportionality constant whose value is $5.672 \times 10^{-8} \text{ W|m}^2\text{|K}^{-4}$. Equation (7) is also known as Stefan–Boltzmann’s law. It is clear from Figure 2.1 that as the absolute temperature of body increases, λ_{max} or the wavelength corresponding to maximum power emission shifts to lower wavelength side. A more general expression was given by German physicist Wilhelm Wien in 1893. According to the Wien, the absolute temperature of the blackbody is inversely proportional to λ_{max} , that is,

$$\lambda_{\text{max}} T = \text{Constant} = 0.29 \times 10^{-2} \text{ mK} \quad (8)$$

Equation (8) is the well-known Wien’s law. Using Wien’s law, the temperature on the sun’s surface can be calculated by assuming λ_{max} to be 500 nm (blue-green light) as follows:

$$T = \frac{0.29 \times 10^{-2} \text{ mK}}{500 \times 10^{-9} \text{ m}} = 5800 \text{ K}$$

This provides a good agreement with experimental and predicted results. Later on, Wien’s exponential law gave a more generalized form for energy per unit volume per unit frequency of the blackbody radiation. According to Wien’s exponential law,

$$E = Af^3 e^{-\beta f/T} \quad (9)$$

where E is energy density, f is frequency, T is absolute temperature of the blackbody, and A and β are constants. Although Paschen found his experimental studies to be in good agreement with Wien’s study for a body heated upto 1,500 K, other physicists, that is, Lummer et al. and Rubens et al. found some discrepancies in the result.

According to Newton and Maxwell, the average energy of an oscillator, $E_{\text{oscillator}}$, that is in thermal equilibrium with the surroundings is directly proportional to absolute temperature (T):

$$E_{\text{oscillator}} = k_{\text{B}} T \quad (10)$$

where k_{B} is the constant of proportionality and its value is $1.38 \times 10^{-23} \text{ J/K}$. k_{B} is also known as Boltzmann’s constant (Eqn. 10) and is based on the principle of the equipartition of energy. According to principle of equipartition of energy, all the oscillations within a system will exhibit same average energy. The particles, that is, atoms or molecules comprising the system, are treated as oscillators, which generate heat radiations. In other words, the particles also vibrate at a particular frequency corresponding to which they emit heat radiations. Although the principle of equipartition also states that inside a cavity every particle in thermal equilibrium should be allocated equal energy, most of this energy will be associated with higher frequencies. As a result, the cavity must have very high-frequency radiation. Anyhow, the blackbody radiations always pass maximum intensity within the middle range of frequencies, and not high frequencies such as X-rays. This distribution of heat radiations inside the cavity is also known as ultraviolet catastrophe according to which the system should proceed toward explosion due to high-frequency distribution. Figure 2.3 represents the distribution of intensity for blackbody radiation as a function of frequency for different temperatures. The area under the curve for classical prediction is infinite, whereas the area under the curve for experimental distribution is finite. Hence, the distribution according to classical theory is almost impractical.

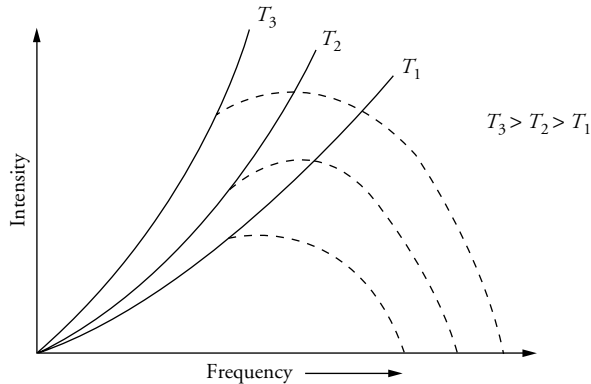


Figure 2.3 Distribution of intensity for blackbody radiation corresponding to different temperatures.

2.3 Quantum of Energy and Planck's Hypothesis

In 1900, Max Planck, a German physicist, derived a function that could correctly explain blackbody radiations. Planck termed the submicroscopic electric charges inside the blackbody as resonators. In addition, he also assumed that the walls of the cavity are composed of billions of such resonators. These resonators were supposed to vibrate at different frequencies. Hence, the energy for every resonator is not continuous but a discrete quantity, which is further composed of an integral number of finite equal parts.

Maxwell proposed that the oscillator can have any energy, and the amplitude is subject to change when the fraction of its energy is radiated out. But Planck gave a revolutionary hypothesis by assuming:

The total energy of resonator with frequency f is discrete and only be integral multiple of hf

In mathematical form, it could be written as follows:

$$E_{\text{oscillator}} = 0, hf, 2hf, 3hf, \dots = nhf \quad (11)$$

$$n = 0, 1, 2, 3, \dots$$

where h is a constant and its value is 6.63×10^{-34} Js; h is also known as Planck's constant. Further, he also proposed that whenever a resonator loses/gains some energy, it is only in finite discrete amount known as quanta. Quanta is a small packet of energy directly proportional to resonator frequency, that is,

$$\Delta E = hf \quad (12)$$

All other energies are forbidden. This is illustrated in Figure 2.4, where all the energy levels are quantized. Based on this hypothesis, Planck was able to derive a mathematical functions to explain the intensity of blackbody radiation. The interpolation between Wien's exponential law and Maxwell's law lead to the formula as follows:

$$E_{\text{oscillator}} = \frac{8\pi hf^3}{c^3} \left[\frac{1}{e^{hf/k_B T} - 1} \right] \quad (13)$$

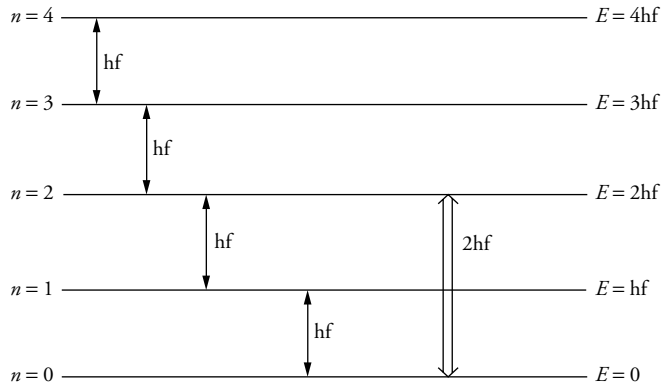


Figure 2.4 According to Planck, the allowed energy transitions are only with energy difference hf ; other transitions are forbidden.

Using this equation, it is easy to explain no occurrence of ultraviolet catastrophe. At normal temperature, the radiations of high frequency possess hf greater than the average kinetic energy $k_B T$. Hence, $hf \gg k_B T$ and

$$\frac{1}{e^{hf/k_B T} - 1} = \frac{1}{e^{hf/k_B T}} \approx e^{-hf/k_B T} \quad (14)$$

Substituting Eqn. (14) into Eqn. (13), we obtain the following:

$$E_{\text{oscillator}} = \frac{8\pi hf^3}{c^3} e^{-hf/k_B T} \quad (15)$$

Under such conditions, the probability of any resonator/oscillator acquiring energy to create such high-energy quantum is almost negligible. Hence, the heat radiations emitted by these radiations do not have high-frequency radiations.

At low frequencies, $hf \ll k_B T$

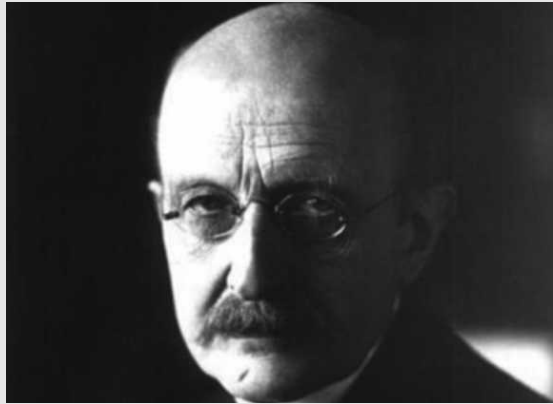
$$\frac{1}{e^{hf/k_B T} - 1} \approx \frac{1}{(1 + hf/k_B T) - 1} \approx \frac{k_B T}{hf} \quad (16)$$

Substituting Eqn. (16) into Eqn. (13), we obtain the following:

$$E_{\text{oscillator}} = \frac{8\pi hf^3}{c^3} \frac{k_B T}{hf} = \frac{8\pi f^2}{c^3} k_B T \quad (17)$$

This is classical regime result, and at low frequencies the energy appear to be continuous.

Max Planck was a German Physicist who made many contributions to theoretical physics. But primarily he is the originator of the quantum theory, which revolutionized our understanding for atomic and sub-atomic processes. Planck was also awarded Nobel Prize in physics in 1918. Max Karl Ernst Ludwig Planck was born in Kiel, Germany, on April 23, 1858. He was very fond of music and was a very disciplined child in school. His teachers assisted him in elevating his interest in physics and mathematics. He was influenced by the law of conservation of energy. One of his famous lines are:



MAX PLANCK

The outside world is something independent from man, something absolute, and the quest for the laws which apply to this absolute appeared to me as the most sublime scientific pursuit in life.

Planck was appointed the professor of theoretical physics at the University of Berlin. He studied the distribution of energy w.r.t. wavelength. He developed Planck's radiation formula by combining the formulae of Wien and Rayleigh. He gave the concept of quanta to the world of quantum mechanics. On December 14, 1900, he presented his theoretical explanation regarding quanta at a meeting of the Physikalische Gesellschaft in Berlin. He demonstrated that energy can take only discrete values instead of continuous values. He defined energy for a resonator of frequency f is hf , where h is a universal constant: " h " is known as universal Planck's constant.

2.4 Rayleigh–Jeans Law

The blackbody radiation energy/volume lying in frequency f and $f + df$ is given as the product of number of resonators/volume ($N(f)$) in frequency range df and average energy $\bar{E}_{\text{oscillator}}$ per oscillator.

$$E(f, T)df = \bar{E}_{\text{oscillator}} N(f)df \quad (18)$$

Usually, Rayleigh–Jeans Law describes the continuous distribution of energy whereas Planck's formulation is based on discrete energy. Rayleigh and Jeans explained that the electromagnetic radiations inside the cavity must be at constant temperature T , as they are in thermal equilibrium. They found that the average energy is independent of frequency, which is equal to $k_B T$. i.e. $\bar{E}_{\text{oscillator}} = k_B T$

Rayleigh and Jeans considered the standing electromagnetic waves as oscillators. According to Maxwell–Boltzmann's law, the probability of finding an oscillator or atom with energy $E > E_0$ at temperature T is

$$P = P_0 e^{-(E-E_0)/k_B T} \quad (19)$$

where P_0 is the probability that the system possesses minimum energy. For discrete distribution of energies, the average energy is given by the following equation:

$$\bar{E} = \frac{\sum E.P(E)}{\sum P(E)} \quad (20)$$

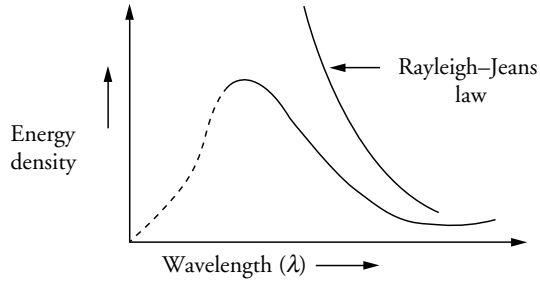


Figure 2.5 Energy density variations for Rayleigh–Jeans law depicting its failure.

For continuous distribution, Σ must be replaced by \int with limits $0 \rightarrow \infty$.

$$\bar{E} = \frac{\int_0^{\infty} E e^{-E/k_B T} dE}{\int_0^{\infty} e^{-E/k_B T} dE} = KT \quad (21)$$

The density of modes can be calculated using free electron model and is

$$N(f)df = \frac{8\pi f^2}{c^3} df \quad (22)$$

Using Eqs (18), (21), and (22), it becomes

$$E(f, T)df = \frac{8\pi f^2}{c^3} k_B T df \quad (23)$$

or

$$E(\lambda, T)d\lambda = \frac{8\pi}{\lambda^4} k_B T d\lambda \quad (24)$$

Figure 2.5 clearly depicts the diverging behavior of energy density as $\lambda \rightarrow 0$, which is referred to as “ultraviolet catastrophe.” Hence, this theory fails to explain blackbody radiation.

Planck considered energy states of oscillators rather than the electromagnetic waves. Planck obtained the following formula:

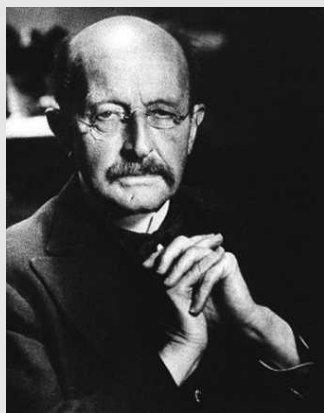
$$E(f, T)df = \frac{8\pi f^2}{c^3} \left(\frac{hf}{e^{hf/k_B T} - 1} \right) df \quad (25)$$

or

$$E(\lambda, T)d\lambda = \frac{8\pi h c d \lambda}{\lambda^5 (e^{hc/\lambda k_B T} - 1)} \quad (26)$$

from Eqs (21) and (22), it is clear that at $\lambda \rightarrow 0$ or $f \rightarrow \infty$, ultraviolet catastrophe is avoided. Hence, Max Planck gave the concept of energy quantization, which laid a strong backbone for explaining blackbody radiations.

After the discovery of Planck's constant, Planck defined physical quantities such as Planck length and Planck mass. Planck's quantum theory was published in the *Annalen der Physik*. In addition, his work is summarized in two books *Thermodynamik* (Thermodynamics) and *Theorie der Wärmestrahlung* (Theory of Heat Radiation). Planck was also a philosopher of science and he wrote in his autobiography "A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die and a new generation grows up that is familiar with it." He died on October 4, 1947 at the age of 89 in Göttingen, West Germany.



"A new scientific truth does not triumph by convincing opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it."
Max Planck

2.5 The Photoelectric Effect

Planck's quantum hypothesis was quite successful in explaining the absorption and emission as discrete processes, but still many researchers believed that radiation is propagated as wave. In 1905, Einstein published his revolutionary theory of photoelectric effect. Hertz found that on illuminating the poles in secondary detector, the sparks were readily induced. He called this effect as photoelectric effect. Subsequently, Hallwach, a German physicist, studied the response of gold leaf electroscope in visible and ultraviolet light. He made the following observations:

1. Irrespective of the material of plate (zinc or iron), no response from positive-charge plate was observed with visible or ultraviolet radiation.
2. Upon changing the intensity of radiation, no charge was lost by the positively charged plate.
3. No response was observed by negative iron plate even after using intense beams of ultraviolet or visible radiations.
4. Even with a weak ultraviolet radiation illuminating the negative zinc plate, the loss of negative charge was observed because the leaves of electroscope closed.
5. The high-intense visible radiation did not exhibit any effect on negative zinc plate. Hence, Hallwach explained that ultraviolet radiations were able to supply the energy required by electrons to set them free from tight bonds. Still some of the important questions could not be neglected and still needs to be addressed as follows:
 - (a) Why the two metals exhibit different behavior?
 - (b) Why did the iron plate not release any electrons even after irradiating with ultraviolet light?
 - (c) Upon increasing the intensity of radiation, the amplitude should be increasing; hence, the frequency should not be a factor for the ejection of electrons.

The classical theory was unable to address these issues, hence a new theory should have been there to answer these questions. Later, Einstein in 1905 proposed his theory and used the Planck's hypothesis of discrete quanta of energy. Einstein proposed that light consists of quanta of energy called photons and energy of each photon is given by the following equation:

$$E_{\text{photon}} = hf \quad (27)$$

where h is Planck's constant and f is frequency of light radiation. When a photon strikes a metal surface, it will lose all its energy to the single electron. i.e. "one photon energy \leftrightarrow one electron energy." The electron will use this energy in the following two steps:

1. First, the electron will break the bond with metal surface using the energy provided by photon.
2. If still some surplus energy is available, then the electron will use it as kinetic energy (KE).

Summarizing it in mathematical form,

$$E_{\text{photon}} = W_0 + \text{KE} \quad (28)$$

where W_0 is the minimum work done to release the electron from metal surface and is known as the work function of metal. Work function is the characteristic property of every metal. From Eqn. (28):

$$\begin{aligned} \text{KE} &= E_{\text{photon}} - W_0 \\ \text{KE} &= hf - W_0 \end{aligned} \quad (29a)$$

If the wavelength of electron just takes out the electron, then $\text{KE} = 0$

$$\text{and} \quad W = hf_0 \quad (29b)$$

Hence, the Hallwachs experiment could be explained successfully using Einstein's hypothesis as illustrated below:

- (a) No electron was liberated from the iron plate even with ultraviolet radiation because the work function of iron is greater than energy of photons ($W_0 > hf$). Hence, radiations of higher frequency must be used to liberate the electrons from the iron surface.
- (b) Although visible light consists of a range of frequencies, no frequency was high enough to eject the electrons out of zinc or iron surface.
- (c) No accumulation of energy takes place as all the electrons are ejected at the same time as soon as the ultraviolet radiations fall on the zinc surface.
- (d) On increasing the intensity of radiation, only the number of photons in the radiation will increase, although still all the photons in the light possess same energy.
- (e) If a beam is more intense, then it will be able to eject more number of electrons from the metal. The electrons that are ejected from the top layers of the metal surface have higher KE. But the electrons that are ejected from the deep layers of metal have lower kinetic energies compared with the KE of surface-ejected electrons. Hence, all the photoelectrons do not possess the same KE.

Thus, Eqn. (29a) can be written as follows:

For surface electrons,

$$\text{KE}_{\text{max}} = hf - W_{\text{min}} \quad (30a)$$

For deeper electrons,

$$\text{KE}_{\text{min}} = hf - W_{\text{max}} \quad (30b)$$

By using the classical theory or Maxwellian equations, it was difficult to arrive at the concept of the photons. Taking into account the discrete nature of light, it was easy to explain "ultraviolet catastrophe and photoelectric effect." Hence, the Planck's hypothesis and Einstein's postulate laid a strong backbone for quantum mechanics.

Further, Millikan designed an experiment in 1916, which validated Einstein's equations and the value of Planck's constant ($h = 6.63 \times 10^{-34}$ Js). He took a vacuum tube of glass known as photoelectric

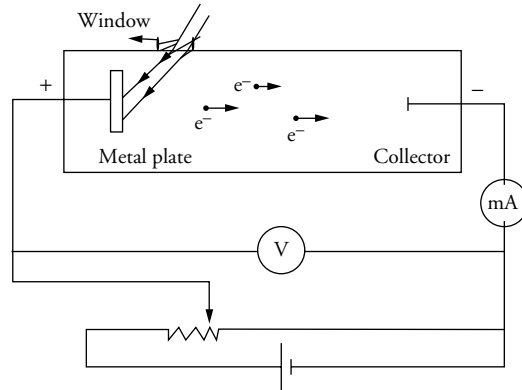


Figure 2.6 Photoelectric effect demonstration using Millikan's experiment.

diode tube and two electrodes were fixed into it; one metal was the emitter and other was collector. The schematic of Millikan's apparatus used to investigate the Einstein's photoelectric effect is shown in Figure 2.6.

The metal plate emits electrons when visible light falls on it. The collector collects these electrons. Both the electrodes are connected to potentiometer such that the metal plate is kept at positive potential and collector is at negative potential. When an electron is emitted from metal plate, it has to overcome the potential between two electrodes at the expense of its KE to reach negative collector plate. When the electrons reach negative collector, the ammeter gives the reading of electric current flowing through the circuit. When the potential is increased, only the most energetic electrons reach the collector. When the potential is raised to a maximum value, then no electron would be able to reach the collector, leading to zero current. The value of potential at which the electric current is reduced to zero due to no flow of electrons from positive metal plate toward the collector plate is called stopping potential, V_o .

The incident radiation has frequency f and the stopping potential is V_o . For an electron to move from metal plate to collector plate through a potential V , the KE is given by

$$\text{KE} = eV \quad (31a)$$

When stopping potential V_o is applied, the electrons have to do maximum work given by the following equation:

$$\text{KE}_{\max} = eV_o \quad (31b)$$

Substituting Eqn. (31b) into Eqn. (30a)

$$eV_o = hf - W_{\min} \quad (32)$$

$$V_o = \frac{hf}{e} - \frac{W_{\min}}{e} \quad (33)$$

This relation (33) gives a straight line fitting according to $y = ax + b$, where $y = V_o$, $a = \frac{h}{e}$, $x = f$, and $b = \frac{-W_{\min}}{e}$.

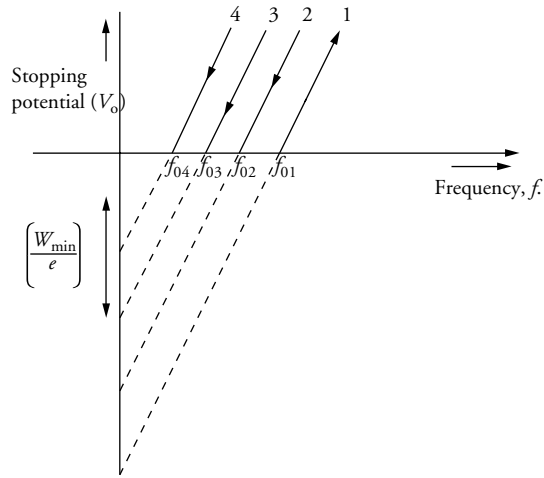
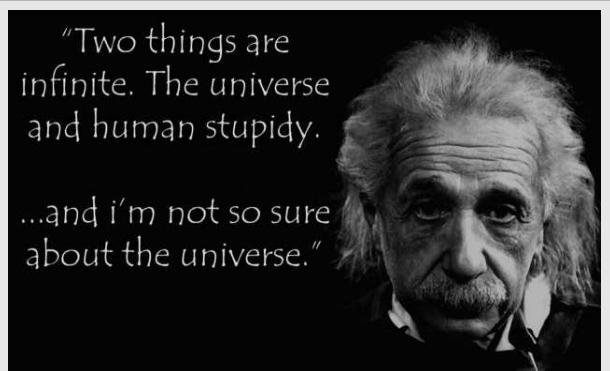


Figure 2.7 Variation of stopping potential V_0 with frequency f . (Planck's constant can be obtained from slope " h/e .")

Eqn. (33) predicts a linear relation between the frequency of incident radiation and stopping potential V_0 (Figure 2.7).

The point on x -axis (frequency axis), where the lines cut, gives the value of minimum frequency known as threshold frequency, f_0 . Any light radiation falling on metal surface must possess this minimum threshold frequency to eject out photoelectrons. The point on y -axis, where these extended lines cut, gives the intercept $\frac{W_{\min}}{e}$, from which the minimum work function can be obtained.

Einstein was awarded doctorate in 1905 from the University of Zurich for his thesis on the different sizes and extent of molecules. Einstein published three important theoretical documents based on the significance of physics during the twentieth century. One of these papers was based on Brownian motion, which discussed motion of particles for any liquid. Einstein's second publication discussed photoelectric effect, which described that light consists of definite packets of energy, which are termed as photons. Photon energy depends directly on radiation's frequency and is given by $E = hf$, where E is defined as the radiation's energy, h is a constant defined as Planck's constant, and f is defined as radiation's frequency. Einstein's idea was rejected by everyone because it opposed the conventional idea stating that transfer of light energy is an ongoing process.



ALBERT EINSTEIN

2.6 The Concept of Photon Mass

According to electromagnetic theory, the light wave is continuous in nature; but the quantum theory postulates that light consists of quanta of energy in discrete packets. The energy of each photon is given by the following equation:

$$E_{\text{photon}} = hf$$

According to Eqn. (64) of Chapter 1, Special theory of Relativity, the total energy is given by the following expression:

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad (34)$$

where p is the linear momentum, c is the velocity of light in vacuum, and m_0 is the rest mass of the particle. Photons are never at rest, hence practically, there is no rest mass for photon, i.e. $m_0 = 0$ for photon. Using rest mass $m_0 = 0$ for photons, Eqn. (34) becomes

$$E_{\text{photon}}^2 = p_p^2 c^2 \quad [p_p = \text{momentum of photon}]$$

$$p_p = \frac{E_p}{c} \quad (35)$$

Substitute $E_{\text{photon}} = hf$ in Eqn. (35) and we get following relation

$$p_p = \frac{hf}{c} = \frac{h}{\lambda_p} \quad (36)$$

The mass of photon (m_p) can also be calculated using $E_{\text{photon}} = m_p c^2$ and $E_{\text{photon}} = hf$, that is,

$$m_p = \frac{hf}{c^2} \quad (37)$$

An American physicist Robert Andrews experimentally proved Einstein's theory. Einstein comprehended the nature of radiations that are electromagnetic. Furthermore, it gave rise to the dual nature of light, that is, light can behave as both wave and particle. This theory too was comprehended by few scientists.

2.7 The Compton Effect

In 1923, Arthur Compton (1892–1962), an American physicist, set another landmark by confirming the quantum theory of light using the concept of conservation of linear momentum and energy. His experiment was based mainly on scattering of X-ray photons by free electrons. The classical electromagnetic theory demonstrates that if radiations are incident on free electrons, then they are scattered in all directions, although they do not undergo any frequency change. If there is no frequency change,

then it implies that the electrons have not taken any energy from incident radiation. But according to quantum hypothesis, all free electrons absorb some energy from the electromagnetic radiation.

If a beam of frequency f passes through a medium containing free electrons, then the transmitted light of some photons with frequency, f' , is lower than incident photons, such that is, $f' < f$.

This fact implies that while passing through the medium, the energy must have been absorbed by the free electrons. Hence, some interaction must have happened between free electrons and X-ray photons. This interaction is known as energy transfer within electron and photon (Figure 2.8).

According to Compton, X-ray photons collide elastically with free electrons of the medium. After collision, the electrons and photons are more in different directions. hf is the energy of incident photon and hf' is the energy of scattered photon. The difference in energy corresponds to KE of electron, that is,

$$KE = h(f - f') \quad (38a)$$

The rest mass energy of electron is m_0c^2 . Hence, the total energy, E_e , of electron after collision is equal to

$$E_e = \underbrace{m_0c^2}_{\text{Rest energy}} + \underbrace{KE}_{\text{Energy from photon}} \quad (38b)$$

From Eqs (38a) and (38b),

$$E_e = m_0c^2 + h(f - f') \quad (39)$$

Using Eqs (35) and (39) can be written as follows:

$$E_e = m_0c^2 + c(p_p - p'_p) \quad (40a)$$

where p_p is the linear momentum of photon before collision and p'_p is the linear momentum of photon after collision.

The total energy of electron after collision can also be obtained using special theory of relativity i.e.

$$E_e^2 = m_0^2c^4 + c^2p_e^2 \quad (40b)$$

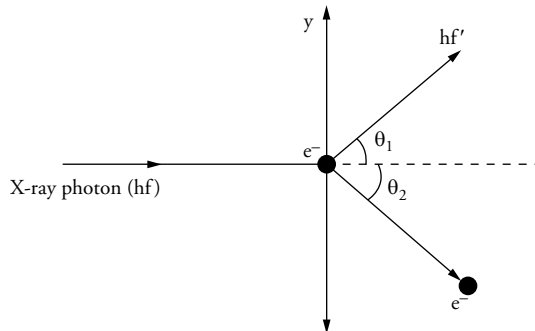


Figure 2.8 Elastic collision between a photon with energy hf and free electron.

where m_o is the rest mass of electron and p_e is the linear momentum of electron after collision.

Combining Eqs (40a) and (40b), we get

$$\left[m_o c^2 + c(p_p - p_p') \right]^2 = m_o^2 c^4 + c^2 p_e^2 \quad (41)$$

$\theta_1 =$ Scattering angle of photon

$\theta_2 =$ Scattering angle of electron or recoil angle of electron.

We can separate the momentum into components along x - and y -axes as shown in Figure 2.9.

Along x -axis

$$p_p = p_p' \cos \theta_1 + p_e \cos \theta_2 \quad (42a)$$

Along y -axis,

$$p_p' \sin \theta_1 = p_e \sin \theta_2 \quad (42b)$$

Equation (42a) can be written as follows:

$$p_p - p_p' \cos \theta_1 = p_e \cos \theta_2 \quad (42c)$$

Squaring and adding Eqs (42b) and (42c), we obtain:

$$\begin{aligned} p_p'^2 \sin^2 \theta_1 + p_p^2 + p_p'^2 \cos^2 \theta_1 - 2p_p p_p' \cos \theta_1 &= p_e^2 \sin^2 \theta_2 + p_e^2 \cos^2 \theta_2 \\ p_p'^2 + p_p^2 - 2p_p p_p' \cos \theta_1 &= p_e^2 \end{aligned} \quad (43)$$

Substituting Eqn. (43) in Eqn. (41), the following expression is obtained:

$$\frac{1}{p_p'} - \frac{1}{p_p} = \frac{(1 - \cos \theta_1)}{m_o c} \quad (44)$$

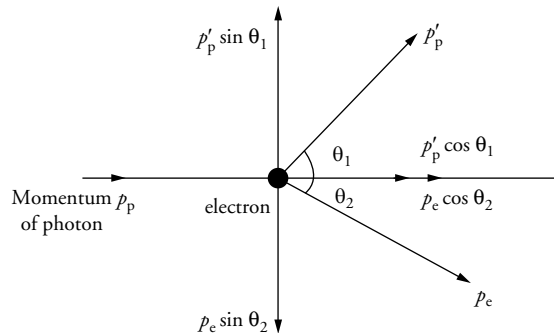


Figure 2.9 Separation of momentum into components.

From Eqn. (34)

$$\lambda_p = \frac{h}{p_p} \Rightarrow \frac{1}{p_p} = \frac{\lambda_p}{h}$$

Hence, substituting into Eqn. (44), we get

$$\frac{\lambda'_p}{h} - \frac{\lambda_p}{h} = \frac{(1 - \cos \theta_1)}{m_0 c}$$

$$(\lambda'_p - \lambda_p) = \frac{h}{m_0 c} (1 - \cos \theta_1) \quad (45)$$

Hence, Compton effect predicted change in wavelength (Compton shift) observed when the X-ray photon passes through the medium. The change in wavelength depends on the scattering angle of photon.

While performing the experiment, Compton used graphite target because electrons in carbon are loosely held and can be treated as free electrons. He performed the experiment and found the difference between scattering angles of 45° , 90° , and 135° . He obtained the difference $\lambda'_p - \lambda_p$ to be same as that predicted by Eqn. (45).

Further, $\lambda'_p - \lambda_p = \Delta\lambda$ and $\frac{\Delta\lambda}{\lambda_p}$ is fractional change, which will be negligible for long wavelengths. Hence, the Compton effect is predominantly shown by short wave, that is, having short wavelength. Light particles such as electrons cause maximum Compton effect and higher mass of particle diminishes the Compton effect.

2.8 X-Rays

In 1895, German physicist Wilhelm Roentgen discovered X-rays. He found X-rays to be propagating in straight line without deflection in electric or magnetic fields. Moreover, they also exhibit ionization effect on the medium through which they propagate. The diffraction experiments indicate that their wavelength is almost 10^{-10} m and frequency is between 10^{17} Hz – 10^{20} Hz. X-rays are electromagnetic radiations that show diffraction and polarization effect. The device used for X-ray production is shown in Figure 2.10.

The electrons are produced through heated cathode filament and are accelerated toward the metal target (anode) in vacuum tube. Electrons stop after hitting metal target and X-rays as well as heat is generated. Only a small fraction of KE of electrons (about 1 percent) is converted to X-rays and rest is converted to heat. Figure 2.11 shows the intensity spectra of X-ray radiation at various potentials.

From Figure 2.11, it is clear that below a minimum wavelength (cut-off wavelength) no radiation is produced. The more the accelerating voltage, the less is the λ_{\min} . At low accelerating voltages, the spectrum is continuous, and as the accelerating voltage increases, some sharp peaks appear in the continuous spectrum. These peaks are known as characteristic peaks as they are characteristic of the material from which the anode target is made up.

Classical electromagnetic theory can explain the continuous spectrum. The continuous spectrum is produced on scattering of electrons from metal atoms during which only a part of electron's energy is converted to electromagnetic radiation. Any decelerated charge would produce Bremsstrahlung or braking radiations. Hence, when the electrons strike the target, they are also decelerated and may

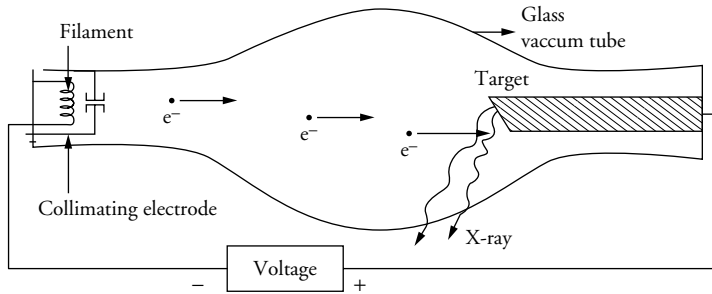


Figure 2.10 X-ray tube.

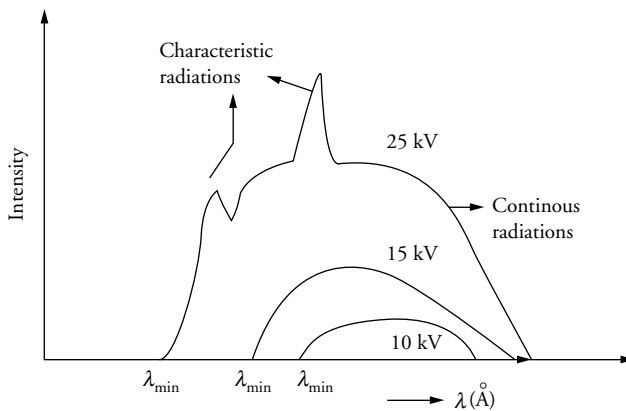


Figure 2.11 X-ray intensity pattern as produced by molybdenum target for different potentials.

produce continuous Bremsstrahlung radiation. But this theory could not explain the existence of λ_{\min} or the dependence of λ_{\min} on accelerating voltage.

But according to quantum theory of radiation, these features are explained as follows:

- When the electrons are produced from the heated filament, they may undergo multiple collisions and hence decelerate. These electrons, which undergo multiple collisions, are responsible for the production of heat in tube.
- Some of the electrons that strike the target directly and lose all their energy in single collision produce X-rays. Hence, production of X-rays can also be regarded as reverse of photoelectric effect.

If an electron is accelerated by potential V , then the most energetic electron will produce energy.

$$\begin{aligned}
 eV &= hf_{\max} \\
 \frac{hc}{\lambda_{\min}} &= eV \\
 \lambda_{\min} &= \frac{hc}{eV}
 \end{aligned} \tag{46}$$

Hence, the minimum cut-off wavelength is inversely proportional to the accelerating voltage.

2.9 Moseley's Law

In 1913, Henry Moseley discovered that the X-ray wavelength is also dependent on the atomic number of the element. Moseley's law describes the relationship between atomic number (Z) and wavelength as

$$\lambda = \frac{K}{(Z - C)^2} \quad (47)$$

C is constant

$C = 1$ for K-lines

$C = 7.4$ for L-lines

$K = 1.042 \times 10^{-2}$ for K-shell

$K = 1.494 \times 10^{-3}$ for L-shell

Moseley's Law can also be given in alternate form as

$$\sqrt{\frac{f}{R}} = \frac{Z - S}{n} \quad (48)$$

where f is the frequency, R is Rydberg constant, Z is atomic number, S is screening constant, and $n = 1, 2, 3$. Figure 2.12 shows the Moseley plots for K_α , L_α , and M_α radiations.

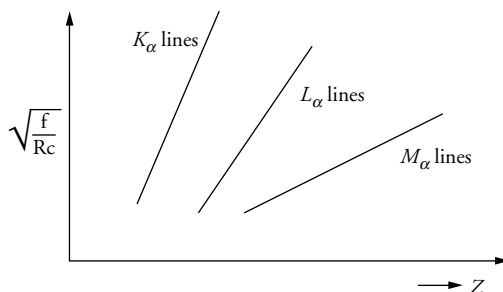


Figure 2.12 Moseley's plot for K_α , L_α , and M_α lines of characteristic X-radiations.

2.10 X-Ray Crystallography

In 1912, William Bragg gave a simple method of analyzing the scattering of X-rays for crystal planes. The wave nature of X-rays was established by Max Von Laue, a German physicist, when he suggested that the crystals could be used as diffraction gratings for X-rays. He anticipated that the spacing between the atoms of crystals is of the order of wavelength of X-rays; hence, the diffraction patterns could be obtained. Every wave has a progressive wavefront, and whenever a wavefront is restricted by some object,

diffraction occurs depending on wavelength and size of the object. William Bragg and his son Lawrence Bragg considered two successive planes of atoms as shown in Figure 2.13 for diffraction studies.

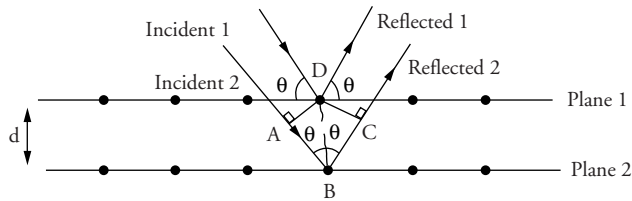


Figure 2.13 Bragg's scattering from the successive plane of atoms.

Atoms in planes 1 and 2 will scatter constructively if the path length between the waves is an integral multiple of wavelength (λ). Therefore, from Figure 2.13

$$AB + BC = n\lambda \quad [n = 1, 2, 3, \dots]$$

Now, $AB = BC = d \sin \theta$

$$n\lambda = 2d \sin \theta \quad (49)$$

where n is the order of reflected beam, d is the interplanar spacing and θ is the glancing angle. Equation (49) is Bragg's equation. Using this equation, the atomic positions can be determined in the crystal. If the wavelength of radiation is known, then the interplanar distances can be measured. The drawback of Bragg's law is that it could be used only for regularly spaced atoms.

SUMMARY

Quantum mechanics laid a strong foundation in physics. Many scientists established classical mechanics after which Pauli, Schrödinger, Heisenberg, and de Broglie worked on quantum mechanics. Hence, quantum mechanics is also called "boys' mechanics." Planck and Einstein led to the formulation of quantum mechanics as Einstein could successfully explain the photoelectric effect using Planck's quantization principle. The concept of thermal radiations and blackbody radiations could be explained. After understanding blackbody radiation, Stefan explained that energy emitted per second per unit area of blackbody radiation is directly proportional to the fourth power of temperature of body. Wien explained the relation between wavelength corresponding to maximum power emission and absolute temperature. Planck's hypothesis is also explained in this chapter according to which energy exists only in discrete packets or quanta. In contrast, Rayleigh–Jeans law states that energy exists in continuous bundles. The results of "Rayleigh–Jeans" law led to "ultraviolet catastrophe" according to which energy density diverges as $\lambda \rightarrow 0$. The quantization of energy could successfully explain the photoelectric effect. Furthermore, the oil drop experiment by Millikan in 1916 validated the value of Planck's constant ($h = 6.63 \times 10^{-34}$ Js) and Einstein's equations. It was found that photon rest mass is zero. In 1923, Compton used the conservation of linear momentum and energy to successfully explain the scattering of X-ray photons by free electrons. This chapter also gives insight into X-rays and crystallography.

SOLVED PROBLEMS

Q. 1: What is the limit (long wavelength) of Planck's law for blackbody radiation?

Ans:
$$E(\lambda, T) d\lambda = \frac{8\pi hcd\lambda}{\lambda^5 (e^{hc/\lambda k_B T} - 1)} \quad (\text{a})$$

For long wavelength limit, $e^{hc/\lambda k_B T} < 1$. Hence,

$$e^{hc/\lambda k_B T} \approx 1 + \frac{hc}{\lambda k_B T} \quad (\text{b})$$

Using result (b) in (a)

$$E(\lambda, T) d\lambda = \frac{8\pi hcd\lambda}{\lambda^5 \left[\frac{hc}{\lambda k_B T} \right]}$$

$$E(\lambda, T) d\lambda = \frac{8\pi k_B T d\lambda}{\lambda^4} \quad (\text{c})$$

Equation (c) is also known as Rayleigh–Jeans law (which leads to ultraviolet catastrophe) as $\lambda \rightarrow 0$.

Q. 2: What is the short wavelength limit of Planck's law for blackbody radiations?

Ans: For Planck's hypothesis of distribution of energy.

$$E(\lambda, T) d\lambda = \frac{8\pi hcd\lambda}{\lambda^5 [e^{hc/\lambda k_B T} - 1]}$$

For short wavelengths, $e^{hc/\lambda k_B T} > 1$. Hence, the factor 1 in denominator can be neglected.

$$E(\lambda, T) d\lambda = \frac{8\pi hcd\lambda}{\lambda^5 (e^{hc/\lambda k_B T})}$$

This is also known as Wien's law for distribution of energy.

Q. 3: Assume that sun behaves like a perfect blackbody of temperature 6,000 K. The radius of sun is 7×10^8 m. Find the rate of emission of energy from sun's surface (given $\sigma = 5.67 \times 10^{-5}$ erg/s/cm²/K⁻⁴).

Ans: Stefan's law states that $E = \sigma T^4$

$$E = 5.67 \times 10^{-5} \times (6000)^4$$

$$E = 7.38 \times 10^{10} \text{ erg/s/cm}^2$$

This represents the energy emitted per unit area per second.

To consider the whole surface, we will obtain the surface area, for sun, that is,

$$\begin{aligned} \text{Area} &= 4\pi R^2 \\ \text{Area} &= 4\pi \times (7 \times 10^{10})^2 = 6.18 \times 10^{22} \text{ cm}^2 \end{aligned}$$

Hence, the rate of emission of energy by the sun is

$$\begin{aligned} E_T &= E \times \text{Area} \\ E_T &= 7.38 \times 10^{10} \times 6.18 \times 10^{22} \\ E_T &= 4.56 \times 10^{33} \text{ erg/s} \end{aligned}$$

Q. 4: If sun has temperature 6,000 K and behaves like a perfect blackbody, obtain the wavelengths of maximum energy density.

Ans: Wien's displacement law states that

$$\lambda_m T = b$$

where $b = 0.29 \text{ cm k}$

$$\begin{aligned} \lambda_m &= \frac{b}{T} \\ \lambda_m &= \frac{0.29}{6000} \text{ cm} \\ \lambda_m &= 4833 \text{ \AA} \end{aligned}$$

Q. 5: Obtain the temperature of sun's surface, if each square centimeter of sun's surface emits energy at a rate of $1.5 \times 10^3 \text{ cal/s/cm}^2$ ($\sigma = 5.67 \times 10^{-5} \text{ erg/s/cm}^2/\text{K}^{-4}$).

Ans: According to Stefan's law,

$$\begin{aligned} E &= \sigma T^4 \\ T^4 &= \frac{E}{\sigma} \\ T^4 &= \frac{1.5 \times 10^3 \text{ cal/s/cm}^2}{5.67 \times 10^{-5} \text{ erg/s/cm}^2/\text{k}^4} \\ T^4 &= \frac{1.5 \times 10^3 \times 4.2 \times 10^7 \text{ erg/s/cm}^2}{5.67 \times 10^{-5} \text{ erg/s/cm}^2/\text{k}^4} \\ T^4 &= 1.1 \times 10^{15} \text{ K}^4 \\ T &= 5765 \text{ K} \end{aligned}$$

Q. 6: The work function of a metal is 5 eV. Obtain the minimum wavelength, which is required to eject the electron from its surface. (given $h = 6.63 \times 10^{-34}$ Js, $c = 3 \times 10^8$ m/s, $1 \text{ eV} = 1.6 \times 10^{-19}$ J)

Ans: Work function = $hf_0 = 5 \text{ eV}$

$$hf_0 = 5 \times 1.6 \times 10^{-19} \text{ J}$$

$$\frac{hc}{\lambda_0} = 5 \times 1.6 \times 10^{-19}$$

$$\lambda_0 = \frac{hc}{8 \times 10^{-19}}$$

$$\lambda_0 = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{8 \times 10^{-19}}$$

$$\lambda_0 = 2.486 \times 10^{-7} \text{ m}$$

$$\lambda_0 = 2486 \text{ \AA}$$

Q. 7: If threshold wavelength for a metal is 5,000 Å, what would be the photoelectric work function for the metal?

Ans:

$$\lambda_0 = 5000 \times 10^{-10} \text{ m}$$

$$\text{Work function} = hf_0$$

$$= \frac{hc}{\lambda_0}$$

$$W_0 = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{5000 \times 10^{-10}}$$

$$W_0 = 3.978 \times 10^{-19} \text{ J}$$

$$W_0 = \frac{3.978 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV}$$

$$W_0 = 2.486 \text{ eV}$$

Q. 8: Calculate the energy of photon with frequency 2000×10^3 cycles/s.

Ans: Energy is given by

$$E = hf$$

$$E = 6.63 \times 10^{-34} \times 2000 \times 10^3$$

$$E = 13260 \times 10^{-31}$$

$$E = 1.326 \times 10^{-27} \text{ J}$$

Q. 9: Find out the energy of photon with frequency $7,000 \text{ \AA}$.

Ans: Energy is given by

$$E = hf = \frac{hc}{\lambda}$$

$$E = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{7000 \times 10^{-10}}$$

$$E = 2.84 \times 10^{-3} \times 10^{-34} \times 10^8 \times 10^{10}$$

$$E = 2.84 \times 10^{-19} \text{ J}$$

Q. 10: Caesium atom has work function of 1.8 eV. Obtain the threshold frequency required to remove photoelectrons from caesium surface.

Ans:

$$W_o = \text{Work function of caesium} = 1.8 \text{ eV}$$

$$= 1.8 \times 1.6 \times 10^{-19} \text{ J}$$

$$W_o = hf_o$$

$$f_o = \frac{W_o}{h}$$

$$f_o = \frac{1.8 \times 1.6 \times 10^{-19}}{6.63 \times 10^{-34}}$$

$$f_o = 4.3 \times 10^{14} \text{ Hz}$$

Q. 11: Platinum has work function of 6.3 eV. What will be the longest wavelength required to eject the electrons from platinum surface?

Ans:

Work function

$$W_0 = 6.30 \text{ eV}$$

$$W_0 = 6.3 \times 1.6 \times 10^{-19} \text{ J}$$

$$W_0 = hf_0 = \frac{hc}{\lambda_0}$$

$$\lambda_0 = \frac{hc}{W_0}$$

$$\lambda_0 = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{6.3 \times 1.6 \times 10^{-19}}$$

$$\lambda_0 = 1.972 \times 10^{-7} \text{ m}$$

$$\lambda_0 = 1972 \text{ \AA}$$

Q. 12: A photon of wavelength 2000 \AA ejects out electron from caesium metal with work function 1.8 eV. Obtain the maximum kinetic energy of the ejected electron.

Ans:

$$\text{KE}_{\text{max}} = hf - W_{\text{min}}$$

$$\text{KE}_{\text{max}} = hf - hf_0$$

$$\text{KE}_{\text{max}} = \frac{hc}{\lambda} - W_{\text{min}}$$

Here $W_{\text{min}} = 1.8 \text{ eV}$ and $\lambda = 2000 \text{ \AA}$

$$\text{KE}_{\text{max}} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{2000 \times 10^{-10} \times 1.6 \times 10^{-19}} - 1.8 \text{ eV}$$

$$= [6.206 - 1.8] \text{ eV}$$

$$\text{KE}_{\text{max}} = 4.406 \text{ eV}$$

Q. 13: Potassium has work function of 2 eV. A light of wavelength 4000 \AA falls on potassium. Obtain the kinetic energy for the most energetic electron.

Ans:

$$\text{KE}_{\text{max}} = hf - hf_0$$

$$hf_0 = W_0 = 2 \text{ eV}$$

$$hf = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{4000 \times 10^{-10} \times 1.6 \times 10^{-19}} \text{ eV}$$

$$hf = 3.107 \times 10^{-3} \times 10^{-34} \times 10^8 \times 10^{29} \text{ eV}$$

$$hf = 3.107 \text{ eV}$$

$$\text{KE}_{\max} = (3.107 - 2) \text{ eV} = 1.107 \text{ eV}$$

Q. 14: Obtain the velocity of photoelectrons emitted when 4000 \AA falls on potassium (work function = 2 eV).

Ans: As described in Question 13, the kinetic energy is obtained to be 1.107 eV.

Hence,

$$\text{KE} = 1.107 \text{ eV}$$

$$\frac{1}{2}mv^2 = 1.107 \times 1.6 \times 10^{-19} \text{ J}$$

$$v^2 = \frac{2 \times 1.107 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}$$

$$v^2 = \frac{2.214 \times 1.6 \times 10^{-19} \times 10^{31}}{9.1}$$

$$v^2 = 0.3892 \times 10^{12}$$

$$v = 0.6238 \times 10^6$$

$$v = 6.238 \times 10^5 \text{ ms}^{-1}$$

Q. 15: The maximum speed of potassium photoelectrons is 10^3 m/s . Obtain the frequency of incident radiation for potassium metal (work function for potassium is 2 eV).

Ans:

$$W_0 = 2 \text{ eV}$$

$$\text{KE}_{\max} = hf - W_0$$

$$hf = \text{KE}_{\max} + W_0$$

$$hf = \frac{1}{2}mv^2 + W_0$$

$$hf = \frac{1}{2} \times 9.1 \times 10^{-31} \times (10)^6 \text{ J} + 2 \text{ eV}$$

$$hf = \frac{9.1}{2} \times 10^{-25} \text{ J} + 2 \text{ eV}$$

$$hf = \frac{9.1 \times 10^{-25}}{2 \times 1.6 \times 10^{-19}} + 2$$

$$hf = (2.84 \times 10^{-6} + 2) \text{ eV}$$

$$f = \frac{(2.00000284) \text{ eV}}{6.63 \times 10^{-34}}$$

$$f = \frac{2.2 \times 1.6 \times 10^{-19}}{6.63 \times 10^{-34}}$$

$$f = 0.483 \times 10^{15}$$

$$f = 4.83 \times 10^{14} \text{ Hz}$$

Q. 16: Prove that during Compton scattering, the energy lost by a photon when it undergoes collision is given by

$$hf \left[\frac{\alpha(1 - \cos\theta_1)}{1 + \alpha(1 - \cos\theta_1)} \right]$$

where θ_1 is angle of scattering of photon and $\alpha = \frac{hf}{m_0 c^2}$.

Ans: The change in wavelength is given by relation:

$$(\lambda'_p - \lambda_p) = \frac{h}{m_0 c} (1 - \cos\theta_1) \quad (\text{a})$$

The loss in energy is given by $hf - hf'$, where f is the frequency of photon and f' is the frequency of scattered photon.

$$\text{Energy lost} = hf - hf'$$

$$= \frac{hc}{\lambda_p} - \frac{hc}{\lambda'_p}$$

$$= hc \left(\frac{\lambda'_p - \lambda_p}{\lambda_p \lambda'_p} \right) \quad (\text{b})$$

Substituting Eqn. (a) in Eqn. (b)

$$\text{Energy lost} = \frac{hc \left[\frac{h}{m_0 c} (1 - \cos\theta_1) \right]}{\lambda_p \left[\lambda_p + \frac{h}{m_0 c} (1 - \cos\theta_1) \right]}$$

$$\begin{aligned}
 &= \frac{h^2(1 - \cos \theta_1)}{m_o \left(\lambda_p^2 \left[1 + \frac{h}{m_o c \lambda_p} (1 - \cos \theta_1) \right] \right)} \\
 &= \frac{h^2 f^2}{m_o c^2} \left[\frac{(1 - \cos \theta_1)}{1 + \frac{h}{m_o c \lambda_p} (1 - \cos \theta_1)} \right] \\
 &= hf \left(\frac{hf}{m_o c^2} \right) \left[\frac{(1 - \cos \theta_1)}{1 + \frac{hf}{m_o c^2} (1 - \cos \theta_1)} \right]
 \end{aligned}$$

Substitute $\frac{hf}{m_o c^2} = \alpha$, and hence

$$\text{Energy lost} = hf \left[\frac{\alpha(1 - \cos \theta_1)}{1 + \alpha(1 - \cos \theta_1)} \right]$$

Q. 17: The wavelength of incident photon is 2 \AA . After it collides with electron the wavelength becomes 2.8 \AA . Obtain the energy of scattered electron.

Ans: Wavelength on incident and scattered photon is 2 and 2.8 \AA , respectively.

$$\text{Energy of scattered electron is} = hf - hf'$$

$$\text{Energy} = hc \left[\frac{1}{\lambda_p} - \frac{1}{\lambda'_p} \right]$$

$$\text{Energy} = 6.63 \times 10^{-34} \times 3 \times 10^8 \left[\frac{10^{10}}{2} - \frac{10^{10}}{2.8} \right]$$

$$\text{Energy} = 19.89 \times 10^{-26} \times 10^{10} \left[\frac{2.8 - 2}{5.6} \right]$$

$$\text{Energy} = 19.86 \times 10^{-16} \left[\frac{0.8}{5.6} \right]$$

$$\text{Energy} = 2.787 \times 10^{-16} \text{ J}$$

Q. 18: What should be the wavelength of incident photon, such that there is 2 percent increase in the wavelength of scattered photon at a scattering angle of 90° ?

Ans: Given

$$\frac{\Delta\lambda}{\lambda_p} = \frac{2}{100} \quad (a)$$

$$\lambda_p = 50\Delta\lambda$$

The Compton shift is given by

$$\lambda'_p - \lambda_p = \frac{h}{m_0c}(1 - \cos\theta_1)$$

$$\Delta\lambda = \frac{h}{m_0c}(1 - \cos\theta_1) \quad \theta_1 = 90^\circ$$

$$\Delta\lambda = \frac{h}{m_0c} = 0.0243 \text{ \AA}$$

Substituting Eqn. (b) in Eqn. (a)

$$\lambda_p = 50 \times 0.0243 \text{ \AA}$$

$$= 1.215 \text{ \AA}$$

Q. 19: The wavelength of scattered radiation is 0.022 \AA (at an angle of 60°). Calculate the wavelength for incident radiation.

Ans:

$$\lambda'_p - \lambda_p = \frac{h}{m_0c}(1 - \cos\theta_1)$$

$$\theta_1 = 60^\circ \quad \lambda'_p = 0.022 \text{ \AA}$$

$$\lambda_p = \lambda'_p - \frac{h}{m_0c}(1 - \cos\theta_1)$$

$$\lambda_p = 0.022 \times 10^{-10} - 0.0243 \times 10^{-10} (1 - \cos 60^\circ)$$

$$\lambda_p = 0.022 \times 10^{-10} - 0.0243 \times 10^{-10} \times 0.5$$

$$\lambda_p = (0.022 - 0.012) \times 10^{-10}$$

$$\lambda_p = 0.010 \times 10^{-10}$$

$$\lambda_p = 0.01 \text{ \AA}$$

Q. 20: Obtain the change in wavelength for photon scattered through electron at 45° and 30° .

Ans:

For $\theta_1 = 45^\circ$

$$\lambda'_p - \lambda_p = \frac{h}{m_0 c} (1 - \cos \theta_1)$$

$$\Delta \lambda = 0.0243 \times 10^{-10} (1 - \cos 45^\circ)$$

$$\Delta \lambda = 0.0243 \times 10^{-10} \times 0.293$$

$$\Delta \lambda = 7.119 \times 10^{-3} \times 10^{-10}$$

$$\Delta \lambda = 0.0071 \text{ \AA}$$

For $\theta_1 = 30^\circ$

$$\lambda'_p - \lambda_p = \frac{h}{m_0 c} (1 - \cos 30^\circ)$$

$$\Delta \lambda = 0.0243 \times 10^{-10} (1 - 0.866)$$

$$\Delta \lambda = 0.0243 \times 10^{-10} \times 0.134$$

$$\Delta \lambda = 3.256 \times 10^{-3} \times 10^{-10}$$

$$\Delta \lambda = 0.0033 \text{ \AA}$$

Q. 21: An X-ray tube is operating at 40 kV. Calculate shortest wavelength of X-rays produced.

Ans:

$$V = 40 \text{ kV}$$

$$e = 1.6 \times 10^{-19} \text{ C}, h = 6.63 \times 10^{-34} \text{ Js}$$

$$c = 3 \times 10^8 \text{ m/s}$$

We know,

$$\lambda_{\min} = \frac{hc}{eV}$$

$$\lambda_{\min} = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \times 40 \times 1000}$$

$$\lambda_{\min} = 0.310 \times 10^{-34} \times 10^8 \times 10^{16}$$

$$\lambda_{\min} = 0.310 \text{ \AA}$$

Q.22: In a Coolidge tube, electrons bombarding the target produce X-rays of wavelength 5 \AA . Calculate the impact energy of electron.

Ans: As

$$\lambda_{\min} = \frac{hc}{eV}$$

$$eV = \frac{hc}{\lambda_{\min}} = \text{KE}$$

$$\text{KE} = eV = \frac{hc}{\lambda}$$

$$\text{KE} = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{5 \times 10^{-10}}$$

$$\text{KE} = 3.97 \times 10^{-34} \times 10^{18}$$

$$\text{KE} = 3.97 \times 10^{-16} \text{ J}$$

$$\text{KE} = \frac{3.97 \times 10^{-16}}{1.6 \times 10^{-19}} \text{ eV}$$

$$\text{KE} = 2.48 \times 10^3 \text{ eV}$$

$$\text{KE} = 2.48 \text{ KeV}$$

OBJECTIVE QUESTIONS

1. Velocity of photon of ultraviolet light is

- (a) $2c$
(c) c

- (b) $3c$
(d) $c/2$

2. Perfect emitter is

- (a) perfect absorber
(c) dielectric

- (b) insulator
(d) all of the above

3. Stefan's law gives the dependence of

- (a) energy and wavelength
(c) energy and velocity

- (b) energy and time
(d) energy and temperature

4. According to Stefan's law

- (a) $E = \sigma T^4$
(c) $E = \sigma T$

- (b) $E = \sigma / T^4$
(d) $E = \sigma / \sqrt{T}$

5. The Wien's displacement law states
- (a) $\lambda_m = b/T$ (b) $\lambda_m = bT$
(c) $\lambda_m T = b$ (d) $\lambda_m / b = T$
6. According to Planck's quantum hypothesis, energy is
- (a) discrete (b) continuous
(c) both discrete and continuous (d) neither discrete nor continuous
7. The limiting case of Planck's energy distribution is
- (a) Wien's distribution law (b) Rayleigh–Jeans law
(c) photoelectric effect (d) Stefan's law
8. According to ultraviolet catastrophe:
- (a) at $\lambda \rightarrow 0, E \rightarrow 0$ (b) at $\lambda \rightarrow \infty, E \rightarrow \infty$
(c) at $\lambda \rightarrow 0, E \rightarrow \infty$ (d) at $\lambda \rightarrow \infty, T \rightarrow 0$
9. Corpuscular nature of radiations could be proved by
- (a) interference (b) Compton effect
(c) polarization (d) dispersion
10. The velocity of photoelectrons depend on
- (a) frequency of incident light (b) intensity of incident light
(c) both frequency and intensity (d) neither frequency nor intensity
11. When intensity is doubled,
- (a) energy of electrons is doubled
(b) number of photoelectrons are doubled
(c) energy gets halved
(d) velocity is four times
12. Photoelectric effect is based on
- (a) conservation of energy (b) conservation of momentum
(c) conservation of angular momentum (d) conservation of charge
13. To explain photoelectric effect, the main condition is
- (a) light is having continuous nature (b) light has pulsating nature
(c) none of these (d) light consists of quanta
14. The dimension of Planck's constant is same as
- (a) mass (b) angular momentum
(c) Energy (d) charge

15. Compton shift depends on
(a) angle of incidence
(b) scattering angle of photon
(c) recoil angle
(d) all of the above
16. The Compton shift is independent of
(a) material of target
(b) energy of incident radiation
(c) recoil angle
(d) all of the above
17. The photo electron effect occurs for
(a) free electrons
(b) bound electrons
(c) both
(d) none of the above
18. The photon mass is given by
(a) $hf c^2$
(b) hc
(c) hf
(d) hf/c^2
19. Characteristic X-rays are
(a) emitted from cathode
(b) emitted from anode
(c) emitted from filament
(d) all of the above
20. Continuous X-rays are also known as
(a) Bremsstrahlung rays
(b) Compton radiations
(c) discrete radiations
(d) visible radiations

ANSWERS

- | | | | |
|--------|---------|---------|---------|
| 1. (c) | 6. (a) | 11. (b) | 16. (d) |
| 2. (a) | 7. (b) | 12. (a) | 17. (a) |
| 3. (d) | 8. (c) | 13. (d) | 18. (d) |
| 4. (a) | 9. (b) | 14. (b) | 19. (b) |
| 5. (c) | 10. (a) | 15. (b) | 20. (a) |

Micro-Assessment Questions

1. What are the assumptions made by Planck for blackbody radiation?
2. An X-ray photon is scattered by an electron. What happens to the frequency of the scattered photon w.r.t. incident photon?
3. If the photoelectric effect occurs in a gaseous target rather than a solid, will photoelectrons be produced at all frequencies of the incident photon?
4. How does the Compton effect differ from the photoelectric effect?
5. If the photoelectric effect is observed for one metal, will the effect be observed for another metal under the same conditions? Explain.
6. What are the assumptions made by Compton during scattering of a photon from an electron?
7. What do you understand by Compton shift?
8. Why does the existence of a cut-off frequency in the photoelectric effect favour a particle theory for light rather than a wave theory?
9. Explain Rayleigh–Jeans law.
10. Is every photon responsible for the photoelectric effect or emission of an electron?
11. Wave nature of matter is not apparent during daily observations. Explain.
12. Explain the variation of kinetic energy of photoelectrons with frequency of light.
13. What is work–function of material? Give its relation with the threshold frequency.
14. Why the electrons emitted from the metal surface have different velocities inspite of the fact that the incident light is monochromatic?
15. When the wavelength of incident light is decreased, how will the velocity of photoelectrons be change?
16. Alkali metals are preferred photocathodes. Explain.

Critical Thinking Questions

1. Which stars have the higher surface temperature. Red or blue?
2. Explain that a perfect emitter is a perfect absorber.
3. All objects radiate energy but we cannot see the objects in dark room. Explain?
4. What is ultraviolet catastrophe?
5. Explain the stopping potential.
6. Derive Einstein's photoelectric equation. How will it explain the photoelectric laws?
7. How classical theory failed to explain the photoelectric equation?
8. Show that the wavelength change for scattered photons is independent of wavelength of incident radiation during Compton experiment.
9. Which one possesses more energy electron or proton, both having same wavelength?
10. What is the source of continuous X-rays?
11. State and explain Moseley's law.
12. What is the difference between characteristic and continuous X-rays?
13. What are X-rays diffraction and Bragg's planes?
14. If a high-energy photon strikes the metal surface, then how will the kinetic energy for the photoelectron vary?

15. Calculate the energy of a photon whose frequency is (a) 80 GHz, (b) 30 GHz, and (c) 20 MHz. Express your answers in electron volts.
16. The temperature of human skin is approximately 35°C. What would be the peak wavelength for radiations emitted from skin?

Graded Questions

1. The photocurrent of a photocell is cut-off by a retarding potential of 3.92 V for radiation of wavelength 250 nm. Obtain the work function for the material.
2. Light of wavelength 200 nm is incident on a metallic surface. If the stopping potential for the photoelectric effect is 0.45 V, find (a) the maximum energy of the emitted electrons, (b) the work function, and (c) the cut-off wavelength.
3. X-rays with an energy of 200 keV undergo Compton scattering. If the scattered rays are detected at 60° relative to the incident rays, find (a) the Compton shift at this angle, (b) the energy of the scattered X-ray, and (c) the energy of the recoiling electron.
4. Find the energy of an X-ray photon that can impart a maximum energy of 30 keV to an electron by Compton collision.
5. A photon undergoing Compton scattering has an energy after scattering of 20 keV, and the electron recoils with an energy of 15 keV. (a) Find the wavelength of the incident photon, (b) Find the angle at which the photon is scattered, and (c) Find the angle at which the electron recoils.
6. A 2 Å X-ray photon is deflected through 134° in a Compton scattering event. What is the recoiling angle?
7. Calculate the energy and momentum of a photon of wavelength 300 nm.
8. The work function for potassium is 2 eV. If light of wavelength 450 nm, incident on it find (a) the maximum kinetic energy of the photoelectrons and (b) the cut-off wavelength.
9. Find out the shortest wavelength of X-rays produced for a tube operating at 55 kV.
10. The work-function of a metal is 3 eV. What should be its maximum wavelength so that photoelectrons can be ejected from its surface.
11. A metal has threshold voltage of 6,000 Å. Find out the work function and threshold frequency.
12. Caesium metal has a work function of 1.8 eV. Light radiation of wavelength 2,000 Å is incident on the metal. Find out the maximum possible kinetic energy of electrons ejected.
13. What is the frequency of photon with energy 80 eV?
14. Find out the Compton shift for X-ray beam of wavelength 3 Å and scattered through an angle of 90°.

Remember and Understand

1. The energy in electromagnetic wave is carried in packets known as photons. The energy is given by $E = hf$ and momentum is given by $p = E/c$.
2. According to Wien's displacement law, the wavelength of maximum emittance is inversely proportional to absolute temperature T . This is known as Wien's displacement law.
3. According to photoelectric effect, threshold energy is required to eject electron out of metal surface. Extra energy is imparted as the kinetic energy to electrons.
4. The Rayleigh–Jeans law could explain only the lower part of blackbody radiation. This predicted ultraviolet catastrophe at higher energy part.

5. Planck's law could explain the ultraviolet catastrophe and Rayleigh–Jeans law was a special case of it.
6. Continuous X-rays are produced due to Bremsstrahlung, whereas characteristic X-rays are produced due to photoelectric process.
7. According to Bragg's law of X-ray diffraction, $2d \sin \theta = n\lambda$, d is the interplanar spacing and λ is the wavelength of incident X-rays.
8. In Compton shift, the wavelength shift is independent of nature of scattered. i.e.
$$(\lambda'_p - \lambda_p) = \frac{h}{m_o c} (1 - \cos \theta_1)$$
9. Photoelectric current increases with intensity of light.
10. Photoelectric effect is an instantaneous process and it only occurs for a definite threshold frequency.
11. The rest mass of photon is zero and it travels with velocity of light. Photons cannot be deflected by electric and magnetic field as they are electrically neutral.

Quantum Mechanics—II

Uncertainty Principle and Schrödinger Equations

Keywords: de-Broglie waves, quantum mechanics, uncertainty principle, Schrödinger equations, wave function, orthonormality, Schwarz inequality, expectation values, orthogonality

Learning Objectives

- ◆ To study the matter waves and de-Broglie relation
- ◆ To obtain de-Broglie wavelength in terms of energy and temperature
- ◆ To understand Davisson and Germer experiment
- ◆ To understand phase velocity, group velocity, and particle velocity
- ◆ To get an insight into wave packet and group of waves
- ◆ To understand Heisenberg's uncertainty principle of, i.e, position and momentum cannot be measured simultaneously
- ◆ To learn about differential equations and well-behaved wave functions
- ◆ To learn Schrödinger's time-dependent and time-independent equations
- ◆ To understand the probabilistic approach
- ◆ To know about the expectation values and average values
- ◆ To obtain the Schwarz's inequality, i.e, product of wave functions
- ◆ To learn that Ehrenfest theorem which bridges the gap between classical and quantum mechanics
- ◆ To learn about operators and their types
- ◆ To understand Eigen values, Eigen functions, and Eigen equations
- ◆ To know about Hermitian operators

Electromagnetic radiations have dual characteristics: particle and wave. The particle characteristic of electromagnetic wave can be demonstrated by photoelectric and Compton effects, whereas the wave characteristic can be verified by the interference and diffraction. Hence, electromagnetic radiations can show particle and wave characteristics. Both the characteristics cannot be shown in a single experiment. de-Broglie proposed that due to symmetry in nature, light should also be exhibiting dual characteristics. Photon is associated with light wave; similarly, material particles such as electron, proton, etc., have matter waves associated with them. These matter waves are known as de-Broglie waves (different from electromagnetic waves).

3.1 de-Broglie Hypothesis

de-Broglie hypothesis states that the wave–particle dualism is not only limited to radiations, but also valid for fundamental entities such as material particles. Hence, de-Broglie waves are associated with particles matter. The energy of photon is given by the following expression:

$$E = hf = \frac{hc}{\lambda} \quad (1)$$

According to the principle of relativity, the energy is given by the following equation:

$$E = (\text{photon mass})c^2$$

$$E = mc^2 \quad (2)$$

From Eqs (1) and (2),

$$\frac{hc}{\lambda} = mc^2$$

$$\lambda = \frac{h}{mc} \quad (3)$$

For matter particle of mass m and velocity v , Eqn. (3) is given by

$$\lambda = \frac{h}{mv} \quad (4)$$

Equation (4) gives the de-Broglie wavelength for matter particle. de-Broglie wavelength is independent of charge of particle. For the particle with heavy mass, the wavelength is small and vice versa.

3.2 de-Broglie Wavelength of Temperature and Potential

The kinetic energy of a particle with mass m and velocity v is given by

$$E = \frac{1}{2}mv^2 \quad [p = mv]$$

$$E = \frac{p^2}{2m} \quad (5)$$

$$p = \sqrt{2mE} \quad (6)$$

From Eqs (4) and (6),

$$\lambda = \frac{h}{\sqrt{2mE}} \quad (7)$$

According to kinetic theory of gas, the kinetic energy for material particle is given by

$$E = \frac{3}{2}k_B T \quad (8)$$

Using Eqs (7) and (8),

$$\lambda = \frac{h}{\sqrt{3mk_B T}} \quad (9)$$

Let the electron with charge e and mass m are under the effect of accelerating voltage V . During the process of acceleration, electron acquires velocity v and the kinetic energy of acceleration. Electron energy is given by

$$E = eV \quad (10)$$

Put Eqn. (10) in Eqn. (7)

$$\lambda = \frac{h}{\sqrt{2meV}} \quad (11)$$

and

$$p = \sqrt{2meV} \quad (12)$$

Hence, the de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p} = \frac{h}{\sqrt{2meV}} \quad (13)$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times V}}$$

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA} \quad (14)$$

3.3 Davisson and Germer Experiment

To predict the waves associated with electron, Davisson and Germer performed experiments in 1927. Figure 3.1 shows the Davisson–Germer experimental setup. Electron gun (G) produces the electron beam and F is the filament inside the electron gun. Due to thermionic emission, electrons are emitted from the filament. A is a set of plates with pinholes and B is the hole from which the narrow beam of electrons emerge out. These electrons have energy eV and are well collimated. When the high-tension voltage is varied, the velocity of electrons get changed. After the beam comes out through hole B, it falls on the nickel target and the electrons get scattered. These scattered electrons are collected by detector D. The detector D is movable such that the electrons from all directions can be measured. The electrons collected using a collector coin can be amplified and then measured using a galvanometer. The detector D collects fast-moving electrons only. This whole arrangement is enclosed inside high vacuum. The apparatus operated in two modes as described below:

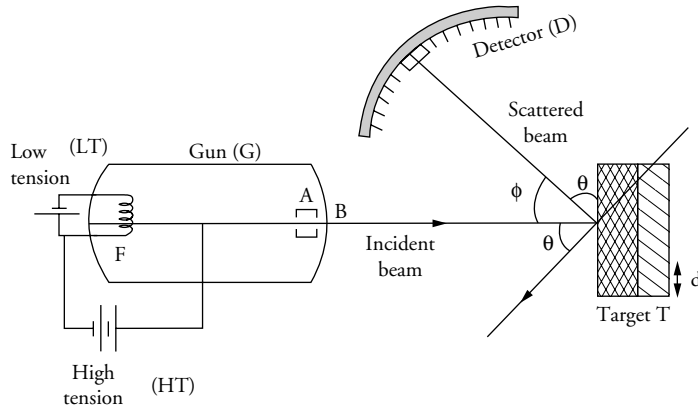


Figure 3.1 The Davisson–Germer experimental setup.

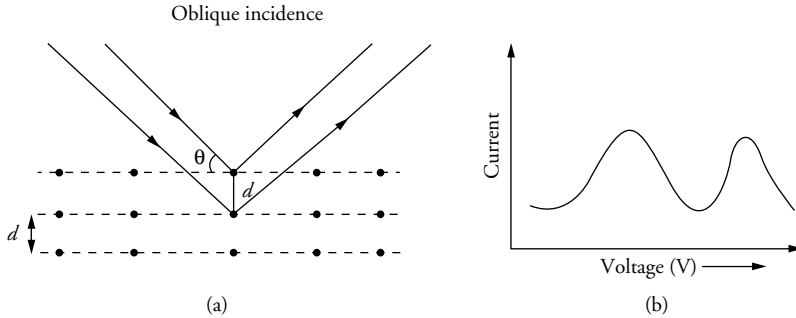


Figure 3.2 (a) Bragg's Reflection, and (b) current versus voltage for oblique incidence.

1. Oblique Incidence

The angle of incidence is kept at 10° and the accelerating voltage is varied to vary electron's wavelength. The electrons suffer Bragg's reflection and satisfy the Bragg's condition (Figure 3.2(a))

$$n\lambda = 2d \sin \theta \tag{15}$$

where d is interplanar distance.

The characteristics between current and \sqrt{V} are shown in Figure 3.1(b). From Eqn. (15),

$$n \propto \frac{1}{\lambda} \tag{16}$$

Comparing (13) and (16),

$$n \propto \frac{\sqrt{2meV}}{h}$$

$$n \propto (V)^{1/2} \tag{17}$$

Equation (17) is validated from Figure 3.2(b), which indicates that order of Bragg's reflection is proportional to square root of accelerating potential.

2. Normal Incidence

In this case, the electrons fall normally on the surface of target. The accelerating voltage was changed and graph was plotted between the current and angle between the incident beam and scattered beam. Figure 3.3 shows the plots at different accelerating voltages. It is observed that at a voltage of 40 V, no bump is there. A bump appears at voltage of 44 V and this bump gets very prominent at an accelerating voltage of 54 V. After 54 V, the bump starts decreasing with further increase in voltage. Hence, it is concluded that at 54 V the electron waves show constructive interferences at that voltage. According to Bragg's diffraction, condition,

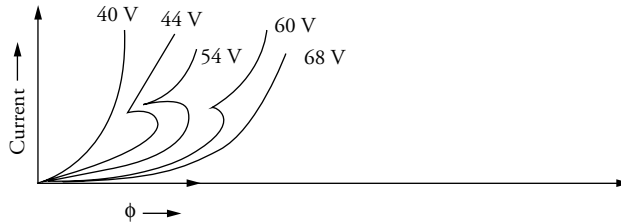


Figure 3.3 Variation of galvanometric current and co-latitude angle(ϕ). [Co-latitude is the angle between incident ray and scattered beam entering the detector]

$$n\lambda = 2d \sin\theta$$

From Figure 3.1,

$$\theta + \phi + \theta = 180^\circ$$

Hence, $\theta = 65^\circ$ for $\phi = 50^\circ$ at 54 V

For $n = 1$

$$\lambda = 2d \sin(65^\circ) \quad (18)$$

For Ni crystal, $d = 0.91 \text{ \AA}$, hence Eqn. (18) becomes

$$\lambda = 2 \times (0.91 \times 10^{-10}) \sin 65^\circ = 1.65 \text{ \AA} \quad (19)$$

At 54 V, the de Broglie wavelength is given by

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{12.27 \text{ \AA}}{\sqrt{V}} = \frac{12.27 \times 10^{-10}}{\sqrt{54}}$$

$$\lambda = 1.66 \text{ \AA} \quad (20)$$

Hence, the theoretical and experimental results are in good agreement with each other.

3.4 Relation Between Momentum and Propagation Constant

de-Broglie explained the dual nature of matter, i.e., matter waves exhibit particle as well as wave nature. When the matter exhibits particle nature, it has localized position in space. But wave is not located at a particular position because wave is basically a function of position and time. The wave associated with a particle is given by (in x -direction)

$$\frac{\partial^2 A(x,t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 A}{\partial t^2} \quad (21)$$

$A(x, t)$ represents the displacement of wave traveling with velocity v . For a wave to propagate, $A(x, t)$ should always exist. For three-dimensional wave, Eqn. (21) is given by

$$\frac{\partial^2 A(x, y, z, t)}{\partial r^2} = \frac{1}{v^2} \frac{\partial^2 A(x, y, z, t)}{\partial t^2} \quad (22)$$

The matter wave is represented by $\Psi(x, y, z, t)$. This wave function gives complete information of the matter wave $\Psi(x, y, z, t)$ as given by

$$\Psi(r, t) = C e^{i(kx - \omega t)} \quad (23)$$

For a wave in x -direction, it is given by

$$\Psi(x, t) = C e^{i(kx - \omega t)} \quad (24)$$

In Eqn. (24), C is the constant and k is wave number/propagation constant. If at time $t = 0$, we have knowledge of $\Psi(x, t)$, then we can find out $\Psi(x, t)$ at time t . One must take into account that electromagnetic wave may be represented by either the real part or imaginary part, but the matter waves have both the parts. Propagation constant and momentum can be related by the following relation:

$$\lambda = \frac{h}{p} \quad \text{and} \quad k = \frac{2\pi}{\lambda}$$

Hence

$$k = \frac{2\pi p}{h}$$

$$p = \frac{h}{2\pi} k$$

$$p = \hbar k \quad \left(\text{where } \hbar = \frac{h}{2\pi}\right) \quad (25)$$

3.5 Velocity of de-Broglie Wave and Need of Wave Packet

Let us suppose the particle is traveling with velocity; hence, one can assume the velocity of matter wave to be same as particle velocity. Let us take the de-Broglie wave velocity to be D , such that

$$D = f\lambda \quad (26)$$

We know, from Planck's law

$$E = hf \quad (27a)$$

[From Eqn. (3) $\lambda = \frac{h}{mc}$]

and from Einstein's mass-energy relation

$$E = mc^2 \quad (27b)$$

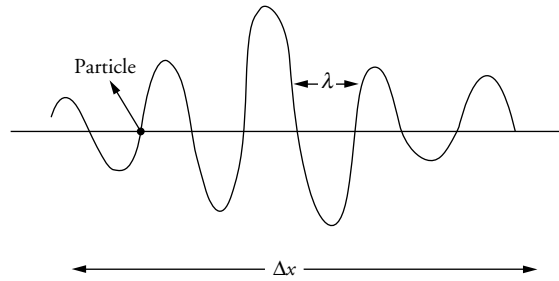


Figure 3.4 Wave packet associated with particle.

From Eqn. (27a–b)

$$f = \frac{mc^2}{h} \quad (28)$$

Using Eqn. (28) and de-Broglie wavelength for mater wave [velocity = v] in Eqn. (26),

$$D = \frac{mc^2}{h} \times \frac{h}{mv}$$

$$D = \frac{c^2}{v} \quad (29)$$

Equation (29) implies that the velocity of matter wave is more than velocity of light, which is a contradictory situation. Hence, Schrödinger postulated the concept of wave packet according to which moving particle is not associated with a single wave but with a group of waves. Such group of waves is called wave packet. According to Eqn. (29) the matter wave is extended infinitely in space. But the actual particle is represented by finite wave, i.e., the wave function associated with a particle should be zero everywhere except the position where particle exists (Figure 3.4).

Wave packet has a group of waves that travel with different speed. Many waves interfere to give rise to wave packet where amplitude is quite large in a small region of space. The probability of finding a particle varies directly as the amplitude. The probability of finding a particle is minimum, where the amplitude is small and vice versa.

3.6 Wave and Group Velocity

Till now, we have understood the following points regarding wave packet:

- When many waves combine linearly, then they give rise to wave packet.
- The wave packet is associated with localised partical.
- Many waves combine to form a wave packet; every wave has different wavelengths $\lambda = \frac{h}{mv}$

corresponding to different velocity, hence different wave numbers also. When these waves are added together to form a single wave packet, the momentum of wave packet is uncertain.

- The velocity of every individual de Broglie wave is known as phase velocity of wave (v_p).
- The velocity with which the wave packet travels is known as group velocity (v_g) of packet.

Mathematical Treatment

Let us take two waves represented by

$$y_1 = A \cos(kx - wt) \quad (30a)$$

$$y_2 = A \cos((k + dk)x - (w + dw)t) \quad (30b)$$

where dk and dw are small changes in wave number and angular velocity.

The resultant is given by

$$y = y_1 + y_2$$

$$y = A \left[\cos(kx - wt) + \cos\left[(k + dk)x - (w + dw)t\right] \right]$$

$$y = 2A \cos\left[\frac{(2k + dk)x - (2w + dw)t}{2}\right] \cos\left[\frac{(dk)x - (dw)t}{2}\right]$$

where dk and dw are very small; hence, they are negligible compared with k and w , respectively.

$$y = 2A \cos(kx - wt) \cos\left[\frac{dk}{2}x - \frac{dw}{2}t\right] \quad (31)$$

In Eqn. (31), $\left(\frac{dk}{2}\right)$ and $\left(\frac{dw}{2}\right)$ are the modulation factors. This modulating wave number and angular frequency produce successive “wave groups.” The phase velocity is given by

$$v_p = f\lambda = \frac{2\pi f\lambda}{2\pi}$$

$$v_p = \frac{w}{(2\pi/\lambda)} = \frac{w}{k} \quad (32)$$

The group velocity (v_g) is given by

$$v_g = \frac{dw}{dk} \quad (33)$$

Substituting Eqn. (32) in Eqn. (33)

$$v_g = \frac{d}{dk}(v_p k)$$

$$v_g = v_p + \frac{k dv_p}{dk} \quad (34)$$

Furthermore,

$$k = \frac{2\pi}{\lambda} \quad (35a)$$

$$\frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2}$$

$$dk = -\frac{2\pi}{\lambda^2} d\lambda \quad (35b)$$

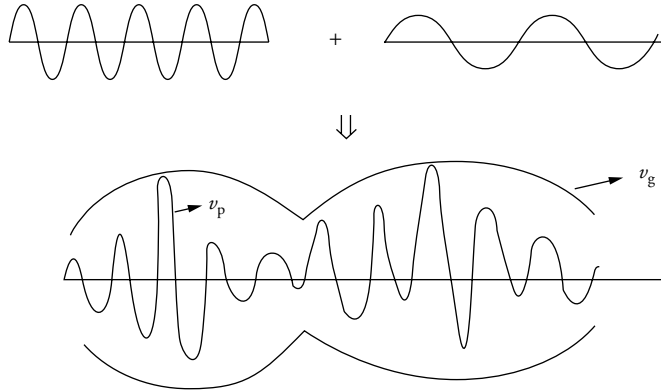


Figure 3.5 Superposition of waves resulting in group wave.

Dividing Eqn. (35a) and Eqn. (35b),

$$\frac{k}{dk} = -\frac{\lambda}{d\lambda} \tag{36}$$

Substituting Eqn. (36) in Eqn. (34),

$$v_g = v_p - \frac{\lambda}{d\lambda} dv_p \tag{37}$$

Figure 3.5 depicts the modulated wave form for wave packet. The wave moves with group velocity v_g and particle has velocity v_p .

3.7 Equivalence of Group and Particle Velocity

The group velocity is given by $v_g = \frac{dw}{dk}$

$$v_g = \left(\frac{dw/dv}{dk/dv} \right) \tag{38}$$

As

$$w = 2\pi f$$

$$w = 2\pi \left(\frac{mc^2}{h} \right) \text{ from Eqn. (28)}$$

$$w = \frac{2\pi c^2}{h} \frac{m_o}{\sqrt{1 - v^2/c^2}}$$

The particle is supposed to move in relativistic regime and hence relativistic mass is taken with rest mass zero.

$$\frac{dw}{dv} = \frac{2\pi m_o v}{h} \left(1 - \frac{v^2}{c^2} \right)^{-3/2} \tag{39}$$

Now, we have to find $\frac{dk}{dv}$

$$\begin{aligned}
 k &= \frac{2\pi}{\lambda} \\
 k &= \frac{2\pi}{(h/mv)} = \frac{2\pi mv}{h} \\
 k &= \frac{2\pi v}{h} \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \\
 \frac{dk}{dv} &= \frac{2\pi m_0}{h} \left(1 - \frac{v^2}{c^2}\right)^{-3/2}
 \end{aligned} \tag{40}$$

Using Eqs. (39) and (40) in Eqn. (38),

$$\begin{aligned}
 v_g &= \frac{\frac{2\pi m_0 v}{h} \left(1 - \frac{v^2}{c^2}\right)^{-3/2}}{\frac{2\pi m_0}{h} \left(1 - \frac{v^2}{c^2}\right)^{-3/2}} \\
 v_g &= v
 \end{aligned} \tag{41}$$

Hence, group velocity and phase velocity are the same. Therefore, the moving particle and wave packet travel with same velocity.

3.8 The Uncertainty Principle

The principle of uncertainty states that “The position and momentum of a particle cannot be measured precisely and simultaneously.” This relation was given by Werner Heisenberg. If Δp_x is the uncertainty in momentum of particle and Δx is the uncertainty in position of particle, then

$$\Delta x \Delta p_x \geq \hbar \tag{42}$$

From Eqn. (42), we can say that the product of uncertainties in position and momentum is always greater than Planck’s constant. Momentum and position cannot be measured simultaneously. If we measure position with great certainty, then the momentum has large uncertainty. If $\Delta x = 0$ or $\Delta p = 0$, then the other term is completely uncertain. Hence, uncertainty can be regarded as an inherent property of every natural object. For microscopic objects, the uncertainty principle holds good. But in macroscopic regime, it is no longer valid. Moreover, position can be measured with great accuracy and momentum can also be measured with certainty but not simultaneously. The uncertainty in y and z direction can be given by

$$\Delta y \Delta p_y \geq \hbar$$

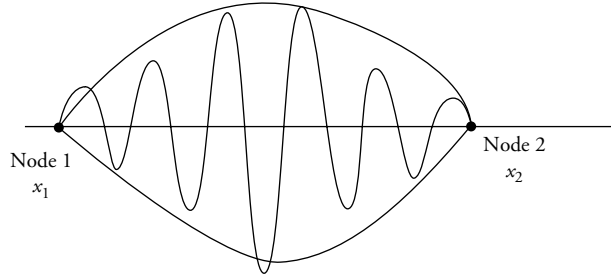


Figure 3.6 Uncertainty of particle within the wave packet.

and

$$\Delta z \Delta p_z \geq \hbar$$

The general expression can be given by:

$$\Delta r \Delta p_r \geq \hbar \quad (43)$$

Proof of Heisenberg Uncertainty Principle

From Eqn. (31), the superposition of waves gives the resultant as

$$y = 2A \cos(kx - wt) \cos\left(\frac{(dk)x}{2} - \frac{(dw)t}{2}\right)$$

Figure. 3.6 depicts the probability of finding the particle in between the nodes. The node can be formed if following condition is satisfied, that is,

$$\cos\left(\frac{(dk)}{2}x - \frac{(dw)}{2}t\right) = 0$$

$$\cos\left(\frac{\Delta k}{2}x - \frac{\Delta w}{2}t\right) = 0$$

or

$$\frac{(\Delta k)}{2}x - \left(\frac{\Delta w}{2}\right)t = (2n+1)\frac{\pi}{2}$$

$$x \Delta k - t \Delta w = (2n+1)\pi \quad (44)$$

Δx can be given by (Fig. 3.6)

$$\Delta x = x_2 - x_1 \quad (45a)$$

and

$$x_2 \Delta k - t \Delta w = (2n+3)\pi \quad (45b)$$

$$x_1 \Delta k - t \Delta w = (2n+1)\pi \quad (45c)$$

Using (45b) and (45c) in (45a),

$$\Delta x = \left(\frac{(2n+3)\pi + t\Delta w}{\Delta k} \right) - \left(\frac{(2n+1)\pi + t\Delta w}{\Delta k} \right)$$

$$\Delta x = \frac{2\pi}{\Delta k} \quad (46)$$

Furthermore, by using $k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}$,

$$\Delta x = \frac{2\pi}{\Delta \left(\frac{2\pi p}{h} \right)} = \frac{2\pi}{\frac{2\pi}{h} \Delta p}$$

$$\Delta x = \frac{h}{\Delta p}$$

$$\Delta x \cdot \Delta p = h$$

or $\Delta x \cdot \Delta p \geq \hbar$ [h and \hbar have same order] (47)

This is the uncertainty principle with reference to a wave packet.

Werner Heisenberg was a German physicist who was born in Würzburg, Germany, in 1901. His father was a prominent secondary school teacher. He was a student of Ludwig-Maximilians-Universität, München, and the Georg-August-Universität, Göttingen. He earned his doctorate in 1923. He contributed significantly to particle physics, nuclear physics, and quantum field theory. He formulated quantum mechanics in terms of matrices. Hence, he developed quantum mechanics and its modern interpretation. One of the earliest breakthroughs to quantum mechanics was in 1925, when Heisenberg formulated the uncertainty principle. For this contribution, he was awarded the Nobel Prize for Physics in 1932 at a young age of 31 years. Heisenberg is widely considered as one of the most influential figures.



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3.9 Applications of Heisenberg Principle

Using Heisenberg uncertainty principle, the probable position or momenta of particle can be elucidated. Uncertainty principle can be used to extract lots of information for many systems as discussed below:

1. No Electron Within Nucleus

The size of atomic nucleus is of the order of 10^{-14} m as determined by Rutherford's gold foil experiment. Hence, the uncertainty in position is given by

$$\Delta x = 10^{-14} \text{ m}$$

Using uncertainty principle,

$$\Delta x \Delta p = \hbar$$

$$\Delta p = \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 10^{-14}}$$

$$\Delta p = 1.048 \times 10^{-20} \text{ kg m/s} \quad (48)$$

The kinetic energy of particle is

$$E = \frac{p^2}{2m}$$

Uncertainty in momentum represents minimum momentum of electron, hence

$$E = \frac{(1.048 \times 10^{-20})^2}{2 \times 9.1 \times 10^{-31}} \times \frac{1}{1.6 \times 10^{-19}} \text{ eV}$$

$$E = 370 \text{ MeV} \quad (49)$$

Therefore, the electrons must possess at least energy of the order of 370 MeV, whereas the electrons emitted out from the nucleus is only upto 3–4 MeV. This clearly validates the fact that the electrons cannot exist inside the nucleus.

2. Energy of Particle in a Box

Let the particle is contained in box (one-dimensional), such that its linear dimension is L . Hence, the uncertainty of particle can be given by dimension L as particle can lie anywhere in the box. Hence,

$$\Delta x = L \quad (50)$$

From uncertainty principle,

$$\Delta x \cdot \Delta p = \hbar$$

$$\Delta p = \frac{\hbar}{L} \quad (51)$$

Again the kinetic energy can be written as

$$E = \frac{p^2}{2m} \quad (52)$$

From Eqs (51) and (52),

$$E = \frac{\hbar^2}{2mL^2} \quad (53)$$

Equation (53) represents minimum zero point energy for a particle in box. Classically, the minimum energy for particle in box is zero; but quantum mechanically, the minimum energy for a particle is never zero.

3. Strength of Nuclear Force

The nuclear forces are short-range forces that exist inside the nucleus. The nuclear radius is of the order of Fermi = $[10^{-15} \text{ m}]$.

The kinetic energy is given by

$$E = \frac{p^2}{2m} = \frac{\hbar^2}{\Delta x^2 (2m)} \quad (\text{from } \Delta x \cdot \Delta p = \hbar)$$

$$E = \frac{(6.63 \times 10^{-34})^2}{4 \times 3.14 \times 3.14 \times (10^{-15})^2 \times 2 \times (1.67 \times 10^{-27})}$$

$$E = 9.6 \text{ MeV} \quad (54)$$

Hence, binding energy of nuclear is of the order of 10 MeV.

4. Hydrogen Atom

Hydrogen atom consists of an electron around the nuclei. The radius of orbit is a and hence uncertainty is given by

$$\Delta x = a \quad (55)$$

The total energy is given by following expression:

$$E = \text{Kinetic energy} + \text{potential energy}$$

$$[\text{potential energy due to Coulomb field is } \frac{-Ze^2}{4\pi\epsilon_0 a}]$$

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 a} \quad [\text{For hydrogen atom, } Z = 1]$$

$$E = \frac{1}{2m} \left(\frac{\hbar}{\Delta x} \right)^2 - \frac{e^2}{4\pi\epsilon_0 a}$$

$$E = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_0 a} \quad (56)$$

The radius of hydrogen atom can be obtained using equation $\frac{dE}{da} = 0$. (minimum energy condition)

$$\frac{dE}{da} = \frac{-\hbar^2}{ma^3} + \frac{e^2}{4\pi\epsilon_0 a^2}$$

Hence, using $(dE/da) = 0$,

$$a = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad (57)$$

Equation (57) gives the radius of first orbit of hydrogen when $n = 1$.

Substituting Eqn. (57) in Eqn. (56),

$$\begin{aligned}
 E &= \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2} - \frac{me^4}{16\pi^2\epsilon_0^2\hbar^2} \\
 E &= \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2} \\
 E &= \frac{-(9.1 \times 10^{-31})(1.6 \times 10^{-19})^4 (3.14)^2 \times 4}{32 \times (3.14)^2 \times (8.85 \times 10^{-12})^2 (6.63 \times 10^{-34})^2} \\
 E &= -13.6 \text{ eV}
 \end{aligned} \tag{58}$$

Equation (58) represents ground state energy of hydrogen atom.

5. Energy of Harmonic Oscillator

As per classical mechanics, the energy of oscillator is minimum at rest, i.e., $E = 0$. Oscillator is represented by mass m , which is attached to spring of constant k , when the oscillator is considered at rest than $\Delta x = 0$, and hence $\Delta p = \infty$, which is impossible as, energy will also be infinite. Hence, the oscillator must be given quantum mechanical treatment as follows:

Energy of oscillator = kinetic energy + potential energy

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{59}$$

$$E = \frac{\Delta p^2}{2m} + \frac{1}{2}k(\Delta x)^2$$

$$E = \left(\frac{\hbar}{\Delta x}\right)^2 \frac{1}{2m} + \frac{1}{2}k(\Delta x)^2$$

$$E = \frac{\hbar^2}{2m\Delta x} + \frac{1}{2}mw^2\Delta x^2 \tag{60}$$

$$[w^2 = \frac{k}{m} \Rightarrow k = mw^2, \text{ where } w \text{ is angular frequency}]$$

To find the minimum energy of oscillator, $\frac{dE}{d(\Delta x)} = 0$ must be satisfied

$$\frac{dE}{d(\Delta x)} = \frac{-\hbar^2}{m(\Delta x)^3} + mw^2(\Delta x) = 0$$

$$\Delta x = \pm \left(\frac{\hbar}{mw}\right)^{1/2} \tag{61}$$

Substituting Eqn. (61) in Eqn. (60)

$$E = \hbar w \tag{62}$$

Equation (62) gives minimum energy of oscillator, which is same as obtained from Schrödinger equation.

Heisenberg also formulated the neutron–proton model of the nucleus, the quantum theory of ferromagnetism, and the S-matrix theory of particle scattering. He has more than 600 original research papers, philosophical essays, and explanations for general audiences. His work is compiled in the nine volumes of the “Gesammelte Werke.” During the years of the Hitler regime, Heisenberg preferred staying in Germany. He also contributed to the effort of scientific community on the applications of nuclear fission during World War II. Heisenberg helped in reconstructing West Germany’s nuclear and high-energy physics research programs. Throughout his career, he was appointed at various influential positions in Germany and abroad. He died on February 1, 1976, at the age of 74 years due to cancer of the kidneys and gall bladder.



**WERNER
HEISENBERG**

3.10 Differential Equations

Till now, we have seen that position and momentum cannot be measured simultaneously with precision. But according to Newtonian mechanics, under the effect of forces, motion, mass, force, and other physical entities of particle can be measured accurately. Rather than giving an exact location or exact value of some physical quantity, quantum mechanics defines the probabilities. Conclusively, Newtonian approach is the limiting case of quantum mechanics. We need differential equation to describe the motion of particles. To describe the motion of the particle and its complete information, we need wave function $\psi(x, t)$. By using wave function, we need to formulate and solve the Schrödinger’s equation. Schrödinger equation gives the space–time behavior of particle. If $\psi(r, t)$ represents the position of particle at time t , then the probability is given by (P):

$$P = |\psi(x, t)^* \psi(x, t)|$$

$$P = |\psi(x, t)|^2 \quad (63)$$

The generalized Eqn. (63) can be written as

$$P = |\psi(r, t)|^2 \quad (64a)$$

The probability can be normalized as

$$P(r, t) = |\psi(r, t)|^2 = \int_{-\infty}^{\infty} \psi(r, t) \psi^*(r, t) d^3r = 1 \quad (64b)$$

An appropriate constant is required to define a wave function. Then the wave function can be normalized such that, we can obtain the value of constant. Wave function should be single valued and finite

at every point in space. The wave function and its first derivative is continuous. We will discuss the Schrödinger equation in the next section.

3.11 Time-Dependent Schrödinger Equation

The Schrödinger wave equation should have first- and second-order derivative of wave function in order to completely describe a wave function. The wave equation is different for a free particle and particle under the influence of force.

1. Schrödinger Equation for Free Particle

When we say free particle, it means no force is acting on the particle. Hence, $F = 0$. From Newton's second law

$$F = \frac{dp}{dt}$$

$$p = \text{constant} \quad (65a)$$

$$\text{Hence, energy } E = \frac{p^2}{2m} = \text{constant} \quad (65b)$$

The wave function can be given from Eqn. (24) as

$$\psi(x, t) = C e^{i(kx - \omega t)} \quad (65c)$$

The momentum in relation to propagation constant is

$$p = \hbar k \quad (66)$$

Substituting Eqn. (66) in Eqn. (65b),

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\hbar f = \frac{\hbar^2 k^2}{2m} \quad [\text{as } E = \hbar f \text{ from Planck's hypotheses}]$$

$$\hbar \omega = \frac{\hbar^2 k^2}{2m} \quad (67)$$

We need to calculate ω and k and then substitute in Eqn. (67). Differentiating Eqn. (65c) w.r.t. x ,

$$\frac{\partial \psi}{\partial x} = ik C e^{i(kx - \omega t)} \quad (68a)$$

Again differentiating Eqn. (68a) w.r.t. x ,

$$\frac{\partial^2 \psi}{\partial x^2} = i^2 k^2 C e^{i(kx - \omega t)} \quad (i^2 = -1)$$

$$k^2 = \frac{-1}{\psi} \frac{\partial^2 \psi}{\partial x^2} \quad (68b)$$

Differentiate Eqn. (65c) w.r.t. time,

$$\omega = \frac{i}{\psi} \frac{\partial \psi}{\partial t} \quad (68c)$$

Using Eqs (68b) and (68c) in Eqn. (67),

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (69)$$

Equation (69) represents the Schrödinger equation in one dimension for a free particle, which is under the effect of nil force.

2. Schrödinger Equation for a Particle Under Some Force

The total energy is not constant for a particle when it is under the influence of some external force. Then, energy E is the sum of potential and kinetic energy

$$E = \frac{p^2}{2m} + V(x)$$

Hence, Eqn. (67) becomes

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x) \quad (70)$$

Using Eqs (68b) and (68c) in Eqn. (70)

$$\left(i\hbar \frac{\partial \psi}{\partial t} \right) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \quad (71)$$

Equation (71) represents the Schrödinger equation in one dimension for a bound particle, $\psi(x, t)$ is the solution of Eqn. (71) and it describes the behavior of a particle.

The generalized Schrödinger equation can be written as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] + V(x, y, z)\psi \quad (72)$$

Erwin Schrödinger was born in Vienna on August 12, 1887. He was the single child of Rudolf Schrödinger who was from a Bavarian family settled in Vienna. Schrödinger was a God-gifted person who had multidisciplinary interests. He did Italian painting after finishing his chemistry studies. He also studied botany from which he published a series of papers on plant phylogeny. He also studied ancient grammar and German poetry. He was a student at the University of Vienna from 1906 to 1910. During this time, he was deeply influenced by Fritz Hasenöhl, who was Boltzmann's successor. Schrödinger became a master of eigen value problems of quantum physics during these years. He along with his friend K.W.F. Kohlrusch assisted Franz Exner. He also served as an artillery officer during World War II. He assisted Max Wien in 1920. Afterwards, he got many influential academic positions such as professor at Stuttgart and Breslau. He replaced Von Laue at University of Zurich and settled for almost six years. This was among his most fruitful period where was recognized for his work on thermodynamics, specific heats of solids, physiological studies of color, and atomic spectra.



ERWIN SCHRÖDINGER

3.12 Time-Independent Schrödinger Equation

Usually potential energy is not a function of time t and it depends only on position coordinates. Hence, the variables used in Schrödinger Equation can be separated. Let us take $\psi(x, t)$ to be a product of two functions, that is, $\psi(x)$ dependent only on position and $T(t)$, which is function of time.

We know

$$\begin{aligned}\psi(x, t) &= C e^{i(kx - \omega t)} \\ \psi(x, t) &= C \left[e^{ikx} \cdot e^{-i\omega t} \right] \\ \psi(x, t) &= C \left[e^{\frac{ipx}{\hbar}} \cdot e^{\frac{-iEt}{\hbar}} \right] \quad (73)\end{aligned}$$

$$(p = \hbar k, k = p/\hbar \text{ and } \omega = \frac{E}{\hbar})$$

$$\psi(x, t) = [\varphi(x) \cdot T(t)] \quad (74)$$

where
$$\varphi(x) = C e^{\frac{ipx}{\hbar}} \quad (75a)$$

and
$$T(t) = e^{-iEt/\hbar} \quad (75b)$$

Double differentiating Eqn. (74), w.r.t x ,

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = T(t) \frac{d^2 \varphi(x)}{dx^2} \quad (76)$$

Differentiating Eqn. (74) w.r.t. time t ,

$$\frac{\partial \Psi(x,t)}{\partial t} = \varphi(x) \frac{dT}{dt} \quad (77)$$

Substituting Eqs (76) and (77) in Eqn. (71),

$$\begin{aligned} i\hbar \left(\varphi(x) \frac{dT}{dt} \right) &= -\frac{\hbar^2}{2m} \left[T(t) \frac{d^2 \varphi(x)}{dx^2} \right] + V(x) T(t) \varphi(x) \\ i\hbar \varphi(x) \frac{dT}{dt} &= -\frac{\hbar^2}{2m} T(t) \frac{d^2 \varphi(x)}{dx^2} + V(x) T(t) \varphi(x) \\ \frac{i\hbar}{T(t)} \frac{dT}{dt} &= -\frac{\hbar^2}{2m \varphi(x)} \frac{d^2 \varphi(x)}{dx^2} + V(x) \\ \frac{i\hbar}{T} \frac{dT}{dt} &= \frac{-\hbar^2}{2m \varphi} \left(\frac{d^2 \varphi}{dx^2} \right) + V \end{aligned} \quad (78)$$

The left-hand side (L.H.S.) of Eqn. (78) represents the time-dependent wave function and right-hand side (R.H.S.) represents the position-dependent wave function only.

[From Eqn. (75b)], $T(t) = e^{-iEt/\hbar}$

$$\frac{dT}{dt} = \frac{-iE}{\hbar} T(t)$$

$$\frac{i\hbar}{T} \frac{dT}{dt} = E$$

Hence, R.H.S. can be written as

$$\frac{-\hbar^2}{2m \varphi} \frac{d^2 \varphi}{dx^2} + V = E \quad (79)$$

where E is a constant.

$$+\frac{\hbar^2}{2m} \frac{d^2\varphi}{dx^2} + (E - V)\varphi = 0$$

$$\frac{d^2\varphi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\varphi = 0 \quad (80)$$

Equation (80) is time-independent Schrödinger equation in one dimension as the equation is independent of time. These wave equations represent stationary wave functions.

Note: For $T(t) = e^{-iEt/\hbar}$, $\frac{Et}{\hbar}$ is dimensionless, hence E has the dimension of energy and E is total energy of particle.

From Eqn. (74),

$$\Psi(x) = \varphi(x)e^{-iEt/\hbar} \quad (81)$$

Equation (80) represents a second-order linear and homogenous equation. Schrödinger equation can have n -solutions. Let Ψ_n be the n th solution given by

$$\Psi_n(x, t) = \varphi_n(x)e^{-iE_n t/\hbar} \quad (82)$$

The generalized solution can be given by

$$\Psi(x, t) = c_1\Psi_1 + c_2\Psi_2 + \dots$$

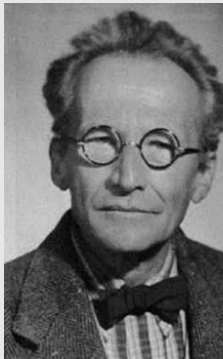
$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n\Psi_n \quad (83)$$

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n\Psi_n e^{-iE_n t/\hbar} \quad (84)$$

Equation (84) shows that the sum or linear combinations of wave functions also satisfy Schrödinger equation. Hence, Eqn. (84) is superposition of wave functions.

Schrödinger made a great discovery in 1926, i.e. "Schrödinger's wave equation." He shared Nobel Prize with Dirac in 1933. This theory was an outcome of his belief that some eigen values should describe atomic spectra. He was not satisfied with Bohr's theory. Schrödinger moved to Berlin as Planck's successor in 1927. Schrödinger decided not to continue his research in Germany when Hitler came to power. Hence, he came to England with a fellowship at Oxford. He was offered a permanent position at Princeton University in 1934, where he was invited to lecture. He refused that offer and accepted a position at the University of Graz in 1936. During 1933, leaving Germany was an offense.

Anyhow, he managed to escape to Italy, thereby to Oxford and subsequently to University of Ghent. Later, he moved to Institute for Advanced Studies in Dublin. He was appointed as Director of the School for Theoretical Physics there and then retired in 1955. He returned to an honored position in Vienna after his retirement. He was also the author of the book *What is Life?* Schrödinger was more interested in wave nature of matter and generally disliked the dual nature, that is, waves and particles. Therefore, he was opposed by many other leading physicists. He died on January 4, 1961, after a long illness and left the world with his achievements.



"The mathematical framework of quantum theory has passed countless successful tests and is now universally accepted as a consistent and accurate description of all atomic phenomena."

Erwin Schrodinaer

3.13 Expectation Values

When we take the average number of measurements of a physical quantity to define its space–time coordinates, it is known as expectation value of the quantity. Suppose, we perform n trials to measure a quantity, the expectation value of the quantity is the sum of individual quantities divided by number of trials. Probability is given as $|\varphi(x)|^2$ or $|\psi(r,t)|^2$ in more generalized form. It gives the probability of finding a particle at particular point of time. For a function $F(r)$, the expectation value is given by

$$\langle F(r) \rangle = \int_{-\infty}^{\infty} F(r) \psi^*(r,t) \psi(r,t) d^3r \quad (85)$$

The expectation value for position coordinate can be given by following demonstration:

Let the particle be found n_1 times at position coordinate (x_1, y_1, z_1, t_1) and n_2 times with position coordinates (x_2, y_2, z_2, t_2) , then the expectation value in x is given by

$$\langle x \rangle = \frac{n_1 x_1 + n_2 x_2 + \dots}{n_1 + n_2 + n_3 + \dots} = \frac{\sum x_i n_i}{n} \quad (86)$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x \frac{n_i}{n} dx$$

$$[P_i = \frac{n_i}{n} = \text{probability of occurrence of } x_i]$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x P(x,t) dx \quad (87)$$

Equation (87) is the expectation value of x -coordinate at time t .

$$\left. \begin{array}{l} \text{Similarly} \\ \text{and} \end{array} \right\} \begin{array}{l} \langle y \rangle = \int_{-\infty}^{\infty} y P(y, t) dy \\ \langle z \rangle = \int_{-\infty}^{\infty} z P(z, t) dz \end{array} \quad (88)$$

The generalized form can be

$$\begin{aligned} \langle r \rangle &= \int_{-\infty}^{\infty} r P(r, t) d^3 r \\ \langle r \rangle &= \int_{-\infty}^{\infty} r \psi^*(r, t) \psi(r, t) d^3 r \end{aligned} \quad (89)$$

The expectation value of momentum is given by

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) p \psi(x, t) dx \quad (90)$$

We know from Eqn. (73),

$$\psi(x, t) = C \left[e^{-\frac{iEt}{\hbar}} \cdot e^{\frac{ipx}{\hbar}} \right]$$

$$\begin{aligned} \frac{\partial \psi}{\partial x} &= \frac{ip \psi}{\hbar} \\ p \psi &= -i\hbar \frac{\partial \psi}{\partial x} \end{aligned} \quad (91a)$$

Hence, the momentum operator is given by

$$p = -i\hbar \frac{\partial}{\partial x} \quad (91b)$$

Using Eqn. (91b) in Eqn. (90),

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x, t) \left(\frac{\partial}{\partial x} \right) \psi(x, t) dx \quad (92)$$

Similarly, the value of energy can be obtained as follows:

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) E \psi(x, t) dx \quad (93)$$

Differentiating w.r.t. time,

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{-iE}{\hbar} \psi \\ E \psi &= i\hbar \frac{\partial \psi}{\partial t} \end{aligned} \quad (94)$$

Hence, the energy operator is given by

$$E = i\hbar \frac{\partial}{\partial t} \quad (95)$$

Substituting Eqn. (95) in Eqn. (93),

$$\langle E \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \left(\frac{\partial}{\partial t} \right) \Psi(x,t) dx \quad (96)$$

Hence, the generalized form of expectation value of momentum and energy can be given by

$$\left. \begin{aligned} \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \Psi^*(r,t) \frac{\partial}{\partial r} \Psi(r,t) d^3r \\ \langle E \rangle &= i\hbar \int_{-\infty}^{\infty} \Psi^*(r,t) \frac{\partial}{\partial t} \Psi(r,t) d^3r \end{aligned} \right\} \quad (97)$$

3.14 Proof of Uncertainty Principle Using Expectation Values

After measuring and observing a physical system, when we elucidate some physical quantity out of it, then the physical quantity is said to be an observable. Classically, the observable is not affected by the measurement technique; but according to quantum mechanics, it depends on the device and the technique used. Let A be an observable, then its uncertainty is given by

$$\Delta A = \left[\langle A^2 \rangle - \langle A \rangle^2 \right]^{1/2} \quad (98a)$$

where

$$\langle A^2 \rangle = \int \Psi^*(r,t) A^2 \Psi(r,t) d^3r \quad (98b)$$

Hence, the uncertainty in the measurement of observable A is given by the square root of difference of mean of square and square of mean of observable A. This is the precise definition of uncertainty principle, whereas the exact definition of uncertainty principle says that the positions and momentum of particle cannot be determined accurately simultaneously, i.e.,

$$\Delta x \Delta p \geq \hbar$$

We will have to arbitrarily assume some functions and three integrals as follows:

$$\left. \begin{aligned} U &= \int a^* a d^3r \\ V &= \int a^* b d^3r \\ W &= \int b^* b d^3r \end{aligned} \right\} \quad (99)$$

Let us take a parameter λ , which assumes only real values such that

$$\int |\lambda a + b|^2 d^3r = \int (\lambda a^* + b^*)(\lambda a + b) d^3r \quad (100)$$

Substituting Eqn. (99) in Eqn. (100),

$$\int |\lambda a + b|^2 d^3r = \lambda^2 U + \lambda(V + V^*) + W$$

↓
Positive Quantity

$$(101)$$

Therefore, R.H.S. should be satisfied for all λ values which leads to condition

$$UW \geq \frac{1}{4}(V + V^*)^2 \quad (102)$$

Substituting Eqn. (99) in Eqn. (102),

$$\int a^* a d^3 r \int b^* b d^3 r \geq \frac{1}{4} \left[\int (a^* b + ab^*) d^3 r \right]^2 \quad (103)$$

Let
$$\left. \begin{aligned} a &= -i\hbar \frac{\partial \varphi}{\partial x} \\ \text{and } b &= ix\varphi \end{aligned} \right\} \quad (104)$$

Then L.H.S of Eqn. (103) becomes

$$\begin{aligned} \int a^* a d^3 r \int b^* b d^3 r &= \hbar^2 \int \frac{\partial \varphi^*}{\partial x} \cdot \frac{\partial \varphi}{\partial x} d^3 r \underbrace{\int \varphi^* x^2 \varphi d^3 r}_{\langle x^2 \rangle} \\ &= \hbar^2 \iiint \frac{\partial \varphi^*}{\partial x} \cdot \frac{\partial \varphi}{\partial x} dx dy dz \int \varphi^* x^2 \varphi d^3 r \\ &= \hbar^2 \iiint \frac{\partial \varphi^*}{\partial x} \cdot \frac{\partial \varphi}{\partial x} dy dz dx \langle x^2 \rangle \\ &= \hbar^2 \langle x^2 \rangle \iint dy dz \underbrace{\int \frac{\partial \varphi^*}{\partial x} \cdot \frac{\partial \varphi}{\partial x} dx}_{\text{Solving the integral}} \\ &= \hbar^2 \langle x^2 \rangle \iint dy dz \left[\varphi^* \frac{\partial \varphi}{\partial x} \Big|_{-\infty}^{\infty} - \int \varphi^* \frac{\partial^2 \varphi}{\partial x^2} dx \right] \\ &= -\langle x^2 \rangle \iiint \varphi^* \hbar^2 \frac{\partial^2 \varphi}{\partial x^2} dx dy dz \\ &= \langle x^2 \rangle \iiint \varphi^* \left(-\hbar^2 \frac{\partial^2 \varphi}{\partial x^2} \right) dx dy dz \\ &\quad \downarrow \\ &\quad \text{(momentum)}^2 \\ &= \langle x^2 \rangle \langle p^2 \rangle \quad (105) \end{aligned}$$

Similarly solving R.H.S. of eqn (103), the following relation is obtained:

$$\int (a^* b + ab^*) d^3 r = \hbar \int \underbrace{\varphi^* \varphi d^3 r}_{\text{it represents probability}} \quad (106)$$

Comparing Eqs (105), (103), and (106),

$$\langle x^2 \rangle \langle p^2 \rangle \geq \frac{\hbar^2}{4}$$

$$\begin{aligned} [\langle x^2 \rangle]^{1/2} [\langle p^2 \rangle]^{1/2} &\geq \hbar / 2 \\ \Delta x \cdot \Delta p &\geq \hbar / 2 \end{aligned} \quad (107)$$

Equation (107) gives the uncertainty principle. One should understand that \hbar and $\hbar / 2$ have same order of magnitude.

3.15 Schwarz Inequality

Consider two wave functions φ_n and φ_m such that their scalar product is given by

$$\int \varphi_n^* \varphi_m d^3 r = (\varphi_n, \varphi_m) \quad (108)$$

The wave function φ_n and φ_m are said to be orthogonal if their scalar product is zero, such that

$$\int \varphi_n^* \varphi_m d^3 r = 0 \quad (\text{for } n \neq m) \quad (109)$$

$$\text{When} \quad \int \varphi_n^* \varphi_m d^3 r = 1 \quad (\text{for } n = m) \quad (110)$$

Equation (110) represents the orthonormality condition.

Schwarz inequality states that the absolute value of scalar product of state φ_n and φ_m is less than the product of norm of φ_n and φ_m individually.

$$|(\varphi_n, \varphi_m)| \leq \|\varphi_n\| \|\varphi_m\| \quad (111)$$

where $\|\varphi_n\|$ and $\|\varphi_m\|$ are norms and are given by

$$\|\varphi_n\| = \sqrt{(\varphi_n, \varphi_n)} \quad \text{and} \quad \|\varphi_m\| = \sqrt{(\varphi_m, \varphi_m)}$$

The norm is real number, which is greater than or equal to zero. Hence, the norm of a wave function is the positive square root of its scalar product. Consider φ to be a linear combination of φ_n and φ_m such that

$$\varphi = \varphi_n + \lambda \varphi_m \quad (112)$$

(λ being a real number)

Take norm on both sides,

$$\|\varphi\| = \|\varphi_n + \lambda \varphi_m\| \quad (113a)$$

as $\|\varphi\| \geq 0$, hence $\|\varphi_n + \lambda \varphi_m\| \geq 0$

Squaring both sides,

$$\|\varphi_n + \lambda \varphi_m\|^2 \geq 0 \quad (113b)$$

Using Eqn. (110) when $n = m$,

$$\int \varphi_n^* \varphi_n dV = 1$$

In generalized form,

$$\int \varphi^* \varphi dV = 1 \quad (114)$$

Hence, the norm of $\|\varphi_n + \lambda\varphi_m\|$ can be written as

$$\begin{aligned} & \int (\varphi_n + \lambda\varphi_m)^* (\varphi_n + \lambda\varphi_m) dV \geq 0 \\ & \int \varphi_n^* \varphi_n dV + \lambda \int \varphi_m^* \varphi_n dV + \lambda \int \varphi_n^* \varphi_m dV + \lambda^2 \int \varphi_m^* \varphi_m dV \geq 0 \\ & \|\varphi_n\|^2 + \lambda(\varphi_m, \varphi_n) + \lambda(\varphi_n, \varphi_m) + \lambda^2 \|\varphi_m\|^2 \geq 0 \end{aligned}$$

The scalar product satisfies the condition,

$$\begin{aligned} & (\varphi_n, \varphi_m) = (\varphi_m, \varphi_n)^* \quad (115) \\ & \Rightarrow \|\varphi_n\|^2 + \lambda^2 \|\varphi_m\|^2 + \lambda \left[(\varphi_n, \varphi_m) + (\varphi_n, \varphi_m)^* \right] \geq 0 \end{aligned}$$

We will take only real part of the complex conjugate. Hence, the above equation can be written as

$$\lambda^2 \|\varphi_m\|^2 + \|\varphi_n\|^2 + 2\lambda \operatorname{Re}(\varphi_n, \varphi_m) \geq 0 \quad (116)$$

Equation (116) has negative values for real roots and positive values for equal/imaginary roots. Hence, for imaginary roots, the condition $b^2 - 4ac \leq 0$ should be satisfied.

$$\begin{aligned} \therefore & 4 \operatorname{Re}(\varphi_n, \varphi_m)^2 \leq 4 \|\varphi_n\|^2 \|\varphi_m\|^2 \\ & \operatorname{Re}(\varphi_n, \varphi_m) \leq \|\varphi_n\| \|\varphi_m\| \quad (117) \end{aligned}$$

The maximum value of $\operatorname{Re}(\varphi_n, \varphi_m)$ is the modulus of scalar product, Hence,

$$|(\varphi_n, \varphi_m)| \leq \|\varphi_n\| \|\varphi_m\| \quad (118)$$

The relation (118) is known as Schwarz inequality.

3.16 Ehrenfest Theorem (Wave Packet Motion)

This theorem acts as a bridge between the classical and quantum mechanics. According to Ehrenfest theorem, "The particle for which the expectation values of physical dynamical quantities are involved, the classical and quantum mechanics yield same result."

The formula for equations of motion is as follows:

$$(i) \quad \frac{m d \langle x \rangle}{dt} = \langle p_x \rangle \quad (119)$$

$$(ii) \quad \frac{d \langle p_x \rangle}{dt} = - \left[\frac{\partial V}{\partial x} \right] \quad (120)$$

where V is the potential energy of particle, when it is under the influence of force. Equation (119) can be proved as follows:

The expectation value of x for a time-dependent $\psi(x, t)$ state is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) x \psi(x, t) dx$$

Differentiating both sides,

$$\begin{aligned}\frac{d}{dt} \langle x \rangle &= \frac{d}{dt} \int_{-\infty}^{\infty} \psi^*(x,t) x \psi(x,t) dx \\ \frac{d \langle x \rangle}{dt} &= \int_{-\infty}^{\infty} \left[\psi^* x \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} x \psi \right] dx\end{aligned}\quad (121)$$

The Schrödinger equation and its complex conjugate is given by the following equation (time dependent and under the influence of a force):

$$\text{Time dependent Schrodinger equation} \Rightarrow \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V \psi \quad (122)$$

$$\text{Complex conjugate} \Rightarrow \frac{\partial \psi^*}{\partial t} = \frac{-i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V \psi^* \quad (123)$$

Substituting Eqs (122–123) in Eqn. (121),

$$\begin{aligned}\frac{d \langle x \rangle}{dt} &= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \left(\psi^* x \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} x \psi \right) dx \\ \frac{d \langle x \rangle}{dt} &= \frac{i\hbar}{2m} \left[\int_{-\infty}^{\infty} \psi^* x \frac{\partial^2 \psi}{\partial x^2} dx - \int_{-\infty}^{\infty} \psi^* \frac{\partial^2}{\partial x^2} (x \psi) dx \right]\end{aligned}\quad (124)$$

In Eqn. (124), we have used the properties of Hermitian operator as follows:

$$\int A^* \frac{\partial^2 B}{\partial x^2} dx = \int \left(\frac{\partial^2}{\partial x^2} A \right)^* B dx$$

After solving Eqn. (124),

$$\begin{aligned}\frac{d \langle x \rangle}{dt} &= \frac{-i\hbar}{m} \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx \\ \frac{d \langle x \rangle}{dt} &= \frac{i}{m} \int_{-\infty}^{\infty} \psi^* \underbrace{\left(-i\hbar \frac{\partial}{\partial x} \right)}_{\text{Momentum operator}} \psi dx \\ \frac{d \langle x \rangle}{dt} &= \frac{\langle p_x \rangle}{m}\end{aligned}\quad (\text{Eq. 119})$$

Hence, this is the first equation of motion.

To prove Eqn. (120), we will use the expectation value of momentum:

$$\begin{aligned}\langle p_x \rangle &= \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t) dx \\ &= \frac{\hbar}{i} \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\partial}{\partial x} \psi(x,t) dx\end{aligned}\quad (125)$$

Differentiating w.r.t. time,

$$\frac{\partial \langle p_x \rangle}{\partial t} = \frac{\hbar}{i} \int_{-\infty}^{\infty} \left(\frac{\partial \psi^*}{\partial t} \cdot \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi}{\partial x \partial t} \psi^* \right) dx \quad (126)$$

$$\frac{\partial \langle p_x \rangle}{\partial t} = \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \psi^*}{\partial t} \cdot \frac{\partial \psi}{\partial x} - \psi^* i\hbar \frac{\partial^2 \psi}{\partial x \partial t} \right) dx \quad (127)$$

Differentiating Eqn. (122) w.r.t x ,

$$i\hbar \frac{\partial^2 \psi}{\partial x \partial t} = \frac{-\hbar^2}{2m} \frac{\partial^3 \psi}{\partial x^3} + \frac{\partial(V\psi)}{\partial x} \quad (128a)$$

Equation. (123) can be written as

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \quad (128b)$$

Substituting Eqns (128a) and (128b) in Eqn. (127),

$$\begin{aligned} \frac{d \langle p_x \rangle}{dt} &= \frac{-\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\frac{\partial^2 \psi^*}{\partial x^2} \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^3} \right) dx + \int_{-\infty}^{\infty} \left[V\psi^* \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial}{\partial x}(V\psi) \right] dx \\ \frac{d \langle p_x \rangle}{dt} &= \frac{-\hbar^2}{2m} \left(\frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right)_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi^* \frac{\partial V}{\partial x} \psi dx \end{aligned} \quad (129)$$

The first term in Eqn. (129) tends to zero, because ψ and $\frac{\partial \psi}{\partial x}$ tend to zero as $x \rightarrow -\infty$ or ∞ . Hence,

$$\begin{aligned} \frac{d \langle p_x \rangle}{dt} &= - \int_{-\infty}^{\infty} \psi^* \frac{\partial V}{\partial x} \psi dx \\ \frac{d \langle p_x \rangle}{dt} &= - \langle \frac{\partial V}{\partial x} \rangle \\ \frac{d \langle p_x \rangle}{dt} &= - \langle F_x \rangle \end{aligned} \quad (130)$$

Equation (130) represents the second equation of motion. Hence, by using expectation values, the quantum and classical mechanics give same result.

3.17 Operators

The rules by means of which we can map elements A of a linear space on elements B of another linear space leading to an equation is called operators (Figure 3.7).

$$B = OA \quad (131)$$

B = range of operator

A = domain of operator

O = operator

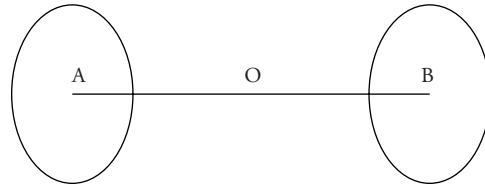


Figure 3.7 Mapping of operators

An operator may also be defined as the mathematical term used for operating a function such that the original function transforms to another function. If A is operator applied to function $\phi(x)$, then $A\phi(x) = \psi(x)$, where $\psi(x)$ is the transformed function. If X is rotated about an axis and Y is obtained, then the relationship between X and Y is given by $Y = \hat{A}X$, where \hat{A} represents rotation operation. \hat{A} has meaning in the domain of \hat{A} only, that is, space within a set of vectors. The set of vectors Y defines the range of \hat{A} .

3.18 Different Types of Operators

This section describes the most commonly used operators:

3.18.1 Linear Operators

An operator is linear if it satisfies the following conditions:

$$A(U + V) = AU + AV \quad (132)$$

and $AC = CA \quad (C \text{ is constant}) \quad (133)$

3.18.2 Identity Operators and Null Operators

When null or identity operator (I) is applied to a function, then the function remains unchanged after the operation, and is given by,

$$IA = AI = A \quad (134)$$

The null operator makes the function zero. Thus, $OA = 0$, where O is null operator.

3.18.3 Inverse Operators

When T is applied on any linear operators A and B , such that

$$B = TA \quad (135)$$

$$\Rightarrow A = T^{-1}B \quad (136)$$

then T^{-1} is the inverse operator. $TA = B$ is unique correspondence that could be proved as follows:

Consider $TA' = B$ and $TA'' = B$

$$T(A' - A'') = 0$$

$A' = A''$ but T cannot be zero.

3.18.4 Differential Operators

Consider any function $\phi(x)$. The expression $[d/dx]\phi(x)$ consists of the operator $[d/dx]$ and the operand $\phi(x)$.

$$[d/dx]\phi(x) = \phi'(x) \quad (137)$$

where (d/dx) is called differential operator.

3.18.5 Singular and Nonsingular Point Operators

If the two operators A and B satisfy the following relation:

$$AB = BA = I$$

where I is the identity operator, then A and B are reciprocal to each other, that is, $A^{-1} = B$ and $B^{-1} = A$. An operator for which a reciprocal exists is called nonsingular operator. If $A = TB$, then $B = T^{-1}A$. Hence, T^{-1} is regarded as a nonsingular operator. If for non zero B , $TB = 0$, then operator T has no reciprocal and hence it is singular, hence, the operator with no reciprocal is called singular operator. Moreover, inverse of a product of operators is the product of the inverse of operators in reverse order.

$$\text{i. e.} \quad (ABC)(ABC)^{-1} = 1 \quad (138)$$

$$\text{Now} \quad (ABC)^{-1} = C^{-1}B^{-1}A^{-1} \quad (139)$$

3.19 Laws of Operators

Let us take X and Y to be two operators, such that they satisfy following rules:

- (i) $(X + Y)A = XA + YA$
- (ii) $(XY)A = X(YA)$
- (iii) $XY \neq YX$
- (iv) $X + Y = X + Y$

Although addition is commutative, multiplication is not. When multiplication is commutative, that is, when $XY = YX$, then the operators X and Y are said to be commuting. For example, Let us take two operators X and Y :

$$X = x, Y = d/dx$$

$$\text{Therefore,} \quad XY[\phi(x)] = x(d/dx)[\phi(x)] \quad (140)$$

$$YX[\phi(x)] = (d/dx) \times [\phi(x)] \quad (141)$$

Therefore, $XY \neq YX$ which shows that, X and Y do not commute.

3.19.1 Power of Linear Operators

Consider X is any linear operator.

Now $X^3 = X.X.X$, then 3 is the power of operator.

For $X^n = X.X \dots X$, n is the power.

3.20 Eigen Functions and Eigen Values

When the function satisfies the continuity conditions as well as boundary condition, it is said to be an eigen function. Let X be an operator, such that $X\phi(x) = \lambda\phi(x)$, where λ is a complex number and $\phi(x)$ is an eigen function, then λ is called eigen value of operator X . For example, let us take function $\cos 2x$ and operator is $-(d^2/dx^2)$.

$$-(d^2/dx^2)(\cos 2x) = 4(\cos 2x) \quad (142)$$

$\phi(x) = \cos 2x$ is an eigen function and $\lambda = 4$ is the eigen value of operator (d^2/dx^2) .

But if operator X operates on a vector, then it yields different vector, that is, $XV = U$, some vectors satisfy the property of $XV = \alpha U$, α is the scalar operation. We can consider the vector V multiplied by a scalar. V is the eigen vector of X with eigen value α and $XV = \alpha V$ is the eigen value equation of X .

A linear operator may have several eigen values and eigen vectors.

i. e.
$$XV_k = \alpha_k V_k \quad (143)$$

The eigen values may be continuous or discrete. An eigen vector can have only one eigen value. But many linearly independent eigen vectors may have same eigen values. Then the eigen value is said to be degenerate and number of linearly independent eigen vectors defines the degree of degeneracy. The set $\{a_n\}$ of all the eigen values constitute the regime/spectrum of the operator X . Let us consider the eigen value equation.

$$(-d^2/dx^2)\phi(x) = E\phi(x) \quad (144)$$

For $\phi(x) = \phi_p(x)e^{ipx}$ and $\phi_{-p}(x) = e^{-ipx}$, the eigen value E remains the same and E is two-fold degenerate. Both the eigen vectors correspond to the same eigen value E .

3.21 Special Operators

3.21.1 Continuous and Bounded Operators

An operator X is continuous if $\{XA_n\} \rightarrow XA$, for every Cauchy sequence of vector $\{A_n\}$ converging to limit A . X is bounded for positive number "x" such that the inequality $\|XA\| \leq x\|A\|$ exists corresponding to every A in the domain of X . The norm is the smallest "x" value satisfying this criterion and is denoted by $\|X\|$. For $\|XA_n - XA\| = \|X\|\|A_n - A\| \rightarrow 0$, if X is bounded. Thus, $XA_n \rightarrow XA$, for $n \rightarrow \infty$. Every operator that is defined for finite dimensions is bounded.

3.21.2 Positive Definite Operators

If $X > 0$ and $X^{-1} > 0$, then X is positive definite operator. The eigen values of a positive definite operator are positive.

$$\text{If } X > Y > 0, \text{ then } Y^{-1} > X^{-1} > 0$$

Now for $X > Y$,

$$\begin{aligned} X^{-1}X &> X^{-1}Y \\ X^{-1}XX^{-1} &> X^{-1}YX^{-1} \end{aligned}$$

$$X^{-1}[1 - YX^{-1}] > 0$$

Hence

$$1 - YX^{-1} > 0$$

$$Y^{-1} > X^{-1}$$

Now again for $X > Y$

$$Y^{-1}X > Y^{-1}Y \Rightarrow Y^{-1} > X^{-1} \quad \text{for } Y^{-1}Y = 1$$

3.21.3 Commuting Operators

If X and Y are linear operators, which satisfy the same equation in eigen function ψ , then ψ is called simultaneous eigen function of X and Y with Eigen values α and β , respectively.

$$\text{i. e.} \quad X\psi = \alpha\psi \quad (145)$$

$$\text{and} \quad Y\psi = \beta\psi \quad (146)$$

For example, consider a well-behaved function e^{5ix} and an operator $-i(d/dx)$ belonging to eigen value. Now,

$$-i(d/dx)e^{5ix} = 5e^{5ix}$$

$$\text{Also} \quad (d^2/dx^2)e^{5ix} = 25e^{5ix}$$

Hence, operand e^{5ix} can be operated by two more operators. Such functions are called as simultaneous Eigen functions.

$$\text{Consider the Eqn. (145),} \quad X\psi = \alpha\psi$$

Multiplying on left by Y

$$Y(X\psi) = Y\alpha\psi = \alpha\beta\psi \quad (147)$$

Consider second equation $Y\psi = \beta\psi$ and multiply by X on both sides

$$XY(\psi) = X\beta\psi = \beta\alpha\psi \quad (148)$$

Subtracting Eqs (147) and (148),

$$[XY - YX]\psi = 0 \quad (149)$$

$$[XY - YX]\psi = 0\psi \quad (150)$$

Hence, ψ is eigen function of operator $[XY - YX]$ having eigen value zero. The mandatory condition for the two observables X and Y to be measured simultaneously is that X and Y should commute. $[X, Y] = XY - YX$ is called the commutator and the operators, which satisfy the equation $[X, Y] = 0$, are said to commute. If the two operators X and Y commute with each other and have simultaneous eigen function ψ , then $Y\psi$ is also eigen function of X , belonging to the same eigen value. This is proved as follows:

Suppose ψ is an eigen function of X , that is,

$$X\psi = \alpha\psi \quad (151)$$

$$\text{If } X \text{ and } Y \text{ commute then } XY = YX \quad (152)$$

Multiplying Eqn. (151) by Y ,

$$YX\psi = Y\alpha\psi = \alpha Y\psi \quad (153)$$

From Eqn. (152),

$$XY\psi = \alpha Y\psi \Rightarrow X(Y\psi) = \alpha(Y\psi)$$

Hence $Y\psi$ is also an eigen function of X .

3.21.4 Hermitian Operators

If arbitrary vectors A and B lie in the domain of two linear operators X and Y , then X and Y are said to be adjoint of each other. The Hermitian operators are represented by

$$(XA, B) = (A, XB) \quad (154)$$

Y is denoted by X^+ . X is self-adjoint or Hermitian if $X = X^+$ and anti-Hermitian if $X = -X^+$. The expectation value of an operator (variable) represents the arithmetic means of the precise measurement. If S is the Schrödinger operator associated with a dynamical variable z and if ψ is a normalized wave function, then according to expectation results

$$\langle S \rangle = \left(\int \psi^* S \psi dz \right) / \left(\int \psi^* \psi dz \right) = \int \psi^* S \psi dz \quad (155)$$

($\left[\int \psi^* \psi dz = 1 \right]$ orthonormality condition, ψ^* complex conjugate)

An operator S is said to be Hermitian if its expectation/average value is real or the imaginary factor is zero. If S is to be Hermitian, then $\int \psi^* S \psi dz$ must be real or

$$\text{Im} \int \psi^* S \psi dz = 0 \quad (156)$$

\Rightarrow Let us take $(a + ib) = x$, a is the real part, ib is the imaginary part

\Rightarrow If $b = 0$, then $x = a$ $(a + ib)^* = a - ib$

For real function, the complex conjugate of function $\int \psi^* S \psi dz = \int (S\psi)^* \psi dz$. i.e, if $b = 0$, then the function is equal to its complex conjugate, that is, $\int \psi^* S \psi dz = \int (S\psi)^* \psi dz$. Let u and v be two normalizable and acceptable wave functions of z such that

$$\int [(u + v)]^* S(u + v) dz = \int S^*(u + v)^* (u + v) dz \quad (157)$$

Upon solving,

$$\begin{aligned} & \int u^* S u dz + \int u^* S v dz + \int v^* S u dz + \int v^* S v dz \\ & = \int S^* u^* u dz + \int S^* u^* v dz + \int S^* v^* u dz + \int S^* v^* v dz \end{aligned}$$

As the complex conjugates are equal, hence

$$\begin{aligned} & \int u^* S v dz - \int S^* v^* u dz = \int S^* u^* v dz - \int v^* S u dz \\ & \int u^* S v dz - \int (u^* S v)^* dz = \int S^* u^* v dz - \int (S^* u^* v)^* dz \end{aligned} \quad (158)$$

If we put iv instead of v , then

$$\int u^* S iv dz - \int (u^* S iv)^* dz = \int S^* u^* iv dz - \int (S^* u^* iv)^* dz \quad (159)$$

$$\int u^* S v dz + \int (u^* S v)^* dz = \int S^* u^* v dz + \int (S^* u^* v)^* dz \quad (160)$$

Hence,
$$\int u^* S v dz = \int S^* u^* v dz \quad (\text{complex conjugate is equal to function}) \quad (161)$$

Hence, when u and v are normalizable, we call them Hermitian, self-adjoint, or Hermitian real.

Properties

1. The eigen values of Hermitian operators are real. Let H be a Hermitian operator and let V be an eigen vector belonging to the eigen value α .

By definition
$$(HV, V) = (V, HV) \quad (162)$$

Also
$$(\alpha V, V) = [\alpha V, V]^* \quad (163)$$

$$\alpha [V, V] = \alpha^* [V, V]$$

$$(\alpha - \alpha^*)(V, V) = 0$$

$$(V, V) \neq 0; \quad \alpha^* = \alpha \quad (164)$$

Let S be the Hermitian operator belonging to the Eigen value α . According to condition of Hermitian operator

$$\int u^* S v dz = \int S^* u^* v dz$$

If $v = u$

$$\int u^* S u dz = \int S^* u^* u dz \quad (165)$$

According to eigen value equation

$$S u = \alpha u \quad (166)$$

Hence,

$$\int u^* \alpha u dz = \int \alpha^* u^* u dz$$

$$\alpha \int u^* u dz = \alpha^* \int u^* u dz$$

$$\alpha = \alpha^* \quad (167)$$

This verifies that every Hermitian operator gives real eigen values.

2. If same Hermitian operator operates on two eigen functions, then the functions will be orthogonal functions. Let V_1 and V_2 be eigen vectors of H belonging to the eigen values α_1 and α_2

$$H V_1 = \alpha_1 V_1 \quad \text{and} \quad H V_2 = \alpha_2 V_2 \quad (168)$$

Then

$$[V_2, H V_1] = (H V_2, V_1)$$

$$[V_2, H V_1] - (H V_2, V_1) = 0$$

$$\alpha_1 [V_2, V_1] - \alpha_2 (V_2, V_1) = 0$$

Since

$$(\alpha_1 - \alpha_2) \neq 0 \quad (\text{both } \alpha_1 \text{ and } \alpha_2 \text{ are real})$$

Hence, $(V_2, V_1) = 0$

$$\begin{aligned} \|V_2\| \|V_1\| \cos \theta_{V_2 V_1} &= 0 \\ \theta_{V_2 V_1} &= \pi/2 \end{aligned} \quad (169)$$

Hence, the functions are orthogonal functions.

$$\text{Alternatively, } S\psi_1 = \alpha_1 \psi_1 \quad (170)$$

$$\text{and} \quad S\psi_2 = \alpha_2 \psi_2 \quad (171)$$

Scalar product of $S\psi_1$ and ψ_2 is given as

$$(\psi_2, S\psi_1) = (\psi_2, \alpha_1 \psi_1) = \alpha_1 (\psi_2, \psi_1) \quad (\alpha_1 - \text{real}) \quad (172)$$

Scalar product of $S\psi_2$ and ψ_1 is

$$(S\psi_2, \psi_1) = \alpha_2 (\psi_2, \psi_1) \quad (\alpha_2 - \text{real}) \quad (173)$$

$$\text{But} \quad (S\psi_2, \psi_1) = (\psi_2, S\psi_1) \quad \text{as } S \text{ is Hermitian} \quad (174)$$

From Eqs (172)–(174),

$$(\alpha_2 - \alpha_1)(\psi_2, \psi_1) = 0$$

But $\alpha_2 - \alpha_1 \neq 0$

$$(\psi_2, \psi_1) = \int \psi_2^* \psi_1 dz = 0 \quad (175)$$

Hence, ψ_2 and ψ_1 are mutually orthogonal functions.

3. The set of all eigen vectors that are bounded by Hermitian operators form a complete set of values. Eigen vectors form a basis for space because the Eigen vectors are orthogonal and can be normalized.

If H_1 and H_2 are commuting Hermitian operator, then $H_1 H_2$ is also Hermitian, which can be proved as follows:

When H_1 is Hermitian, then

$$\int u^* H_1 H_2 v dz = \int u^* H_1 (H_2 v) dz \quad (176)$$

$$\int u^* H_1 H_2 v dz = \int H_1^* u^* H_2 v dz \quad (177)$$

If H_2 is also Hermitian, then

$$\int u^* H_1 H_2 v dz = \int H_1^* H_2 u^* v dz$$

$$\int u^* H_1 H_2 v dz = \int (H_1 H_2)^* u^* v dz$$

$$\int u^* H_1 H_2 v dz = \int (H_2 H_1)^* u^* v dz$$

When H_1 and H_2 commute, then

$$[H_1, H_2] = 0 \quad \Rightarrow \quad [H_1 H_2 - H_2 H_1] = 0 \quad (178)$$

$$\int u^* H_1 H_2 v dz = \int (H_1 H_2)^* u^* v dz$$

$$\int u^* S v dz = \int S^* u^* v dz$$

where $S = H_1 H_2$

Hence, $H_1 H_2$ is also Hermitian.

3.21.5 Unitary Operators

A linear operator U is said to be unitary if under a similarity transformation, U preserves the Hermitian character for an operator. The condition for U to be unitary is

$$(U X U^{-1})^+ = U X U^{-1} \quad [X^+ = X \text{ for hermitian character}] \quad (179)$$

Such that
$$(U X U^{-1})^+ = (U^{-1})^+ X U^+ = U X U^{-1} \quad (180)$$

Multiplying Eqn. (180) from left by U^+ and right by U

$$U^+ (U^{-1})^+ X U^+ U = U^+ U X U^{-1} U \quad (181)$$

$$X (U^+ U) = (U^+ U) X$$

as
$$U^+ (U^{-1})^+ = (U^{-1} U)^+ = 1 \quad (182)$$

$$U^+ = U^{-1}$$

$$U U^+ = U U^{-1} = 1$$

Hence,
$$U U^+ = U^+ U = 1 \quad (183)$$

Under the operation of U , a vector X is transformed into vector X' . If two vectors X and Y are transformed by the same unitary operator U , then following condition is satisfied:

$$(X' Y') = (U X, U Y) = (X, Y) \quad (184)$$

The scalar product of vectors is preserved by the transformation of unitary operators. The norm of a vector is also unchanged under unitary transformation, that is, $\|U X\| = \|X\|$ and U is bounded $\|U\| = 1$. Hermitian operators H corresponding to every unitary operator is defined as

$$U = \exp(i \Sigma H) \quad (185)$$

where Σ is a parameter

$$U^+ = \exp(i \Sigma H)^+ = \exp(-i \Sigma H) = U^{-1} \quad (186)$$

Hence, Hermitian operator generates unitary transformation. In addition, the product of two or more unitary operators is also unitary. Eigen vectors belonging to different eigen values are also orthogonal. The eigen values are unimodular, that is, if $U X = \alpha X$ then $|\alpha| = 1$.

3.21.6 Momentum Operators

The relation between classical variables and quantum mechanical operator ($(\hbar/i) \nabla$) is momentum operator. The eigen value of momentum operator is defined by

$$P_{\text{op}} \psi = (\hbar/i) (d\psi/dx) = \alpha \psi \quad (187)$$

$$(\hbar/i) (d\psi/dx) = \alpha \psi$$

$$d\psi/\psi = (i/\hbar) \alpha dx \quad (188)$$

Integrating Eqn. (188),

$$\ln \psi = i\alpha x/\hbar + \ln c$$

$$\ln(\psi/c) = i\alpha x/\hbar$$

$$\psi/c = e^{i\alpha x/\hbar}$$

$$\psi = ce^{i\alpha x/\hbar} \quad (189)$$

Here

$$c = 1/\sqrt{2\pi\hbar} \quad (190)$$

$$\psi = (1/\sqrt{2\pi\hbar})e^{(i/\hbar)px} \quad [\text{for } \alpha = p] \quad (191)$$

3.21.7 Hamiltonian Operators

The expectation values of position and momentum are given by

$$\langle x \rangle = \int \psi^* x \psi dx / \int \psi^* \psi dx \quad (192)$$

and

$$\langle p \rangle = \int \psi^* p \psi dx / \int \psi^* \psi dx \quad (193)$$

$p_{\text{op}} \rightarrow [(\hbar/i)d/dx]$ is the momentum operator.

Schrödinger equation is given by

$$\hbar^2/2m(d^2\psi/dx^2) + V\psi = E\psi \quad (194)$$

Classically, Hamiltonian $H = (p^2/2m) + V$ and quantum mechanically Hamiltonian is given by

$$H_{\text{op}} = (p_{\text{op}}^2/2m) + V \quad (195)$$

In three dimensions, $H_{\text{op}} = -(\hbar^2/2m)[d^2/dx^2 + d^2/dy^2 + d^2/dz^2] + V(x, y, z)$

In one dimension $H_{\text{op}} \rightarrow -(\hbar^2/2m)(d^2/dx^2) + V(x)$ (196)

in three dimensions $[p_{\text{op}} \rightarrow (\hbar/i)(id/dx + jd/dy + kd/dz)]$ (197)

Or $p_{\text{op}} \rightarrow (\hbar/i) \blacktriangledown$ (198)

Eigen values of Hamiltonian operator can be obtained by $H_{\text{op}}\psi = E\psi$, where ψ is an Eigen function and E is the Eigen value. The Eigen value of E is real. For imaginary value of E , ψ would be divergent at either $x = \infty$ or $x = -\infty$.

3.21.8 Reflection Operator

If we take an operator R , which obeys

$$RA(x)R^{-1} = A(-x) \quad (199)$$

where $A(x)$ is operator function of x , then R is called reflection operator. In terms of x, y, z and bracket notation coordinate system,

$$\begin{aligned} \langle x', y', z' | R_y A_y R_y^{-1} | x'', y'', z'' \rangle &= (R_y \psi(x', y', z') A_y R_y \psi(x'', y'', z'')) \\ \langle x', y', z' | A_y | x'', -y'', z'' \rangle &= \psi(x', -y', z') A_y \psi(x'', -y'', z'') \end{aligned} \quad (200)$$

If $A_y = p_y =$ momentum

$$- \langle x', y', z' | A_y | x'', y'', z'' \rangle = (i\hbar d/dy) \delta(x' - x'') \delta(y' - y'') \delta(z' - z'') \quad (201)$$

$$[\delta(x' - x'') \delta(y' - y'') \text{ and } \delta(z' - z'')]$$

are Dirac-delta functions which are equal to 1 for $x'=x''$, $y'=y''$ and $z'=z''$.

We conclude that $R_y p_y R_y^{-1} = p_y$ (202)

Reflection operator R_y do not change x or z components of momentum. Only y component is changed.

3.21.9 Parity Operator

The parity operator satisfies the relation $\pi\psi(x) = \psi(-x)$, where π is the parity operator. π -operator is a linear operator and it satisfies the following operations:

- (i) $\pi(\psi_1(x) + \psi_2(x)) = (\pi\psi_1(x) + \pi\psi_2(x))$
- (ii) $\pi(\psi_1(x) + \psi_2(x)) = \psi_1(-x) + \psi_2(-x)$
- (iii) $\pi[c\psi(x)] = c\psi(-x) = c\pi\psi(x)$

Properties

1. The eigen value of operator π is given by

$$\pi\psi = \lambda\psi \quad (203)$$

where λ is the eigen value of π . Again operating Eqn. (203) by π

$$\pi^2\psi = \lambda\pi\psi = \lambda\lambda\psi = \lambda^2\psi = \psi \quad (204)$$

$$\text{so here } \lambda^2 = 1$$

$$\Rightarrow \lambda = \pm 1 \quad (205)$$

The eigen function corresponding to the eigen values $\lambda = \pm 1$ of parity operator are

(i) The even function ψ_e , corresponding to $\lambda = +1$

$$\psi_e(x) = +\psi_e(-x) \quad (206)$$

(ii) The odd given function ψ_o correspond to the eigen value $\lambda = -1$

$$\psi_o(x) = -\psi_o(-x) \quad (207)$$

2. π -operator is Hermitian

The scalar product of $\pi\psi$ and ϕ function is given by

$$(\pi\psi, \phi) = \int \psi^*(-x)\phi(x) dx = \int \psi^*(x')\phi(-x') dx' \quad [x' = -x]$$

$$\text{Also, } (\pi\psi, \phi) = \int_{-\infty}^{+\infty} \psi^*(x)\phi(-x) dx = (\psi, \pi\phi)$$

Value of integral is unaffected by renaming the variable of integration. This relation shows that π is also Hermitian operator.

3. The operator commuting with Hamiltonian is known as the Hamiltonian operator and is

$$H = (p^2/2m) + V(x) \quad (208)$$

Let it be operated on a function $\phi(x)$

$$H\phi(x) = -(\hbar^2/2m)(d^2/dx^2)\phi(x) + V(x)\phi(x) \quad (209)$$

Then

$$\begin{aligned} \pi H\phi(x) &= -(\hbar^2/2m)\pi(d^2/dx^2)\phi(x) + \pi V(x)\phi(x) \\ &= -(\hbar^2/2m)(d^2/dx^2)\phi(-x) + V(-x)\phi(-x) \\ &\quad [V(-x) = V(x)] \\ &= [-(\hbar^2/2m)(d^2/dx^2) + V(-x)]\phi(-x) \\ &= H\pi\phi(x) \end{aligned}$$

Hence,

$$[H\pi - \pi H] = [H, \pi] = 0 \quad (210)$$

The eigen values of a Hermitian operator A are real, the Eigen kets of A corresponding to different eigen values are orthogonal.

SUMMARY

The chapter deals with the Heisenberg's uncertainty principle, de-Broglie hypothesis and Schrödinger formulation of wave equations. de-Broglie hypothesis states that the moving particles always have matter waves associated with them. These matter waves are also known as de-Broglie waves. Davisson and Germer performed the experiments to prove the presence of matter waves associated with electron. But, then it was found that waves do not travel as a single wave, rather as a wave packet. Many waves interfere with each other to form a wave packet. Wave packet travels with group velocity (v_g) and every individual wave travels with a phase velocity (v_p). Furthermore, the relation of equivalence of group and phase velocity is established. But, it was well demonstrated by Heisenberg that the position and momentum cannot be measured accurately simultaneously, that is, if position is measured with greater accuracy, then the momentum remains uncertain and vice versa. The product of uncertainties of position and momentum are greater than or equal to Planck's constant. The need of differential equations was there, as exact location and momentum of particle could not be determined. Hence, the probabilistic approach is required. Hence, differential equation describes the motion of particles. Schrödinger used wave functions for the formulation of Schrödinger's equation. Wave functions are continuous, single-valued, and finite at every point in the space. The expectation values have been used to obtain uncertainty principle. The product of two wave functions satisfying Schwarz inequality has also been demonstrated. The bridge between classical and quantum mechanics is demonstrated by Ehrenfest theorem. Eigen values and eigen value equations have also been explained for different operators.

SOLVED PROBLEMS

Q. 1: The de-Broglie wavelength of an electron is 4 \AA . Calculate its momentum.

Ans: $\lambda = 4 \text{ \AA}$

According to de-Broglie hypothesis,

$$\lambda = \frac{h}{mv}$$

$$mv = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34}}{4 \times 10^{-10}}$$

$$p = 1.65 \times 10^{-24} \text{ kg m/s}$$

Q. 2: The speed of a proton is 10^5 m/s . Calculate its de-Broglie wavelength.

Ans:

Velocity of proton = 10^5 m/s

Mass of proton = $1.67 \times 10^{-27} \text{ kg}$

According to de Broglie relation

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{1.67 \times 10^{-27} \times 10^5}$$

$$\lambda = \frac{6.63 \times 10^{-2}}{1.67} = 3.97 \times 10^{-2} \text{ m.}$$

Q. 3: Calculate the de-Broglie wavelength of an electron if it has a velocity of 10^5 m/s .

Ans:

Mass m of electron = $9.1 \times 10^{-31} \text{ kg}$

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^5} = \frac{6.63}{9.1} \times 10^{-8}$$

$$\lambda = 7.28 \times 10^{-9} \text{ m}$$

Q. 4: The mass of a material particle is 207 times the mass of an electron. Calculate its de Broglie wavelength if its velocity is 10^4 m/s .

Ans:

Mass = $207 \times 9.1 \times 10^{-31} \text{ kg}$

Velocity = 10^4 m/s

According to de-Broglie hypothesis,

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{207 \times 9.1 \times 10^{-31} \times 10^4}$$

$$\lambda = 3.51 \times 10^{-3} \times 10^{-34} \times 10^{+31} \times 10^{-4}$$

$$\lambda = 3.51 \times 10^{-10} \text{ m} = 3.51 \text{ \AA}$$

Q. 5: An electron has been accelerated through a potential difference of 400 V. Calculate its de-Broglie wavelength.

Ans: The relation between de-Broglie wavelength and voltage is

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$$

$$\lambda = \frac{12.27}{\sqrt{200}} = \frac{12.27}{10 \times 1.41} \text{ \AA}$$

$$\lambda = \frac{12.27}{14.1} \text{ \AA} = 0.87 \text{ \AA}$$

Q. 6: An electron microscope used 2 keV electrons. Find out its resolving power.

Ans:

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$$

$$\lambda = \frac{12.27}{\sqrt{2000}} \text{ \AA} = \frac{12.27}{44.72} \text{ \AA}$$

$$\lambda = 0.274 \text{ \AA}$$

Q. 7: Calculate the energy of electrons (in eV) when its de-Broglie wavelength is 2 \AA.

Ans:

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}}$$

$$2 \times 10^{-10} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times E}}$$

$$(2 \times 10^{-10})^2 = \frac{(6.63 \times 10^{-34})^2}{18.2 \times 10^{-31} \times E}$$

$$E = \frac{(6.63 \times 10^{-34})^2}{4 \times 10^{-20} \times 18.2 \times 10^{-31}}$$

$$E = \frac{43.95 \times 10^{-68}}{72.8 \times 10^{-51}} = 0.603 \times 10^{-17} \text{ J}$$

$$E = \frac{6.03 \times 10^{-18}}{1.6 \times 10^{-19}} = 37.68 \text{ eV}$$

Q.8: What would be the energy of an electron if its wavelength is $4.2 \times 10^{-4} \text{ m}$. ?

Ans:

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$E = \frac{h^2}{2m\lambda^2}$$

$$E = \frac{(6.63 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times 17.64 \times 10^{-8}}$$

$$E = \frac{43.95 \times 10^{-68}}{321.048 \times 10^{-39}}$$

$$E = 0.1368 \times 10^{-29} \text{ J}$$

$$E = \frac{0.1368 \times 10^{-29}}{1.6 \times 10^{-19}} = 0.0855 \times 10^{-10}$$

$$E = 8.55 \times 10^{-12} \text{ eV}$$

Q. 9: Calculate the de-Broglie wavelength of thermal neutrons at 25°C (given the mass of neutron $1.67 \times 10^{-27} \text{ kg}$ and Boltzmann constant $8.6 \times 10^{-5} \text{ eV/C}$).

Ans:

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{h}{\sqrt{2mk_B T}}$$

$$T = 25^\circ\text{C} = 298 \text{ K}$$

$$k_B = 8.6 \times 10^{-5} \text{ eV/C}$$

$$= 1.376 \times 10^{-23} \text{ J/C}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 1.376 \times 10^{-23} \times 298}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{1369.56 \times 10^{-50}}}$$

$$\lambda = \frac{6.63 \times 10^{-34} \times 10^{+25}}{37}$$

$$\lambda = 0.179 \times 10^{-9}$$

$$\lambda = 1.79 \times 10^{-10}$$

$$\lambda = 1.79 \text{ \AA}$$

Q. 10: The energy of proton is 10^4 eV . Calculate its de-Broglie wavelength and velocity.

Ans: The energy of proton is

$$\frac{1}{2}mv^2 = 10^4 \text{ eV} = 10^4 \times 1.6 \times 10^{-19} \text{ J}$$

$$v^2 = \frac{2 \times 1.6 \times 10^{-19} \times 10^4}{1.67 \times 10^{-27}}$$

$$v^2 = \frac{3.2 \times 10^{-15}}{1.67 \times 10^{-27}}$$

$$v^2 = \frac{3.2}{1.67} \times 10^{+12}$$

$$v^2 = 1.91 \times 10^{12}$$

$$v = \sqrt{1.91 \times 10^{12}} = 1.38 \times 10^6 \text{ m/s}$$

The de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 10^4 \times 1.6 \times 10^{-19}}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{5.344 \times 10^{-42}}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{2.31 \times 10^{-21}} = 2.86 \times 10^{-13} \text{ m}$$

Q. 11: Evaluate the group and phase velocity of electron whose de-Broglie wavelength is 1 \AA .

Ans:

$$\lambda = 10^{-10} \text{ m}$$

Energy $E = \hbar\omega$ and momentum $p = \hbar k$

$$\frac{E}{p} = \frac{\omega}{k} = v_p$$

$$v_p = \frac{E}{p} = \frac{p^2/2m}{p} = \frac{p}{2m}$$

$$v_p = \frac{h}{2m\lambda} \quad (\text{using de Broglie's theorem})$$

$$v_p = \frac{6.63 \times 10^{-34}}{2 \times 9.1 \times 10^{-31} \times 10^{-10}}$$

$$v_p = 0.364 \times 10^{-34} \times 10^{41}$$

$$v_p = 0.364 \times 10^7 = 3.64 \times 10^6 \text{ m/s}$$

Group velocity is equal to the particle velocity

$$v_g = \frac{p}{m} = 2v_p = 2 \times 3.64 \times 10^6 \text{ m/s}$$

$$v_g = 7.28 \times 10^6 \text{ m/s}$$

Q. 12: A proton is moving with velocity 10^5 m/s and located with an accuracy of 10^{-3} cm. Calculate the fractional uncertainty in momentum.

Ans: According to Heisenberg uncertainty principle,

$$\Delta x \Delta p \geq \hbar$$

$$\Delta p \geq \frac{\hbar}{\Delta x} \quad \left(\begin{array}{l} \Delta x = 10^{-3} \text{ cm} \\ = 10^{-5} \text{ m} \end{array} \right)$$

$$\Delta p \geq \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 10^{-5} \text{ m}}$$

$$\Delta p \geq 1.05 \times 10^{-29} \text{ kg m/s}$$

The fractional uncertainty in momentum is given by

$$\frac{\Delta p}{p} = \frac{\Delta p}{mv} = \frac{1.05 \times 10^{-29}}{1.67 \times 10^{-27} \times 10^5}$$

$$\frac{\Delta p}{p} = 0.628 \times 10^{-29} \times 10^{22}$$

$$\frac{\Delta p}{p} = 6.28 \times 10^{-29} \times 10^{21} = 6.28 \times 10^{-8}$$

Q. 13: An electron is correct up to 0.05 percent while moving with a velocity of 300 m/s. What should be the minimum accuracy for the location of particle?

Ans:

$$p = mv$$

$$= 9.1 \times 10^{-31} \times 300 = 27.3 \times 10^{-29}$$

$$= 2.73 \times 10^{-28} \text{ kg m/s}$$

$$\Delta p = m\Delta v$$

$$\Delta p = mv \frac{\Delta v}{v} = p \frac{\Delta v}{v}$$

$$\Delta p = 2.73 \times 10^{-28} \times \frac{0.05}{100}$$

$$\Delta p = 0.1365 \times 10^{-30}$$

$$\Delta p = 1.365 \times 10^{-31} \text{ kg m/s}$$

According to uncertainty principle,

$$\Delta x \Delta p \geq \hbar$$

$$\Delta x \geq \frac{\hbar}{2\pi} \times \frac{1}{\Delta p}$$

$$\Delta x \geq \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 1.365 \times 10^{-31}}$$

$$\Delta x \geq 0.77 \times 10^{-3} \text{ m}$$

$$\Delta x = 0.77 \text{ mm}$$

Q. 14: A bullet of 100 g mass is shot out with a velocity of 600 m/s with an uncertainty of 0.01 percent in momentum. What would be the accuracy of its position with which it will be located?

Ans:

$$\text{Mass } m = 100 \text{ g} = 100 \times 10^{-3} \text{ kg}$$

$$m = 10^{-1} \text{ kg}$$

Momentum of bullet

$$p = mv = 10^{-1} \times 600 = 60 \text{ kg m/s}$$

Uncertainty in momentum is given by

$$\Delta p = \frac{0.01}{100} \times 60 = 60 \times 10^{-4} \text{ kg m/s}$$

According to uncertainty principle,

$$\Delta x \Delta p \geq \hbar$$

$$\Delta x \geq \frac{\hbar}{\Delta p}$$

$$\Delta x \geq \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 60 \times 10^{-4}}$$

$$\Delta x \geq 0.0175 \times 10^{-34} \times 10^4$$

$$\Delta x \geq 1.75 \times 10^{-34} \times 10^2$$

$$\Delta x \geq 1.75 \times 10^{-32} \text{ m}$$

Q. 15: Electron is confined to a box of dimension 10^{-10} m. Obtain the minimum uncertainty in its velocity.

Ans: According to uncertainty principle,

$$\Delta x \Delta p \geq \hbar$$

$$\Delta p \geq \frac{\hbar}{\Delta x} \quad [\Delta x = 10^{-10} \text{ m}]$$

$$m\Delta v \geq \frac{\hbar}{\Delta x}$$

$$\Delta v \geq \frac{\hbar}{m\Delta x} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^{-10} \times 2 \times 3.14}$$

$$\Delta v = \frac{6.63 \times 10^{-34} \times 10^{41}}{9.1 \times 2 \times 3.14}$$

$$\Delta v = \frac{6.63 \times 10^7}{9.1 \times 2 \times 3.14} = \frac{0.728}{2 \times 3.14} \times 10^7$$

$$\Delta v = 0.116 \times 10^7$$

$$\Delta v = 1.16 \times 10^6 \text{ m/s}$$

Q. 16: The one-dimensional wave function is given by $\varphi = \sqrt{a}e^{-\sqrt{ax}}$. Obtain the probability of finding a particle between $x = \frac{1}{a}$ and $x = \frac{2}{a}$.

Ans: Probability is given by

$$P = \varphi(x)\varphi^*(x)$$

$$P(x)dx = \varphi(x)\varphi^*(x)dx$$

$$P(x)dx = \sqrt{a}e^{-\sqrt{ax}} \sqrt{a}e^{-\sqrt{ax}} dx$$

$$P(x)dx = a e^{-ax} dx$$

$$P = \int_{1/a}^{2/a} P(x) dx = \int_{1/a}^{2/a} a e^{-ax} dx$$

$$P = a \int_{1/a}^{2/a} e^{-ax} dx = a \left[\frac{e^{-ax}}{-a} \right]_{1/a}^{2/a}$$

$$P = -\left[e^{-ax} \right]_{1/a}^{2/a}$$

$$P = -\left[e^{-a\left(\frac{2}{a}\right)} - e^{-a\left(\frac{1}{a}\right)} \right]$$

$$P = -\left[e^{-2} - e^{-1} \right]$$

$$P = \left[e^{-1} - e^{-2} \right]$$

$$P = e^{-1} - e^{-2}$$

Q. 17: Normalize the wave function $\varphi(x) = e^{iax}$, where a is constant over the region $0 < x < a$.

Ans: For normalization, we can calculate the wave function as

$$\int_0^a \varphi^*(x) \varphi(x) dx = 1$$

$$\varphi(x) = Ne^{iax} \quad \varphi^*(x) = Ne^{-iax}$$

$$\int_0^a Ne^{iax} Ne^{-iax} dx = 1$$

$$N^2 \int_0^a dx = 1$$

$$N^2 |x|_0^a = 1$$

$$N^2 = \frac{1}{a}$$

$$N = \frac{1}{\sqrt{a}}$$

Hence, $\varphi(x) = \frac{1}{\sqrt{a}} e^{iax}$

Q. 18: The wave function of a particle in one-dimensional box is given by

$$\varphi(x) = \begin{cases} N \sin \frac{2\pi x}{a} & \text{for } 0 < x < a \\ 0 & \text{otherwise} \end{cases}$$

Normalize the wave function.

Ans: The normalization condition is given by

$$\int_{-\infty}^{\infty} \varphi^* \varphi dx = 1$$

$$\int_{-\infty}^0 \varphi^* \varphi dx + \int_0^a \varphi^* \varphi dx + \int_a^{\infty} \varphi^* \varphi dx = 0$$

$$\int_0^a \phi^* \phi dx = 1$$

$$\int_0^a N^2 \sin^2 \frac{2\pi x}{a} dx = 1$$

$$\frac{N^2}{2} \int_0^a \left(1 - \cos \frac{4\pi x}{a}\right) dx = 1$$

$$\frac{N^2}{2} \left[x \Big|_0^a - \int_0^a \cos \frac{4\pi x}{a} dx \right] = 1$$

$$\frac{N^2}{2} (a) = 1$$

$$N = \sqrt{\frac{2}{a}}$$

Hence, the wave function is given by

$$\phi(x) = \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$$

Q. 19: The wave function for a particle is given by $\phi(x) = e^{2x}$. Find the probability of finding the particle between $x = 4$ and $x = 6$.

Ans: The probability is given by $P = \int_4^6 \phi^* \phi dx$

$$P = \int_4^6 e^{4x} dx$$

$$P = \left[\frac{e^{4x}}{4} \right]_4^6 = \frac{1}{4} (e^{24} - e^{16})$$

$$P = \frac{(e^{24} - e^{16})}{4}$$

Q. 20: Prove that probability is real for given wave function $\Psi(x, t)$.

Ans: Let $\Psi(x, t)$ be expressed as a complex quantity.

$$\Psi(x, t) = a + ib$$

Hence,

$$\Psi^*(x, t) = a - ib$$

Therefore, $\Psi(x, t)\Psi^*(x, t) = P = a^2 + b^2 = \text{Real}$

Hence, probability is real.

Q. 21: A particle is described by wave function $\varphi = \sqrt{7}x$ for $0 < x < 1$. Obtain the average position of the particle.

Ans: The expectation value is given by

$$\begin{aligned}\langle x \rangle &= \int_{-\infty}^{\infty} \varphi^* x \varphi dx \\ \langle x \rangle &= \int_0^1 \sqrt{7}x \cdot x \sqrt{7}x dx \\ \langle x \rangle &= \int_0^1 7x^3 dx \\ \langle x \rangle &= 7 \left[\frac{x^4}{4} \right]_0^1 = \frac{7}{4} = 1.75\end{aligned}$$

Q.22: A particle is described by a wave function

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \cos 2x \text{ for } -a < x < a$$

Obtain the expectation value of momentum.

Ans:

$$\begin{aligned}\langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial}{\partial x} (\Psi(x,t)) dx \\ \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \sqrt{\frac{2}{a}} \cos 2x \frac{\partial}{\partial x} \left(\sqrt{\frac{2}{a}} \cos 2x \right) dx \\ \langle p \rangle &= +i\hbar \frac{2}{a} \int_{-a}^a \cos 2x \sin 2x (2) dx \\ \langle p \rangle &= \frac{4i\hbar}{a} \int_{-a}^a \sin 4x dx \\ \langle p \rangle &= -\frac{4i\hbar}{a} \left[\frac{\cos 4x}{4} \right]_{-a}^a \\ \langle p \rangle &= -\frac{i\hbar}{a} (\cos 4a - \cos 4a) \\ \langle p \rangle &= 0\end{aligned}$$

Q.23: The wave function $\Psi(x,t) = \frac{1}{\sqrt{3a}} e^{i(kx - \omega t)}$ is given for a particle in interval $(0, a)$. Obtain the uncertainty in position.

Ans:

$$\langle x \rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{3a}} e^{-i(kx-ut)} x \frac{1}{\sqrt{3a}} e^{i(kx-ut)} dx$$

$$\langle x \rangle = \frac{1}{3a} \int_0^a x dx$$

$$\langle x \rangle = \frac{1}{3a} \left[\frac{x^2}{2} \right]_0^a$$

$$\langle x \rangle = \frac{1}{3a} \left[\frac{a^2}{2} - 0 \right]$$

$$\langle x \rangle = \frac{1}{3a} \times \frac{a^2}{2} = \frac{a}{6}$$

$$\langle x \rangle = \frac{a}{6}$$

Q. 24: Let the particle be described by a wave function $\Psi(x, t) = \sqrt{\frac{2}{L}} e^{ikx}$ in interval $(0, L)$. Obtain the uncertainty in momentum.

Ans:

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} e^{-ikx} \frac{\partial}{\partial x} \left(\sqrt{\frac{2}{L}} e^{ikx} \right) dx$$

$$\langle p \rangle = \frac{-i\hbar 2}{L} \int_0^L e^{-ikx} e^{ikx} (ik) dx$$

$$\langle p \rangle = \frac{2\hbar k}{L} \int_0^L dx$$

$$\langle p \rangle = 2\hbar k$$

Q. 25: Do $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial t}$ commute?

Ans: The operators commute, if

$$[A, B] = AB - BA = 0$$

Here $A = \frac{\partial}{\partial x}$ and $B = \frac{\partial}{\partial t}$

$$[A, B]g = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial t} \right] g$$

where g is $g(x, t)$, that is, continuous function of x and t

$$[A, B]g = \left[\frac{\partial}{\partial x} \frac{\partial}{\partial t} - \frac{\partial}{\partial t} \frac{\partial}{\partial x} \right] g$$

$$\begin{aligned}
 &= \frac{\partial}{\partial x} \frac{\partial g}{\partial t} - \frac{\partial}{\partial t} \frac{\partial g}{\partial x} \\
 &= \frac{\partial^2 g}{\partial x \partial t} - \frac{\partial^2 g}{\partial t \partial x}
 \end{aligned}$$

As
$$\frac{\partial^2 g}{\partial x \partial t} = \frac{\partial^2 g}{\partial t \partial x}$$

Hence, $[A, B]g = 0$

Therefore, A and B commute with each other.

Q. 26: Determine whether the wave function $\Psi = Ae^{ik(x+a)}$ is an Eigen function of momentum operator \hat{p}_x .

Ans:

$$\begin{aligned}
 p_x &= -i\hbar \frac{\partial}{\partial x} \\
 p_x \Psi &= -i\hbar \frac{\partial}{\partial x} (Ae^{ik(x+a)}) \\
 p_x \Psi &= -i\hbar Ae^{ik(x+a)} (ik) \\
 p_x \Psi &= -i\hbar ik \Psi \\
 p_x \Psi &= \hbar k \Psi
 \end{aligned}$$

Hence, it is an eigen function of momentum operator p_x . The Eigen value is $\hbar k$.

Q. 27: Prove that time-independent Schrödinger equation is an example of eigen value equation.

Ans:

$$\begin{aligned}
 \frac{d^2 \varphi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \varphi &= 0 \\
 -\frac{\hbar^2}{2m} \frac{d^2 \varphi}{dx^2} - (E - V) \varphi &= 0 \\
 \left(\frac{-\hbar^2}{2m} \frac{d^2 \varphi}{dx^2} - V \varphi \right) &= E \varphi \\
 \underbrace{\left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V \right)}_H \varphi &= E \varphi \\
 H \varphi &= E \varphi
 \end{aligned}$$

Hence, it represents an eigen-value equation.

OBJECTIVE QUESTIONS

1. de-Broglie wavelength is independent of

- (a) mass (b) velocity
(c) charge (d) all of these

2. de-Broglie wave is related to temperature as

- (a) $\lambda = \frac{h}{\sqrt{2mk_B T}}$ (b) $\lambda = h(\sqrt{2mk_B T})$
(c) $\lambda = m\sqrt{T}$ (d) $\lambda = m\sqrt{3mk_B T}$

3. The de-Broglie wavelength is given by

- (a) $\lambda = \frac{12.27}{\sqrt{mk_B T}} \text{ \AA}$ (b) $\lambda = \frac{6}{\sqrt{3mk_B T}} \text{ \AA}$
(c) $\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$ (d) $\lambda = \frac{10.89}{\sqrt{V}} \text{ \AA}$

4. In Davisson and Germer experiment, no bump was observed at

- (a) 54 V (b) 60 V
(c) 44 V (d) 40 V

5. The propagation constant k and momentum are related to each other by

- (a) $p = \frac{\hbar}{k}$ (b) $p = \hbar k$
(c) $p = mk$ (d) $p = \frac{m}{k}$

6. Wave packet has group of waves that travel with

- (a) different speed (b) different directions
(c) same speed (d) none of these

7. The wave velocity of a particle is given by

- (a) wk (b) \sqrt{wk}
(c) $\frac{w}{k}$ (d) $w^2 k^2$

8. Group velocity is

- (a) greater than particle velocity (b) less than particle velocity
(c) equal to particle velocity (d) none of these

9. According to uncertainty principle, which two things cannot be measured simultaneously?

- (a) mass and velocity (b) position and charge
(c) mass and charge (d) position and momentum

10. Energy of particle in a box is given by

- (a) $E = 2mL^2$ (b) $E = \frac{\hbar^2}{2mL^2}$
(c) $E = \hbar^2 2mL^2$ (d) $E = 2\hbar^2 L$

11. The ground state energy of hydrogen atom is

- (a) 10.2 eV (b) 13.6 eV
(c) 5.6 eV (d) 9 eV

12. Minimum energy of oscillator is given by

- (a) $\hbar w$ (b) $\frac{1}{\hbar} w$
(c) $L\hbar w$ (d) 0

13. The wave function must be

- (a) single valued (b) finite
(c) continuous (d) all of these

14. The probability for a particle is represented by

- (a) φ^* (b) φ
(c) $\varphi^* \varphi$ (d) $\varphi^* \varphi$

15. The probability can be normalized as

- (a) $\int_{-\infty}^{\infty} \varphi(r,t) \varphi^*(r,t) dv = 0$ (b) $\int_{-\infty}^{\infty} \varphi(r,t) \varphi(r,t) dv = 1$
(c) $\int_{-\infty}^{\infty} \varphi^*(r,t) \varphi^*(r,t) dv = 0$ (d) $\int_{-\infty}^{\infty} \varphi^*(r,t) \varphi(r,t) dv = 1$

16. Free particle represents

- (a) no mass (b) no force
(c) no charge (d) all of these

17. The probability density of state is

- (a) imaginary (b) zero
(c) real (d) fluctuates

18. The uncertainty principle is valid for
 (a) subatomic systems (b) large systems
 (c) both small and large (d) none of these
19. The photon of wavelength λ , has mass m is given by
 (a) $\frac{h\lambda}{c}$ (b) $\frac{h}{c\lambda}$
 (c) 0 (d) none of these
20. In terms of expectation values, the uncertainty principle states
 (a) $\Delta A = [\langle A^2 \rangle - \langle A \rangle^2]^{1/2}$ (b) $\Delta A = [\langle A \rangle - \langle A \rangle^2]^{1/2}$
 (c) $\Delta A = [\langle A^2 \rangle - \langle A \rangle]^{1/2}$ (d) none of these
21. Which wave functions do not commute?
 (a) $\frac{\partial}{\partial x}, \frac{\partial}{\partial t}$ (b) x, t
 (c) p_x, p_y (d) p_y, y
22. Which is a nonlinear operator?
 (a) $\sqrt{\quad}$ (b) x
 (c) \exp (d) d/dx

ANSWERS

- | | | | |
|--------|---------|---------|---------|
| 1. (c) | 7. (c) | 13. (d) | 19. (b) |
| 2. (a) | 8. (c) | 14. (d) | 20. (a) |
| 3. (c) | 9. (d) | 15. (d) | 21. (d) |
| 4. (d) | 10. (b) | 16. (b) | 22. (a) |
| 5. (b) | 11. (b) | 17. (c) | |
| 6. (c) | 12. (a) | 18. (c) | |

Micro-Assessment Questions

1. What do you understand by dual nature of material particles?
2. What are matter waves?
3. How do matter waves differ from electromagnetic waves?
4. What is a wave packet?
5. Define group velocity for a wave packet.
6. What is the difference between group and particle velocity?
7. Explain uncertainty principle.
8. What is a wave function?
9. What do you understand by probability for a particle?
10. Define the parameters that define whether a particle is free or bound.
11. What is normalization of wave function?
12. What do you understand by the orthogonality condition?
13. Why the wave function needs normalization?
14. When you say “a wave-function is well behaved,” what does it infer?
15. Explain the conditions that a wave function should obey.
16. What was the need for a wave function?
17. Define the expectation value for an observable.
18. How the behavior of particle is described using differential equation?
19. What do you understand by single-valued function?
20. What do you understand by observable?

Critical Thinking Questions

1. Show that the group velocity associated with the moving particle is equal to velocity of the particle itself.
2. Derive the mathematical relation between group and particle velocity for a wave packet.
3. If matter has a wave nature, then why its wave-like character is not observable in our everyday life?
4. Find out the de Broglie wavelength in terms of potential difference V .
5. Discuss Davisson and Germer experiment for diffraction of electrons.
6. How does uncertainty principle exclude the possibility of existence of electrons inside the nucleus?
7. Heisenberg uncertainty principle is important for microscopic objects. Explain.
8. Calculate the binding energy of hydrogen using uncertainty principle.
9. Explain the zero-point finite energy using uncertainty principle.
10. Obtain the time-dependent Schrödinger wave equation for bound and free particle.
11. Derive the time-independent Schrödinger wave equation in one dimension.
12. Derive the expression for expectation value of position and momentum operators.
13. State and derive the Ehrenfest theorem. Explain its physical significance.
14. Obtain the Heisenberg uncertainty principle using Schwarz inequality.
15. Why the de Broglie waves associated with cricket ball are not observable?
16. Why the wave function and its derivative should be continuous everywhere?
17. Why Schrödinger wave equation has first-order time derivative?

18. An electron and a proton are accelerated from rest through the same potential difference. Which one has the longer wavelength?
19. Why is it impossible to measure the position and speed of a particle simultaneously with infinite accuracy?

Graded Questions

1. Find out the de Broglie wavelength for electron with energy 1 V.
2. Find out the voltage that should be applied to electron source to produce electrons with wavelength 0.6 Å.
3. Find out the momentum for neutron with de Broglie wavelength 1 Å.
4. Find out the uncertainty in position of electron moving with speed 500 ms⁻¹ having accuracy 0.05 per cent.
5. Calculate the de Broglie wavelength for an electron with kinetic energy: (a) 100 eV and (b) 1,000 keV.
6. The wavelength for sodium line is 5,890 Å. Find out the kinetic energy at which the electron will have same energy.
7. Calculate the binding energy of hydrogen atom using uncertainty principle.
8. Calculate the de Broglie wavelength for a proton moving with a speed of 10⁶ m/s.
9. Calculate the de Broglie wavelength of a 90-kg person who is running at a speed of 3.0 m/s.
10. Through what potential difference would an electron have to be accelerated to give it a de Broglie wavelength of 1 Å?
11. A ball of mass 100 g moves with a speed of 20 m/s. If its speed is measured to an accuracy of 0.1 per cent, what is the minimum uncertainty in its position?
12. A proton has a kinetic energy of 2.0 MeV. If its momentum is measured with an uncertainty of 4.0 per cent, what is the minimum uncertainty in its position?
13. Calculate the wavelength in nm of electrons that have been accelerated from rest through a potential difference of 54 V.
14. If $\psi(x) = (A/(x^2 + a^2))$, calculate the normalization constant A.
15. State Ehrenfest's theorem. Show that

$$(a) \quad \frac{d \langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}$$

$$(b) \quad \frac{d \langle p_x \rangle}{dt} = \langle -\partial V / \partial x \rangle$$

Remember and Understand

1. de-Broglie wavelength is independent of charge on the particle. Heavy particle has small wavelength.
2. A particle is said to be free when it is under no force.
3. A wave function representing a wave packet describes a localized particle. The wave packet is superposition of many wavelets. Every wave has its own propagation constant and angular velocity.
4. The group velocity of particle is equal to particle velocity.

5. The wave function is continuous, single valued, finite, and well-behaved. The wave function must vanish at infinity.

6. According to Heisenberg uncertainty principle

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}, \text{ where } \Delta p_x \text{ and } \Delta x \text{ are the uncertainties in momentum and position, respectively.}$$

7. The probability for a particle to be found in interval dx is given by:

$$P(x) dx = |\Psi(x, t)|^2 dx, \text{ where } \Psi(x, t) \text{ represents the wave function defining the particle.}$$

8. The orthonormality condition states:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1.$$

9. When the wave function at time $t = 0$ is given, then the position of particle can be obtained at time t .

10. The generalised time-dependent Schrodinger Equation is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + V(x, y, z) \Psi$$

11. The time-independent Schrodinger equation is given by

$$\frac{d^2 \phi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \phi = 0$$

12. The expectation value of momentum and energy are given by

$$\Delta z \Delta p_z \geq \hbar$$

13. According to Schwarz's inequality, the absolute value of scalar product of state ϕ_n and ϕ_m is less than the product of norm ϕ_n and ϕ_m

14. The Ehrenfest Equations are given by

$$(i) \frac{m d \langle x \rangle}{dt} = \langle p_x \rangle$$

$$(ii) \frac{d \langle p_x \rangle}{dt} = - \left[\frac{\partial V}{\partial x} \right]$$

Quantum Mechanics—III

Solutions of Schrödinger Equations and Hydrogen Problem

Keywords: finite potential well, Step potential, Tunneling effect, 3-D harmonic oscillator, Hydrogen value problem, Radial equation, total quantum number, Spherical coordinates. azimuthal quantum number

Learning Objectives

- ◆ To know about the behavior of Schrödinger equations under different potentials.
- ◆ To obtain the wave function of a particle in one-dimensional infinite potential well.
- ◆ To obtain the particle behavior in step potential for two cases, that is, when energy E is greater than step-potential V and when energy E is less than step-potential V .
- ◆ To understand the tunnel effect for finite potential barrier.
- ◆ To obtain the wave function for scattered and bound state.
- ◆ To calculate the hydrogen value problem in terms of azimuthal, angular, and radial wave functions.
- ◆ To analyze the 3-D harmonic oscillator and square-well potential.
- ◆ To apply separation of variables for solving hydrogen value problem.

Till now, we have studied the time-dependent and time-independent Schrödinger equations. This chapter deals with the time-independent Schrödinger equations under the effect of different potentials. These equations are very helpful to describe the motion of a particle.

4.1 Particle In Infinite Potential Well (1-D)

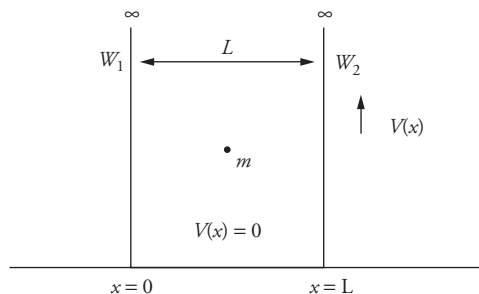


Figure 4.1 The particle in a box (1-D)

Consider a one-dimensional (1-D) (see Figure 4.1) box with dimensions extending from $0 < x < L$. The walls of the well are taken to be rigid, so that when the particle collides with the walls, no loss of energy takes place (square well potential is equivalent to potential of closed box). The variation of potential for this well is given by

$$V(x) = 0 \quad \text{for} \quad 0 < x < L \quad (\text{inside})$$

$$V(x) = \infty \quad \text{for} \quad x < 0 \quad \text{and} \quad x > L \quad (\text{outside})$$

and W_1 and W_2 represent the walls of a closed box or well.

This problem can be analyzed with two treatments, classical and quantum-mechanical. Ideally, the particle of mass m inside the box moves under no force because potential inside the box is zero. But while moving, when the particle reaches boundary walls W_1 and W_2 , the potential changes from 0 to ∞ . Hence, the particle experiences force $F = -\frac{dV}{dx}$, that is, the particles gets reflected back (as the force is in opposite direction). Hence, the particle keeps on moving within the walls W_1 and W_2 .

But the quantum mechanical picture portrays this motion of particle in box using Schrödinger equation as follows:

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\phi = 0 \quad (1)$$

Equation (1) for particle inside the box can be written as $[V(x) = 0]$:

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}E\phi = 0 \quad (2)$$

We can substitute
$$\frac{2mE}{\hbar^2} = k^2 \quad (3)$$

Hence, Eqn. (2) can be written as

$$\frac{d^2\phi}{dx^2} + k^2\phi = 0 \quad (4)$$

Equation (4) has the general solutions

$$\phi(x) = A_1 \sin kx + A_2 \cos kx \quad (5)$$

where A_1 and A_2 are arbitrary constants. Before solving Eqn. (4), we need to determine the boundary conditions first. The potential outside the box is almost infinite, hence the probability and wave function of particle outside the box and at the boundaries is almost zero.

$$\phi(x) = 0 \quad \text{at} \quad x = 0 \quad \text{and} \quad L \quad (6)$$

Apply Eqn. (6) in Eqn. (5)

$$\begin{aligned} \phi(x) = 0 &= A_1 \sin kx + A_2 \cos kx && [\text{at } x = 0] \\ 0 &= A_1 \sin(0) + A_2 \cos(0) \\ A_2 &= 0 \end{aligned} \quad (7)$$

Therefore, the solution from Eqn. (5) becomes

$$\varphi(x) = A_1 \sin kx \quad (8)$$

Using second boundary condition at $x = L$,

$$\varphi(x) = A_1 \sin k(L) = 0$$

$$A_1 \sin kL = 0$$

(A_1 cannot be zero because otherwise both the constants will be zero leading to no particle inside the box)

$$\sin kL = 0$$

$$kL = n\pi \Rightarrow k = \frac{n\pi}{L} \quad (9)$$

where $n > 0$ or $n = 1, 2, 3, \dots$

From Eqs (3) and (9),

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (10)$$

This Eqn. (10) represents energy of states for particle in box. Applying $n = 1, 2, 3, \dots$, the energy values obtained are depicted in Figure 4.2.

Ideally, the particle inside the box can take any arbitrary values. But quantum mechanically, it is not possible. The particles can take only some well-defined energy values, which are defined by $n = 1, 2, 3, \dots$. Hence, in other words, the energy of particle is quantized and discrete. Figure 4.2 shows the energy levels corresponding to $n = 1, 2, 3$, and 4. This diagram is known as energy-level diagram. It is

clear from Figure 4.2 that $E_n = \frac{\pi^2 \hbar^2}{2mL^2}$ for $n = 1$.

This is the minimum energy of a particle in potential well. E_1 is also known as ground-state energy or zero-point energy.

Let us find out the value of constant A_1 by using normalization.

$$\begin{aligned} n=4 & \text{ ————— } E_4 = 16 \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) = 16E_1 \\ n=3 & \text{ ————— } E_3 = 9 \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) = 9E_1 \\ n=2 & \text{ ————— } E_2 = 4 \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) = 4E_1 \\ n=1 & \text{ ————— } E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \end{aligned}$$

Figure 4.2 Energy-level diagram

From Eqn. (8)

$$\varphi(x) = A_1 \sin kx$$

$$\varphi(x) = A_1 \sin\left(\frac{n\pi}{L}x\right) \text{ for } 0 < x < L$$

For the particle outside the box, the wave function $\varphi(x)$ vanishes.

Applying normalization condition,

$$\int_{-\infty}^{\infty} \varphi(x) \varphi^*(x) dx = 1 \quad (11)$$

$$\underbrace{\int_{-\infty}^0 \varphi(x) \varphi^*(x) dx}_{=0 \text{ (outside the box)}} + \int_0^{\infty} \varphi(x) \varphi^*(x) dx = 1$$

$$\int_0^L \varphi(x) \varphi^*(x) dx + \underbrace{\int_L^{\infty} \varphi(x) \varphi^*(x) dx}_{=0 \text{ (outside the box)}} = 1$$

$$\int_0^L \varphi(x) \varphi^*(x) dx = 1$$

$$\int_0^L A_1^2 \sin^2 \frac{n\pi}{L}x dx = 1$$

$$A_1^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$$

$$A_1 = \sqrt{\frac{2}{L}} \quad (12)$$

Hence, using Eqn. (12), Eqn. (8) becomes

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad (13)$$

Figure 4.3 gives the variation of wave function $\varphi_n(x)$ with x .

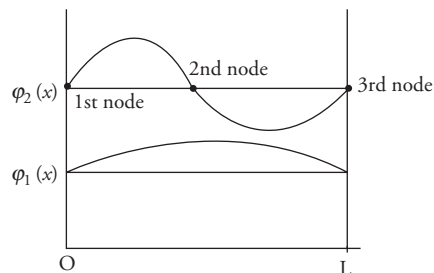


Figure 4.3 The wave function in n th state has $(n + 1)$ nodes of vibration

4.2 Step Potential

Sometimes potential barriers are present for a particle. When we speak of potential barrier, it means the energy of particle is below zero or nearly zero everywhere except for some regions. The potential barrier has some height. The step potential has two cases as follows:

- (i) When energy E of particle is more than the potential barrier height.
- (ii) When energy E of particle is less than the potential barrier height.

Both the cases are discussed in the following sections:

4.2.1 Energy Greater than Potential Step

Figure 4.4 represents single potential step for particle of mass m . V_0 is the height of potential barrier at $x < 0$ and it is constant for $x > 0$. Hence, it can be summarized as

$$V(x) = 0 \quad \text{for} \quad x < 0 \rightarrow \text{region 1}$$

$$V(x) = V_0 \quad \text{for} \quad x > 0 \rightarrow \text{region 2}$$

The total energy E of the incident particle is greater than V_0 , such that $E - V_0 > 0$. Classically, the particle can move freely in region 1, as $V(x) = 0$. But at $x = 0$, a force $F = \frac{-dV}{dx}$ is experienced. This force is retarding in nature, which affects the moving particle, and the velocity of incident particle gets slowed down. Hence, no reflection takes place and the particle is transmitted to region 2, but with lower velocity compared to incident velocity. Hence, the classical viewpoint states that the particle is always transmitted in region 2. Quantum mechanically, the Schrödinger wave equation is used. Time-independent wave equation is used as potential is independent of time.

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\phi = 0 \quad [\text{Eqn. (1)}]$$

For $x < 0$ (region 1), the Schrödinger wave equation can be written as

$$\frac{d^2\phi_1}{dx^2} + \frac{2m}{\hbar^2}E\phi_1 = 0 \quad [V(x) = 0 \text{ for region 1}]$$

$$\frac{d^2\phi_1}{dx^2} + k_1^2\phi_1 = 0 \quad (14)$$

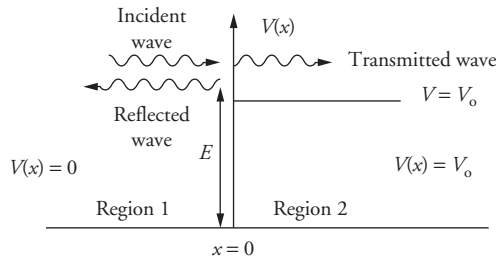


Figure 4.4 Representation of potential barrier when the energy $E > V_0$.

where
$$k_1^2 = \frac{2mE}{\hbar^2} \quad (15)$$

The general solution for Eqn. (14) is given by

$$\varphi_1 = A_1 e^{ik_1 x} + A_2 e^{-ik_1 x} \quad (16)$$

where A_1 and A_2 are arbitrary constants.

For $x > 0$ (region 2), the Schrödinger wave equation is given by

$$\frac{d^2 \varphi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_o) \varphi_2 = 0 \quad [\text{for region 2, } V(x) = V_o]$$

$$\frac{d^2 \varphi_2}{dx^2} + k_2^2 \varphi_2 = 0 \quad (17)$$

where
$$k_2^2 = \frac{2m(E - V_o)}{\hbar^2} \quad (18)$$

The general solution for Eqn. (17) is given by

$$\varphi_2 = B_1 e^{ik_2 x} + B_2 e^{-ik_2 x} \quad (19)$$

For Eqs (16) and (19), the exponential terms can be described as follows:

(a) Equation (16): $e^{ik_1 x} \rightarrow$ wave associated with incident particle in region 1
 $e^{-ik_1 x} \rightarrow$ wave of reflected particle in region 1

(b) Equation (19): $e^{ik_2 x} \rightarrow$ wave of transmitted particle in region 2
 $e^{-ik_2 x} \rightarrow$ wave of reflected particle in region 2

There is no further potential barrier in region 2, hence no wave is associated with reflected particle in region 2. Therefore, $e^{-ik_2 x}$ is 0, and Eqn. (19) is written as

$$\varphi_2 = B_1 e^{ik_2 x} \quad (20)$$

For solving the Schrödinger equation, we need to have boundary conditions. At boundaries, the wave function and its first derivative is continuous. Hence, at boundary $x = 0$

$$\varphi_1(0) = \varphi_2(0) \quad (21a)$$

and

$$\left. \frac{d\varphi_1}{dx} \right|_{x=0} = \left. \frac{d\varphi_2}{dx} \right|_{x=0} \quad (21b)$$

Using Eqs (16), (20), and (21a)

$$A_1 e^{ik_1 \cdot 0} + A_2 e^{-ik_1 \cdot 0} = B_1 e^{ik_2 \cdot 0}$$

$$A_1 + A_2 = B_1 \quad (22)$$

Using Eqs (16), (20), and (21b)

$$ik_1 (A_1 - A_2) = ik_2 B_1$$

$$A_1 - A_2 = \frac{k_2}{k_1} B_1 \quad (23)$$

Adding Eqs (22) and (23),

$$B_1 = \left(\frac{2k_1}{k_1 + k_2} \right) A_1 \quad (24)$$

Then we obtain A_2 from Eqs (22) and (24)

$$A_2 = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A_1 \quad (25)$$

Using Eqs (24) and (25) in Eqs (16) and (20),

$$\varphi_1 = \underbrace{A_1 e^{ik_1 x}}_{\text{I}} + \underbrace{A_1 \left(\frac{k_1 - k_2}{k_1 + k_2} \right) e^{-ik_1 x}}_{\text{II}} \quad (26a)$$

$$\varphi_2 = \underbrace{\left(\frac{2k_1}{k_1 + k_2} \right) A_1 e^{ik_2 x}}_{\text{III}} \quad (26b)$$

From Eqn. (26(a)–(b)), the wave can be written as

$$\varphi_i - A_1 e^{ik_1 x} \rightarrow \text{incident wave. } \varphi_r - A_1 \left(\frac{k_1 - k_2}{k_1 + k_2} \right) e^{-ik_1 x} \rightarrow \text{reflected wave}$$

$$\varphi_t - A_1 \left(\frac{2k_1}{k_1 + k_2} \right) e^{ik_2 x} \rightarrow \text{transmitted wave}$$

We will define two important terms based on these results as follows:

- (i) **Reflection coefficient:** For a free particle, the probability density current is the product of the velocity of particle and its probability density. Let u_1 be the velocity of particle in region 1
Hence, reflected probability density current

$$= u_1 \varphi_r^* \varphi_r$$

Incident probability density current

$$= u_1 \varphi_i^* \varphi_i$$

Reflection coefficient is the ratio of reflected probability density current to the incident probability current density, that is,

$$R = \frac{u_1 \varphi_r^* \varphi_r}{u_1 \varphi_i^* \varphi_i} \quad (27)$$

$$R = \frac{A_1^* \left(\frac{k_1 - k_2}{k_1 + k_2} \right) e^{ik_1 x} A_1 \left(\frac{k_1 - k_2}{k_1 + k_2} \right) e^{-ik_1 x}}{A_1^* e^{ik_1 x} A_1 e^{-ik_1 x}} \quad (28)$$

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

Equation (28) gives the probability of reflection of incident particle. The reflection coefficient is zero only when $k_1 = k_2$. Otherwise, there is always some reflection at the potential barrier. Classical view-point states that no reflection occurs.

- (ii) **Transmission coefficient:** We need transmitted probability density current for calculation of transmission coefficients.

$$\text{Transmitted probability density} = u_2 \varphi_t^* \varphi_t$$

where $u_2 \rightarrow$ velocity of particle in region 2.

Transmission coefficient is defined as the ratio of transmitted probability density to incident probability density, that is,

$$T = \frac{u_2 \varphi_t^* \varphi_t}{u_1 \varphi_i^* \varphi_i} \quad (29)$$

$$\left[u_2 = \frac{p_2}{m} = \frac{\hbar k_2}{m}; \quad u_1 = \frac{p_1}{m} = \frac{\hbar k_1}{m} \right]$$

$$T = \frac{\hbar k_2 / m (2k_1 / (k_1 + k_2))^2 A_1^* A_1}{\hbar k_1 / m A_1^* e^{ik_1 x} A_1 e^{-ik_1 x}}$$

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (30)$$

Transmission coefficient gives the probability of transmission of particle across potential barrier.

Equation (30) gives $T < 1$, but classical mechanics treats $T = 1$. If we add reflection and transmission coefficient, then

$$R + T = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} + \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

$$R + T = 1 \quad (31)$$

4.2.2 Energy Less than Potential Step

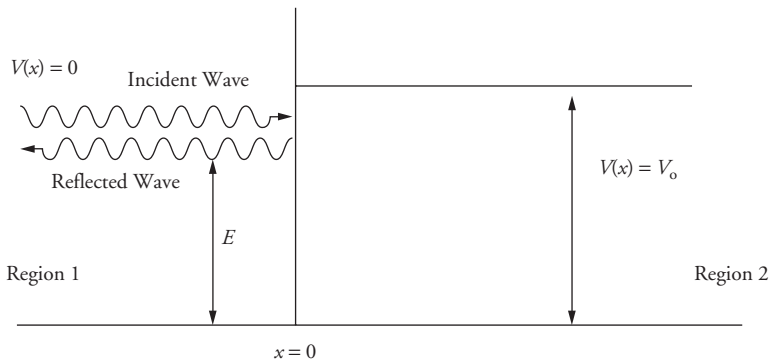


Figure 4.5 Potential step greater than energy E of particle

Figure 4.5 represents the step barrier when energy of particle is less than barrier height, that is, $E - V_0 < 0$. The potential on the left of $x = 0$ vanishes and on the right is constant. It can be summarized as

$$V(x) = 0 \quad \text{for} \quad x < 0 \text{ in region 1}$$

$$V(x) = V_0 \quad \text{for} \quad x > 0 \text{ in region 2}$$

The classical analysis of Figure 4.5 gives the explanation as follows:

When the particle moves in region 1, there is no field on the particle. As it reaches the boundary at $x = 0$, it experiences force due to potential V_0 . The energy of incident particle is less than the potential barrier; hence, it is not able to penetrate the barrier and will remain in region 1. It will be reflected back as soon as it comes across the boundary. For the quantum mechanical treatment, we have to solve the Schrödinger equation

$$\frac{d^2\varphi_1}{dx^2} + \frac{2m}{\hbar^2}(E - V)\varphi_1 = 0$$

for $x < 0$ (region 1 corresponds to zero potential)

$$\frac{d^2\varphi_1}{dx^2} + \frac{2mE}{\hbar^2}\varphi_1 = 0 \quad (32)$$

where m = mass of incident particle.

$$k_1^2 = \frac{2mE}{\hbar^2} \quad (33)$$

The solution is given by

$$\varphi_1 = A_1 e^{ik_1 x} + A_2 e^{-ik_1 x} \quad (34)$$

where A_1 and A_2 are arbitrary constants.

For $x > 0$ (region 2 corresponding to constant potential)

$$\frac{d^2\varphi_2}{dx^2} + \frac{2m}{\hbar^2}[E - V_0]\varphi_2 = 0$$

$$\frac{d^2\varphi_2}{dx^2} - \frac{2m}{\hbar^2}[V_0 - E]\varphi_2 = 0 \quad (35)$$

$$\frac{d^2\varphi_2}{dx^2} - k_2^2\varphi_2 = 0 \quad (36)$$

where

$$k_2^2 = \sqrt{\frac{2m[V_0 - E]}{\hbar^2}} \quad (37)$$

The solution of Eqn. (36) is given by

$$\varphi_2 = B_1 e^{-k_2 x} + B_2 e^{+k_2 x} \quad (38)$$

as x tends toward infinity, $e^{k_2 x}$ becomes infinite; hence, it violates the boundary condition that wave function is finite everywhere. Therefore $e^{k_2 x}$ is neglected and eqn.38 is written as

$$\varphi_2 = B_1 e^{-k_2 x} \quad (39)$$

Before we could solve this equation, we have to use the boundary condition that the wave function and its derivative are continuous at boundary:

$$\text{i. e.} \quad \varphi_1 \Big|_{x=0} = \varphi_2 \Big|_{x=0} \quad (40a)$$

$$\frac{d\varphi_1}{dx} \Big|_{x=0} = \frac{d\varphi_2}{dx} \Big|_{x=0} \quad (40b)$$

Using Eqs (34), (39), and (40a),

$$A_1 + A_2 = B_1 \quad (41a)$$

Using Eqs (34), (39) and (40b),

$$ik_1 (A_1 - A_2) = -B_1 k_2$$

$$A_1 - A_2 = i \frac{k_2}{k_1} B_1 \quad (41b)$$

Adding Eqn. (41a) and (41b),

$$B_1 = \left(\frac{2i k_1 A_1}{ik_1 - k_2} \right) \quad (42)$$

From Eqs (41a) and (42),

$$A_2 = \left(\frac{i k_1 + k_2}{i k_1 - k_2} \right) A_1 \quad (43)$$

Substituting Eqs (42) and (43) in Eqs (34) and (39)

$$\varphi_1 = \underbrace{A_1 e^{ik_1 x}}_I + \underbrace{A_1 \left(\frac{i k_1 + k_2}{i k_1 - k_2} \right) e^{-ik_1 x}}_{II} \quad (44)$$

$$\varphi_2 = \frac{2i k_1 A_1}{ik_1 - k_2} e^{-k_2 x} \quad (45)$$

Equation (44) is interpreted as

$$\varphi_i = A_1 e^{ik_1 x} \rightarrow \text{incident wave part}$$

$$\varphi_r = A_1 \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] e^{-ik_1 x} \rightarrow \text{reflected wave part}$$

We can obtain reflection coefficient as obtained in previous section (Eqn. (27))

$$R = \frac{u_1 \varphi_r^* \varphi_r}{u_1 \varphi_i^* \varphi_i} \quad (\text{where } u_1 \text{ is velocity of particle in region 1})$$

$$R = \frac{A_1^* \left[\frac{-ik_1 + k_2}{-ik_1 - k_2} \right] e^{ik_1 x} A_1 \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] e^{-ik_1 x}}{A_1 e^{-ik_1 x} A_1^* e^{ik_1 x}}$$

$$R = 1 \quad (46)$$

If we compare Eqs (45) and (46), we will obtain that the probability of transmission is zero, although some wave function do exist in region 2. The region $x > 0$ is classically forbidden, but still the probability of finding a particle in $x > 0$ may persist.

4.3 Finite Potential Barrier (Tunnel Effect)

Figure 4.6 shows a barrier potential of width L and a particle of mass m with energy E is incident on the potential. The energy E of particle is small than the potential such that $E - V_0 < 0$. The potential here can be divided into three parts as follows:

$$V(x) = \begin{cases} = 0 & \text{for } x < 0 \rightarrow \text{region 1} \\ = V_0 & \text{for } 0 < x < L \rightarrow \text{region 2} \\ = 0 & \text{for } x > 0 \rightarrow \text{region 3} \end{cases}$$

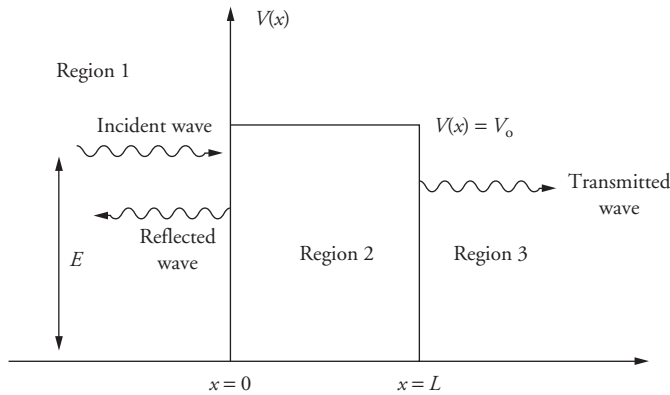


Figure 4.6 Finite potential barrier

The classical explanation states that the energy of particles is less than the potential V_0 . The particle moves freely in region 1, but as its energy is smaller than the potential V_0 , the particle is not able to cross the barrier potential and is reflected back at $x = 0$. We will use time-independent Schrödinger equation for quantum-mechanical treatment.

$$\frac{d^2 \varphi_1}{dx^2} + \frac{2m(E - V)}{\hbar^2} \varphi_1 = 0$$

For $x < 0$, in region 1, the potential $V(x) = 0$

$$\begin{aligned} \frac{d^2 \varphi_1}{dx^2} + \frac{2mE}{\hbar^2} \varphi_1 &= 0 \\ \frac{d^2 \varphi_1}{dx^2} + k_1^2 \varphi_1 &= 0 \end{aligned} \quad (47)$$

where

$$k_1^2 = \frac{2mE}{\hbar^2} \quad (48a)$$

The solution of Eqn. (47) is given as

$$\varphi_1 = A_1 e^{ik_1 x} + A_2 e^{-ik_1 x} \quad (48b)$$

A_1 and A_2 are arbitrary constants

$0 < x < L$, in region 2, the potential $V(x) = V_0$

$$\begin{aligned} \frac{d^2 \varphi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \varphi_2 &= 0 \\ \frac{d^2 \varphi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \varphi_2 &= 0 \\ \frac{d^2 \varphi_2}{dx^2} - k_2^2 \varphi_2 &= 0 \end{aligned} \quad (49)$$

where

$$k_2^2 = \left(\frac{2m}{\hbar^2} (V_0 - E) \right) \quad (50a)$$

General solution of Eqn. (49) is given by

$$\varphi_2 = B_1 e^{-k_2 x} + B_2 e^{+k_2 x} \quad (50b)$$

where B_1 and B_2 are arbitrary constants.

For $x > 0$, is region 3, the potential $V(x) = 0$

$$\begin{aligned} \frac{d^2 \varphi_3}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \varphi_3 &= 0 \\ \frac{d^2 \varphi_3}{dx^2} + \frac{2mE}{\hbar^2} \varphi_3 &= 0 \quad [\text{Using Eqn. 48(a)}] \\ \frac{d^2 \varphi_3}{dx^2} + k_1^2 \varphi_3 &= 0 \end{aligned} \quad (51)$$

The general solution of Eqn. (51) is given by

$$\varphi_3 = C_1 e^{ik_1 x} + C_2 e^{-ik_1 x} \quad (52)$$

where C_1 and C_2 are arbitrary constants. For region 3, there is no further potential barrier. Therefore, there is no possibility of the reflection, hence $C_2 e^{-ik_1 x}$ is zero. Therefore, Eqn. (52) turns out to be

$$\varphi_3 = C_1 e^{ik_1 x} \quad (53)$$

The boundary conditions that are used to solve these time-independent solutions is given by

$$\varphi_1 \Big|_{x=0} = \varphi_2 \Big|_{x=0} \quad (54a)$$

$$\varphi_2 \Big|_{x=L} = \varphi_3 \Big|_{x=L} \quad (54b)$$

$$\frac{d\varphi_1}{dx} \Big|_{x=0} = \frac{d\varphi_2}{dx} \Big|_{x=0} \quad (54c)$$

$$\left. \frac{d\varphi_2}{dx} \right|_{x=L} = \left. \frac{d\varphi_3}{dx} \right|_{x=L} \quad (54d)$$

Hence, the wave function and derivative of the wave function are continuous at the boundary using Eqs (48b), (50b), and (54a),

$$A_1 + A_2 = B_1 + B_2 \quad (55)$$

Using Eqs (50b), (53), and (54b),

$$B_1 e^{-k_2 L} + B_2 e^{k_2 L} = C_1 e^{ik_1 L} \quad (56)$$

Using Eqs (48b), (50b), and (54c),

$$ik_1 A_1 - ik_1 A_2 = -k_2 B_1 + k_2 B_2$$

$$A_1 - A_2 = \frac{ik_2}{k_1} (B_1 - B_2) \quad (57)$$

Using Eqs (50b), (53), and (54d),

$$-B_1 e^{-k_2 L} + B_2 e^{k_2 L} = \frac{ik_1}{k_2} C_1 e^{ik_1 L} \quad (58)$$

Adding Eqs (56) and (58),

$$B_2 = C_1 \frac{e^{ik_1 L}}{2} \left[1 + \frac{ik_1}{k_2} \right] e^{-k_2 L} \quad (59)$$

Subtracting Eqs (56) and (58),

$$B_1 = C_1 \frac{e^{ik_1 L}}{2} \left[1 + \frac{ik_1}{k_2} \right] e^{k_2 L} \quad (60)$$

Adding Eqs (59) and (60) and subtracting Eqs (59) and (60),

$$B_2 + B_1 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) - \frac{ik_1}{k_2} \sin h(k_2 L) \right] \quad (61)$$

$$\left[\text{where } \cos h(k_2 L) = \frac{e^{k_2 L} + e^{-k_2 L}}{2} \text{ and } \sin h(k_2 L) = \frac{e^{k_2 L} - e^{-k_2 L}}{2} \right]$$

$$B_2 - B_1 = C_1 e^{ik_1 L} \left[\sin h(k_2 L) - \frac{ik_1}{k_2} \cos h(k_2 L) \right] \quad (62)$$

Use Eqs (61) and (55),

$$A_1 + A_2 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) - \frac{ik_1}{k_2} \sin h(k_2 L) \right] \quad (63)$$

Use Eqs (62) and (57),

$$A_1 - A_2 = C_1 e^{ik_1 L} \left[\frac{ik_2}{k_1} \sin h(k_2 L) + \cos h(k_2 L) \right] \quad (64)$$

Adding Eqs (63) and (64) gives

$$A_1 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) + \frac{i}{2} \left[\frac{k_2}{k_1} - \frac{k_1}{k_2} \right] \sin h(k_2 L) \right] \quad (65)$$

and

$$A_2 = \frac{-iC_1 e^{ik_1 L}}{2} \left[\left(\frac{k_1}{k_2} - \frac{k_2}{k_1} \right) \sin h(k_2 L) \right] \quad (66)$$

From Eqs (48b) and (53),

$$A_1 e^{ik_1 x} = \text{incident wave} \quad - \quad \varphi_i$$

$$A_2 e^{-ik_1 x} = \text{reflected wave} \quad - \quad \varphi_r$$

$$C_1 e^{ik_1 x} = \text{transmitted wave} \quad - \quad \varphi_t$$

As defined in previous sections, reflection coefficient and transmission coefficient can be described as follows:

$$\text{Reflection coefficient, } R = \frac{\text{Reflected probability density current}}{\text{Incident probability density current}}$$

$$R = \frac{u_1 \varphi_r^* \varphi_r}{u_1 \varphi_i^* \varphi_i}$$

$$R = \frac{A_2 A_2^*}{A_1 A_1^*} \quad (67)$$

Using Eqs (65) and (66) in Eqn. (67),

$$R = \frac{(k_2^2 + k_1^2) \sin^2 h(k_2 L)}{4 \cos^2 h(k_2 L) + \left(\frac{k_2^2 - k_1^2}{k_1 k_2} \right) \sin^2 h(k_2 L)} \quad (68)$$

Equation (68) gives the probability of reflection of particle. To determine transmission coefficient,

$$T = \frac{\text{Transmitted probability density current}}{\text{Incident probability density current}}$$

$$T = \frac{u_3 \varphi_t^* \varphi_t}{u_1 \varphi_i^* \varphi_i} \quad (\text{as } u_3 = u_1)$$

$$T = \frac{C_1^* C_1}{A_1^* A_1} \quad (69)$$

Using Eqs (65) and (66) in Eqn. (69),

$$T = \frac{1}{\cos^2 h(k_2 L) + \left[\frac{k_2^2 - k_1^2}{2k_1 k_2} \right]^2 \sin^2 h(k_2 L)} \quad (70)$$

Substituting $\cos b^2(k_2L) = 1 + \sin b^2(k_2L)$ in (70)

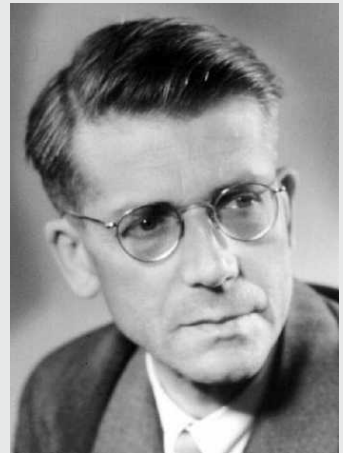
$$T = \frac{1}{1 + \left[\frac{k_2^2 + k_1^2}{2k_1k_2} \right]^2 \sin b^2(k_2L)} \quad (71)$$

Substituting Eqs (48a) and (50a) in Eqn. (71), the following result is obtained:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sin b^2 \sqrt{\frac{2m(V_0 - E)}{\hbar}} L} \quad (72)$$

Equation (72) shows that there is finite probability of penetration of particle into region 3 despite the fact that energy E of particle is less than V_0 . The probability of penetration of particle in region 3 decreases if the width of the barrier gets thicker. This is known as tunneling effect. The emission of α -particles from the nucleus is also an example of quantum mechanical tunneling. The kinetic energy of α -particles is very small compared with the potential wall of 25 MeV. The α -particles have to work and strike a lot with nuclear walls; but somehow, some of the α -particles may be able to tunnel out of nuclei.

F. Hund noticed the possibility of the tunneling phenomena in 1927 while calculating ground-state splitting for a double-well potential known as "barrier penetration." During 1927, L. Nordheim applied the Schrödinger equation for calculating reflection coefficient of an electron when it comes across different interfaces. He observed that even the electron with insufficient energy less than barrier was able to tunnel through the barrier. Hund observed the tunneling in bound state, whereas Nordheim studied tunneling between continuum states. R.W. Gurney, E.U. Condon, and George Gamow explained alpha decay of radioactive nuclei using the tunneling phenomenon. The very first application of tunneling was an atomic clock, which was one of the earliest atomic clocks. This atomic clock was based on the tunneling of the nitrogen atom back and forth across the energy barrier in an ammonia (NH₃) molecule. Scanning tunneling microscopy (STM) is the foremost application of tunneling. This technique accurately maps the surface and is used as a characterization technique for various materials because STM gives high-resolution images of a material.



F. HUND

4.4 Potential Well (Scattering and Bound State)

The potential well can be described by the following three different potential zones (Figure 4.7), that is,

$$\begin{aligned} &= 0 && \text{for } x < 0 && \text{region 1} \\ V(x) &= -V_0 && \text{for } 0 < x < L && \text{region 2} \\ &= 0 && \text{for } x > L && \text{region 3} \end{aligned}$$

4.4.1 Bound State

The depth of the potential is V_o . The particle is considered to be in bound state inside the potential well of depth V_o . The energy of particle is $E < V_o$. Ideally, $(E - V_o)$ cannot be negative. The particle with $E < 0$ cannot enter regions 1 and 2. Hence, the particle will keep on moving within the potential well with a constant speed. To explain the behavior of particle quantum mechanically, the Schrödinger wave equation is used as

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\phi = 0$$

In region $x < 0$, region 1 corresponds to zero potential

$$\frac{d^2\phi_1}{dx^2} + \frac{2m}{\hbar^2}E\phi_1 = 0$$

$E < 0$, hence $E = -|E| = -W$, which implies that particle is bound to well

$\left[\begin{array}{l} \text{Total energy} \\ = \text{KE} + \text{PE} \\ = \text{negative energy} \end{array} \right]$	Total energy
	= KE + PE
	= negative energy

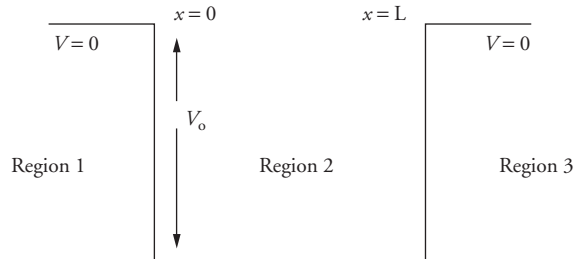


Figure 4.7 The states in potential well

$$\frac{d^2\phi_1}{dx^2} - \frac{2mW}{\hbar^2}\phi_1 = 0$$

$$\frac{d^2\phi_1}{dx^2} - k_1^2\phi_1 = 0 \quad (73)$$

where

$$k_1^2 = \frac{2mW}{\hbar^2} \quad (74)$$

The solution for Eqn. (73) is given by

$$\phi_1 = A_1e^{k_1x} + A_2e^{-k_1x} \quad (75)$$

as $x \rightarrow -\infty$, the term $A_2e^{-k_1x} \rightarrow \infty$; hence, this term is not valid and A_2 should be zero.

$$\text{Therefore } \phi_1 = A_1e^{k_1x} \quad (76)$$

For $0 < x < L$, the region 2, potential is $-V_0$

$$\frac{d^2\varphi_2}{dx^2} + \frac{2m}{\hbar^2}[E + V_0]\varphi_2 = 0$$

$$E = -W$$

$$\frac{d^2\varphi_2}{dx^2} + \frac{2m}{\hbar^2}[V_0 - W]\varphi_2 = 0$$

$$\frac{d^2\varphi_2}{dx^2} + k_2^2\varphi_2 = 0 \quad (77)$$

Here

$$k_2^2 = \frac{2m}{\hbar^2}[V_0 - W] \quad (78)$$

The solution for Eqn. (77) is

$$\varphi_2 = B_1 e^{ik_2 x} + B_2 e^{-ik_2 x} \quad (79)$$

where B_1 and B_2 are arbitrary constants. For $x > L$, the region 3, potential is zero:

$$\frac{d^2\varphi_3}{dx^2} + \frac{2m}{\hbar^2}E\varphi_3 = 0$$

$$\frac{d^2\varphi_3}{dx^2} - \frac{2mW}{\hbar^2}\varphi_3 = 0 \quad [\text{from Eqn. (74)}]$$

$$\frac{d^2\varphi_3}{dx^2} - k_1^2\varphi_3 = 0 \quad (80)$$

General solution of Eqn. (80) is given by

$$\varphi_3 = C_1 e^{k_1 x} + C_2 e^{-k_1 x} \quad (81)$$

As $x \rightarrow \infty$, $C_1 e^{k_1 x} \rightarrow \infty$. Therefore, $C_1 = 0$ and, Eqn. (81) can be written as

$$\varphi_3 = C_2 e^{-k_1 x} \quad (82)$$

To determine the constants, we need to use the following boundary conditions:

$$\varphi_1 \Big|_{x=0} = \varphi_2 \Big|_{x=0} \quad (83a)$$

$$\varphi_2 \Big|_{x=L} = \varphi_3 \Big|_{x=L} \quad (83b)$$

$$\frac{d\varphi_1}{dx} \Big|_{x=0} = \frac{d\varphi_2}{dx} \Big|_{x=0} \quad (83c)$$

$$\frac{d\varphi_2}{dx} \Big|_{x=L} = \frac{d\varphi_3}{dx} \Big|_{x=L} \quad (83d)$$

Hence, the wave functions and their derivation must be continuous at boundaries.

Using Eqs (76), (79), and (83a),

$$A_1 = B_1 + B_2 \quad (84)$$

Using Eqs (79), (82), and (83b),

$$B_1 e^{ik_2 L} + B_2 e^{-ik_2 L} = C_2 e^{-k_1 L} \quad (85)$$

Using Eqs (76), (79), and (83c),

$$B_1 - B_2 = -\frac{ik_1}{k_2} A_1 \quad (86)$$

Use Eqs (79), (82), and (83d),

$$B_1 e^{ik_2 L} - B_2 e^{-ik_2 L} = \frac{ik_1}{k_2} C_1 e^{-k_1 L} \quad (87)$$

Adding Eqs (85) and (87)

$$2B_1 e^{ik_2 L} = C_2 e^{-ik_1 L} \left[1 + \frac{ik_1}{k_2} \right] \quad (88)$$

Adding Eqs (84) and (86)

$$B_1 = \frac{A_1}{2} \left[1 - \frac{ik_1}{k_2} \right] \quad (89)$$

Subtracting Eqs (84) and (86)

$$B_2 = \frac{A_1}{2} \left[1 + \frac{ik_1}{k_2} \right] \quad (90)$$

Put Eqn. (89) in (88),

$$C_2 = \left[\frac{k_2 - ik_1}{k_2 + ik_1} \right] A_1 e^{ik_2 L} e^{k_1 L} \quad (91)$$

Subtracting Eqs (85) and (87), and substituting value of B_2 ,

$$C_2 = A_1 e^{-ik_2 L} \left[\frac{k_2 + ik_1}{k_2 - ik_1} \right] e^{k_1 L} \quad (92)$$

we obtain

Equations (91) and (92) are the same, i.e.

$$\left(\frac{k_2 - ik_1}{k_2 + ik_1} \right) A_1 e^{ik_2 L} e^{k_1 L} = A_1 e^{-ik_2 L} \left[\frac{k_2 + ik_1}{k_2 - ik_1} \right] e^{k_1 L}$$

$$2i(k_2^2 - k_1^2) \sin k_2 L = 4i k_1 k_2 \cos k_2 L$$

$$\tan k_2 L = \frac{2k_1 k_2}{k_2^2 - k_1^2} \quad (93)$$

$$2 \cot k_2 L = \frac{k_2^2 - k_1^2}{k_1 k_2}$$

$$2 \cot k_2 L = \frac{k_2}{k_1} - \frac{k_1}{k_2} \quad (94)$$

Substituting Eqs (74) and (78) in Eqn. (94),

$$2 \cot \left[\frac{2m}{\hbar^2} (V_0 - W) L^2 \right]^{1/2} = \left[\frac{2m}{\hbar^2} (V_0 - W) \right]^{1/2} - \left[\frac{2m}{\hbar^2} W \right]^{1/2} \quad (95)$$

Equation (95) is the transcendental equation, which means the argument of cotangent can determine W . For obtaining energy of particle, the graphical method is used.

Put
$$\beta = \left[\frac{2mV_0 L^2}{\hbar^2} \right]^{1/2} \text{ and } \gamma = \left[1 - \frac{W}{V_0} \right]^{1/2}$$

In Eqn. (95),

$$2 \cot(\beta\gamma) = \frac{\gamma}{\sqrt{1-\gamma^2}} - \frac{\sqrt{1-\gamma^2}}{\gamma}$$

$$2 \cot(\beta\gamma) = \frac{2\gamma^2 - 1}{\gamma\sqrt{1-\gamma^2}} \quad (96)$$

Put
$$\gamma = \cos \alpha / 2 \quad (97)$$

In Eqn. (96),

$$\cot(\beta\gamma) = \cot \alpha$$

$$\beta\gamma = \alpha + n\pi$$

$$\beta\gamma = n\pi + 2 \cos^{-1} \gamma \quad (98)$$

Solving Eqn. (98) requires two new parameters y and x , such that

$$y = \beta\gamma \text{ and } x = n\pi + 2 \cos^{-1} \gamma$$

Allowed values of γ can be obtained from the point of intersection as shown in Figure 4.8.

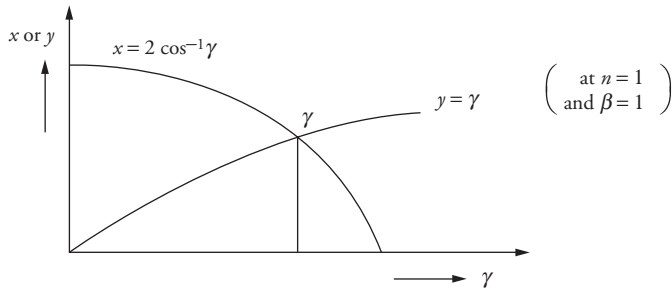


Figure 4.8 Variation of x or y vs γ

These obtained values of γ are then used in $\gamma = \left[1 - \frac{W}{V_0}\right]^{1/2}$, which gives energy values. Figure 4.8 demonstrates the values of γ for $n = 1$ and $\beta = 1$ and only one γ value is obtained. As n increases the energy values also increase. Hence, the particle in well may take discrete value of energies.

4.4.2 Scattered Case

If energy E of particle is greater than zero, then the Schrödinger equations are written as for $x < 0$. Region 1, potential $V(x) = 0$

$$\frac{d^2 \varphi_1}{dx^2} + k_1^2 \varphi_1 = 0 \quad (99)$$

$$\left[k_1^2 = \frac{2mE}{\hbar^2} \right]$$

with solution

$$\varphi_1 = A_1 e^{ik_1 x} + A_2 e^{-ik_1 x} \quad (100)$$

For $0 < x < L$, region 2, potential $V(x) = V_0$

$$\frac{d^2 \varphi_2}{dx^2} + k_2^2 \varphi_2 = 0 \quad (101)$$

$$\left[k_2^2 = \frac{2m(E + V_0)}{\hbar^2} \right]$$

with solution

$$\varphi_2 = B_1 e^{ik_2 x} + B_2 e^{-ik_2 x} \quad (102)$$

For $x > L$, region 3, potential $V(x) = 0$

$$\frac{d^2 \varphi_3}{dx^2} + k_1^2 \varphi_3 = 0 \quad (103)$$

with solution

$$\varphi_3 = C_1 e^{ik_1 x} + C_2 e^{-ik_1 x} \quad (104)$$

Applying the boundary conditions Eqn. 83(a)–(d),

$$A_1 + A_2 = B_1 + B_2 \quad (105a)$$

$$ik_1 (A_1 - A_2) = ik_2 (B_1 - B_2) \quad (105b)$$

$$B_1 e^{ik_2 L} + B_2 e^{-ik_2 L} = C_1 e^{ik_1 L} + C_2 e^{-ik_1 L} \quad (105c)$$

$$k_2 B_1 e^{ik_2 L} - k_2 B_2 e^{-ik_2 L} = k_1 C_1 e^{ik_1 L} - k_1 C_2 e^{-ik_1 L} \quad (105d)$$

For particle incident from left,

$$C_2 = 0$$

The transmission coefficient is obtained as Eqn. (71)

$$T = \left| \frac{C_1}{A_1} \right|^2$$

$$T = \frac{4k_1^2 k_2^2}{4k_1^2 K_2^2 + (k_1^2 - k_2^2) \sin^2 k_2 L} \quad (106)$$

[In this case $k_2 = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}}$ but in Eqn. (50a), it was $k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$]

From Eqn. (68), transmission coefficient can be obtained as

$$R = \left| \frac{A_2}{A_1} \right|^2 = \frac{(k_1^2 - k_2^2) \sin^2 k_2 L}{4k_1^2 k_2^2 + (k_1^2 - k_2^2) \sin^2 k_2 L} \quad (107)$$

From Eqn. (106), maximum T of 1 is obtained for

$$\sin k_2 L = \sin n\pi$$

$$k_2 = \frac{n\pi}{L} \text{ for and } T_{\max} = 1 \quad (108)$$

From Eqn. (106), minimum T is obtained for

$$\sin k_2 L = \sin \left((2n+1) \frac{\pi}{2} \right)$$

$$L = \frac{1}{k_2} \frac{(2n+1)\pi}{2} \quad (109)$$

The transmission increases with energy of incident particle.

4.5 Schrödinger Equation In Spherical Coordinates

Spherical coordinates helps in dealing the problem that involves spherical symmetric potential energy.

Let us write time independent Schrödinger equation for a partied mass, m :

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \varphi = 0 \quad (110)$$

Before solving this equation further, we need to obtain the relation between Cartesian coordinates and spherical coordinates.

Spherical systems have three mutually perpendicular coordinates as given below:

- (a) **Radial distance:** This distance is from origin to the observation point A, and it varies from 0 to ∞ .

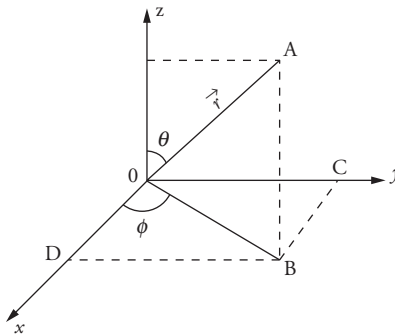


Figure 4.9 Relation between spherical and Cartesian coordinates.

- (b) **Azimuthal angle:** the angle between OB and OX is known as azimuthal angle (ϕ), and its value lie between 0 and 2π .
- (c) **Zenith angle:** the angle between OA and positive OZ is called zenith angle (θ). Its value varies between 0 and π .

All these coordinates are shown in Figure 4.9

The projection of r on x-y plane is given by

$$z = r \cos \theta \quad (111)$$

We obtain

$$x = r \sin \theta \cos \phi \quad (112)$$

and

$$y = r \sin \theta \sin \phi \quad (113)$$

Squaring and adding Eqs (111) through (113), we obtain

$$r^2 = x^2 + y^2 + z^2 \quad (114)$$

Dividing Eqn. (113) by Eqn. (112), we obtain

$$\tan \phi = \frac{y}{x} \quad (115)$$

From Eqn (112), we can write

$$\cos \theta = \frac{z}{r} \quad (116)$$

We have obtained the relations between spherical and Cartesian coordinate; therefore, we should obtain the partial derivative to be used in Eqn. (110). Hence, by chain rule we obtain

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial \varphi}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial \varphi}{\partial \phi} \frac{\partial \phi}{\partial x}$$

From Eqn. (114), we obtain

$$\frac{\partial r}{\partial x} = \frac{x}{r} \quad (117a)$$

Substituting Eqn. (112) in Eqn. (117a), we get

$$\frac{\partial r}{\partial x} = \sin \theta \cos \phi \quad (117b)$$

Similarly, we obtain

$$\frac{\partial \theta}{\partial x} = \frac{\cos \theta \cos \phi}{r} \quad (117c)$$

and

$$\frac{\partial \phi}{\partial x} = \frac{\sin \phi}{r \sin \theta} \quad (117e)$$

Substituting Eqs (117c) through (117e) in Eqn. (117a), we obtain

$$\frac{\partial \varphi}{\partial x} = \sin \theta \cos \phi \frac{\partial \varphi}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial \varphi}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial \varphi}{\partial \phi} \quad (118)$$

Similarly, we obtain other partial derivations as follows:

$$\frac{\partial \varphi}{\partial y} = \sin \theta \sin \phi \frac{\partial \varphi}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial \varphi}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial \varphi}{\partial \phi} \quad (119)$$

and

$$\frac{\partial \varphi}{\partial z} = \cos \theta \frac{\partial \varphi}{\partial r} - \frac{\sin \theta}{r} \frac{\partial \varphi}{\partial \theta}. \quad (120)$$

After performing differentiation on Eqs (118) through (120), we obtain

$$\frac{\partial^2 \varphi}{\partial x^2} = \sin \theta \cos \phi \frac{\partial}{\partial r} \left(\frac{\partial \varphi}{\partial x} \right) + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} \left(\frac{\partial \varphi}{\partial x} \right) - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \left[\frac{\partial \varphi}{\partial x} \right] \quad (121a)$$

$$\frac{\partial^2 \varphi}{\partial y^2} = \sin \theta \sin \phi \frac{\partial}{\partial r} \left(\frac{\partial \varphi}{\partial y} \right) + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} \left(\frac{\partial \varphi}{\partial y} \right) + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \left[\frac{\partial \varphi}{\partial y} \right] \quad (121b)$$

$$\frac{\partial^2 \varphi}{\partial z^2} = \cos^2 \theta \frac{\partial^2 \varphi}{\partial r^2} - \cos \theta \sin \theta \frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial \varphi}{\partial \theta} \right] - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(\cos \theta \frac{\partial \varphi}{\partial r} \right) + \frac{\sin \theta}{r^2} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \varphi}{\partial \theta} \right] \quad (121c)$$

Add Eqs (121a) through c, also use Eqs (118) through (120), we obtain

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = \frac{\partial^2 \varphi}{\partial r^2} + \frac{2}{r} \frac{\partial \varphi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{\cot \theta}{r^2} \frac{\partial \varphi}{\partial \theta} \quad (122)$$

Substituting Eqn. (122) in Eqn. (110), we obtain

$$\Rightarrow \frac{\partial^2 \varphi}{\partial r^2} + \frac{2}{r} \frac{\partial \varphi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{\cos \theta}{r^2} \frac{\partial \varphi}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \varphi = 0 \quad (123)$$

Rewriting Eqn. (123),

$$\Rightarrow \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial \varphi}{\partial r} \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \varphi}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \varphi = 0 \quad (124)$$

Equation 15 is regarded as the Schrödinger equation in spherical polar coordinates.

4.6 Schrödinger Equation for Spherical Symmetric Potential

The time-independent Schrödinger equation in spherical coordinates is

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial \varphi}{\partial r} \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \varphi}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \varphi = 0 \quad [\text{from Eqn. (124)}]$$

Where φ is $\varphi(r, \theta, \phi)$. As wavefunction φ is dependent on three polar coordinator (fig. (4.10)), equation (124) can be separated in the three independent equations:

$$\text{Let} \quad \varphi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Now

$$\frac{\partial \varphi}{\partial r} = \frac{\partial}{\partial r} [R\Theta\Phi] = \Theta\Phi \frac{\partial R}{\partial r} \quad (124a)$$

$$\frac{\partial \varphi}{\partial \theta} = \frac{\partial}{\partial \theta} [R\Theta\Phi] = R\Phi \frac{\partial \Theta}{\partial \theta} \quad (124b)$$

$$\frac{\partial \varphi}{\partial \phi} = \frac{\partial}{\partial \phi} [R\Theta\Phi] = R\Theta \frac{\partial \Phi}{\partial \phi} \quad (124c)$$

$$\frac{\partial^2 \varphi}{\partial \phi^2} = R\Theta \frac{\partial^2 \Phi}{\partial \phi^2} \quad (124d)$$

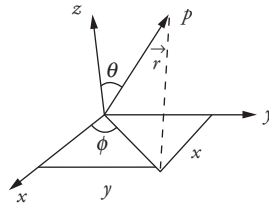


Figure 4.10 Spherical polar coordinates

Substituting Eqs (124a) and (124b) and (124d) in Eqn. (124)

$$\frac{\Theta\Phi}{r^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{R\Phi}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \frac{R\Theta}{r^2 \sin^2 \theta} \frac{d^2 \Phi}{d\phi^2} + \frac{2m(E - V)R\Theta\Phi}{\hbar^2} = 0 \quad (124c)$$

[Here all the partial derivatives are converted to perfect full derivations, because they are dependent on one variable only] Dividing Eqn. (124c) by $R\Theta\Phi$

$$\frac{1}{Rr^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{1}{\Theta r^2 \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{d^2 \Phi}{d\phi^2} + \frac{2m(E-V)}{\hbar^2} = 0 \quad (124d)$$

Multiply both sides by $r^2 \sin^2 \theta$ and rearrange terms

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \frac{2m}{\hbar^2} (E-V) r^2 \sin^2 \theta = \frac{-1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \quad (125a)$$

L.H.S. of Eqn. (125a) is a function of a r and θ where as R.H.S. is a function of ϕ . Put this equal to constant m_l^2 .

$$\frac{-1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m_l^2 \quad (125b)$$

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \frac{2m}{\hbar^2} (E-V) r^2 \sin^2 \theta = m_l^2 \quad (125c)$$

Let us solve Eqn. (125c). Divide (125c) by $\sin^2 \theta$

$$\begin{aligned} \frac{1}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \frac{2mr^2}{\hbar^2} [E-V] &= \frac{m_l^2}{\sin^2 \theta} \\ \frac{1}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{2m}{\hbar^2} r^2 [E-V] &= \frac{m_l^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] \end{aligned} \quad (125d)$$

The L.H.S. of Eqn. (125d) is a function of r and R.H.S. is a function of θ . Hence, put this equation equal to same constant $l(l+1)$

$$\frac{m_l^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] = l(l+1) \quad (125e)$$

$$\frac{1}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{2m}{\hbar^2} r^2 [E-V(r)] = l(l+1) \quad (125f)$$

[For spherical symmetric potential $V = V(r)$]

Rearrange Eqs (125b), (125c), and (125f), and we obtaine following set of equations:

$$\frac{d^2 \Phi}{d\phi^2} + m_l^2 \Phi = 0 \quad (126a)$$

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] + \left[l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right] \Theta = 0 \quad (126b)$$

$$\frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{2m}{\hbar^2} \left[E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right] R = 0 \quad (126c)$$

Hence, the Schrödinger equation is divided into three ordinary differential Eqs (126a), (126b), and (126c). Every equation is dependent on single variable. The solution of these equations gives the value of R , Θ , and Φ . Equations (126a) and (126b) yield the solutions for all cases with spherical symmetric potential.

4.6.1 Solutions of Φ Equation

Take Eqn. (126a)

$$\frac{d^2\Phi}{d\phi^2} + m_l^2\Phi = 0 \quad [\text{from Eqn. (126a)}]$$

It has solution of form $\Phi = Ce^{im_l\phi}$ (127a)

where C is a constant. As ϕ must be single valued, this means Φ should have one value at a given point in space. Hence, $\Phi(\phi)$ has same value at $\phi = 0$ and $\phi = 2\pi$.

$$\begin{aligned} \Phi(0) &= \Phi(2\pi) \\ Ce^{im_l \cdot 0} &= Ce^{im_l \cdot 2\pi} \\ e^{i2\pi m_l} &= 1 \\ \cos 2\pi m_l + i \sin 2\pi m_l &= 1 \end{aligned} \quad (127b)$$

Equating real part [as the imaginary part is 0]

$$\cos 2\pi m_l = 1$$

This condition is satisfied if $m_l = 0, \pm 1, \pm 2, \pm 3, \dots$ where m_l is the magnetic quantum number. As Φ depends on m_l^2 , from (127a)

$$\Phi_{m_l} = C_{m_l} e^{im_l\phi}$$

Normalizing Eqn. (127a) will field,

$$C_{m_l} = \frac{1}{\sqrt{2\pi}}$$

Hence

$$\Phi_{m_l} = \frac{1}{\sqrt{2\pi}} e^{im_l\phi} \quad [m_l = 0 \text{ means no rotation, positive } m_l \text{ corresponds to anticlockwise rotation where as negative } m_l \text{ represents clockwise rotation}] \quad (127c)$$

4.6.2 Solution of Θ Equation

For hydrogen atom, Eqn. (126b) represents Θ equation.

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left[\sin\theta \frac{d\Theta}{d\theta} \right] + \left[l(l+1) - \frac{m_l^2}{\sin^2\theta} \right] \Theta = 0 \quad [\text{from Eqn. (126b)}]$$

Let us introduce new constant x to solve schrodinger's equation such that

$$x = \cos\theta \quad (128a)$$

$$\frac{dx}{d\theta} = -\sin\theta \quad (128b)$$

$$\frac{d\Theta}{d\theta} = \frac{d\Theta}{dx} \frac{dx}{d\theta} = -\sin\theta \frac{d\Theta}{dx} \quad (128c)$$

Multiplying both sides of Eqn. (128c) by $\sin \theta$ to obtain

$$\sin \theta \frac{d\Theta}{d\theta} = -\sin^2 \theta \frac{d\Theta}{dx} \quad (128d)$$

Differentiating w.r.t. θ

$$\begin{aligned} \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] &= \frac{d}{d\theta} \left[-\sin^2 \theta \frac{d\Theta}{dx} \right] \\ \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] &= \frac{d}{d\theta} \left[(\cos^2 \theta - 1) \frac{d\Theta}{dx} \right] \\ \frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] &= \frac{d}{dx} \left[(\cos^2 \theta - 1) \frac{d\Theta}{dx} \right] \frac{dx}{d\theta} \end{aligned}$$

Use Eqs (128a) and (128b) in the above equations.

$$\frac{d}{d\theta} \left[\sin \theta \frac{d\Theta}{d\theta} \right] = -\sin \theta \frac{d}{dx} \left[(x^2 - 1) \frac{d\Theta}{dx} \right] \quad (128e)$$

Substitute Eqn. (128e) in Eqn. (126b)

$$\begin{aligned} \frac{-1}{\sin \theta} \sin \theta \frac{d}{dx} \left[(x^2 - 1) \frac{d\Theta}{dx} \right] + \left(l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right) \Theta &= 0 \quad [\text{using Eqn. (128a)}] \\ \frac{d}{dx} \left[(1 - x^2) \frac{d\Theta}{dx} \right] + \left(l(l+1) - \frac{m_l^2}{1 - x^2} \right) \Theta &= 0 \quad (129) \end{aligned}$$

Equation (129) represents associated Legendre's differential equation. The solution of Eqn. (129) is called associated Legendre's polynomials. Equation (129) clearly indicates that this equation depends on two quantum numbers l and m_l . The solutions are finite for all values of θ such that l should be an integer and $l \geq |m_l|$; $l = 0, 1, 2, 3, \dots$ and is called orbital quantum number.

The acceptable solutions are

$$\Theta_{lm_l} = B_{lm_l} P_l^{m_l}(\cos \theta) \quad (130)$$

where

$$B_{lm_l} = \left[\frac{(2l+1)(l+|m_l|)!}{2(l-|m_l|)!} \right]$$

and hence Eqn. (130) is

$$\Theta_{lm_l} = \sqrt{\frac{(2l+1)(l+|m_l|)!}{2(l-|m_l|)!}} P_l^{m_l}(\cos \theta) \quad (131)$$

$[P_l^{m_l}(\cos \theta)$ is associated Legendre function]

where l should have allowed values $l = |m_l|, |m_l| + 1, |m_l| + 2, \dots$

4.6.3 Solution of Radial Equation

Eqn. (126c) represents radial equation

$$\frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] - \frac{l(l+1)R}{r^2} + \frac{2m}{\hbar^2} [E - V(r)]R = 0 \quad \text{[from Eqn. (126c)]}$$

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left[-\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} [E - V(r)] \right] R = 0 \quad (132a)$$

For a hydrogen-like atoms $V(r) = \frac{-(Ze^2)}{r}$ where Z is atomic number. Substitute it in Eqn. (132a)

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left[-\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} E + \frac{2mZe^2}{\hbar^2 r} \right] R = 0 \quad (132b)$$

Let $E < 0$, so that electron is bound to the atom.

Put $\alpha^2 = \frac{-2mE}{\hbar^2}$ and $\gamma = \frac{mZe^2}{\hbar^2 \alpha}$ in Eqn. (118b)

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \left[-\frac{l(l+1)}{r^2} - \alpha^2 + \frac{2\gamma\alpha}{r} \right] R = 0 \quad (132c)$$

Let us now substitute β such that $\beta = 2\alpha r$

$$\frac{dR}{dr} = \frac{dR}{d\beta} \cdot \frac{\partial \beta}{\partial r} = 2\alpha \frac{\partial R}{\partial \beta} \quad (132d)$$

From Eqn. (132d),

$$\begin{aligned} \frac{d^2 R}{dr^2} &= \frac{d}{dr} \left[\frac{dR}{dr} \right] = \frac{d}{d\beta} \left[2\alpha \frac{dR}{d\beta} \right] \frac{d\beta}{dr} \\ \frac{d^2 R}{dr^2} &= 4\alpha^2 \frac{d^2 R}{d\beta^2} \end{aligned} \quad (132e)$$

Put Eqs (132d) and (132e) in Eqn. (132c) and dividing by

$$\frac{d^2 R}{d\beta^2} + \frac{2}{\beta} \frac{dR}{d\beta} + \left[-\frac{l(l+1)}{\beta^2} + \frac{\gamma}{\beta} - \frac{1}{4} \right] R = 0 \quad (132f)$$

The solution is
$$R = \sqrt{\left(\frac{2Z}{na_0} \right)^2 \frac{(n-l-1)!}{2n\{(n+l)!\}^3}} e^{-Zr/na_0} \left(\frac{2Zr}{na_0} \right) L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right) \quad (132g)$$

We will derive Eqn. (132g) in hydrogen-like atoms (See Section 4.6).

4.7 Hydrogen Atom

For hydrogen atom, the force between electron and proton is given by

$$F = \frac{e^2}{4\pi\epsilon_0 r^2}$$

And the potential energy corresponding to Coulomb's force is given by

$$V = -\frac{e^2}{4\pi\epsilon_0 r}$$

We will take into account radial part. We have derived Eqn. (132f) in the previous section

$$\frac{d^2 R}{d\beta^2} + \frac{2}{\beta} \frac{dR}{d\beta} + \left[-\frac{l(l+1)}{\beta^2} + \frac{\gamma}{\beta} - \frac{1}{4} \right] R = 0 \quad [\text{from Eqn. (132f)}]$$

Now, if $\beta \rightarrow \infty$, then Eqn. (132f) have asymptotic solutions where we neglect terms $\frac{1}{\beta^2}$ and $\frac{1}{\beta}$.

$$\frac{d^2 R(\beta)}{d\beta^2} - \frac{1}{4} R(\beta) = 0 \quad (132h)$$

The solution of the above equation is

$$R(\beta) = e^{+\beta/2} \text{ and } R(\beta) = e^{-\beta/2} \quad (133a)$$

As β may vary from 0 to ∞ , then $e^{\beta/2}$ will increase as β increases, leading to an unacceptable wave function $[R(\beta) = e^{\infty/2} = \infty]$. Hence, the solution is given by

$$R(\beta) = A(\beta) e^{-\beta/2} \quad (133b)$$

$A(\beta)$ is another function of variable β . Now, we will obtain recursion formula.

4.7.1 Recursion Formula

From Eqn. (133b),

$$R(\beta) = A(\beta) e^{-\beta/2}$$

Substitute it in Eqn. (132f)

$$A'' + \left\{ \frac{2}{\beta} - 1 \right\} A' + \left\{ \frac{-l(l+1)}{\beta^2} + \frac{\lambda}{\beta} - \frac{1}{\beta} \right\} A = 0 \quad (134a)$$

where $A' = \frac{dA}{d\beta}$ and $A'' = \frac{d^2 A}{d\beta^2}$

The solution of $A(\beta)$ can be written as

$$A(\beta) = \beta^S \rho(\beta) \quad (134b)$$

where $\rho(\beta)$ is a power series in β and can be written as

$$\rho(\beta) = a_0 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \cdots = \sum_{K=0}^{\infty} a_K \beta^K \quad (134c)$$

[$a_0 \neq 0$]

We obtain following result after differentiating (134b) written β

$$A'(\beta) = \beta^S \rho'(\beta) + S \beta^{S-1} \rho(\beta)$$

For simplicity

$$A' = \beta^S \rho' + S \beta^{S-1} \rho \quad (134d)$$

$$A'' = S(S-1)\beta^{S-2}\rho + 2S\beta^{S-1}\rho' + \beta^S \rho'' \quad (134e)$$

Substituting A , A' , and A'' in Eqn. (134a),

$$\begin{aligned} &\beta^{S+2}\rho'' + 2S\beta^{S+1}\rho' + S(S-1)\beta^S\rho + 2\beta^{S+1}\rho' + 2S\beta^S\rho - \beta^{S+2}\rho' \\ &- S\beta^{S+1}\rho + (\gamma-1)\beta^{S+1}\rho - l(l+1)\beta^S\rho = 0 \end{aligned} \quad (135a)$$

Divide Eqn. (121a) by β^S and then rearrange the terms, we obtain

$$\beta^2\rho'' + \beta[2(S+1)-\beta]\rho' + [\beta(\gamma-S-1) + S(S+1) - l(l+1)]\rho = 0 \quad (135b)$$

Put $\beta = 0$ in Eqn. (135b), and the following result is obtained

$$\begin{aligned} &\{S(S+1) - l(l+1)\}\rho = 0 \quad (\text{as } \rho = a_0) \\ &\{S(S+1) - l(l+1)\}a_0 = 0 \end{aligned} \quad (135c)$$

$$S = l \quad (\text{as } a_0 \neq 0) \quad (135d)$$

or

$$S = -(l+1) \quad (135e)$$

S should be equal to l to keep $R(\beta)$ finite, hence Eqn. (135b) becomes

$$\beta\rho'' + [2(l+1) - \beta]\rho' + (\gamma - l - 1)\rho = 0 \quad (136a)$$

Differentiating Eqn. (134c) w.r.t. β the following result is obtained.

$$\rho' = a_1 + 2a_2\beta + 3a_3\beta^2 + \cdots = \sum_{i=1}^{\infty} ia_i\beta^{i-1} \quad (136b)$$

$$\rho' = \sum_{i=0}^{\infty} a_{i+1}(i+1)\beta^i \quad (136c)$$

$$\begin{aligned} \rho'' &= 2a_2 + 6a_3\beta + 12a_4\beta^2 + \cdots = \sum_{i=2}^{\infty} a_i i(i-1)\beta^{i-2} \\ &= \sum_{i=0}^{\infty} a_{i+2}(i+1)(i+2)\beta^i \end{aligned} \quad (136d)$$

Put Eqs (134c), (136c), and (136d) in Eqn. (136a)

$$\sum_{i=0}^{\infty} a_{i+2} (i+1)(i+2)\beta^{i+1} + \{2(l+1) - \beta\} \sum_{i=0}^{\infty} a_{i+1} (i+1)\beta^i + \{\gamma - l - 1\} \sum_{i=0}^{\infty} a_i \beta^i = 0 \quad [i \text{ can be integer or zero}] \quad (137a)$$

$$\sum_{i=0}^{\infty} a_{i+2} (i+1)(i+2)\beta^{i+1} - \sum_{i=0}^{\infty} a_{i+1} (i+1)\beta^{i+1} + (2l+1) \sum_{i=0}^{\infty} a_{i+1} (i+1)\beta^i + (\gamma - l - 1) \sum_{i=0}^{\infty} a_i \beta^i = 0 \quad (137b)$$

The coefficient of powers of β must vanish to satisfy Eqn. (137b). Hence the coefficient of β^i should be equated to zero separately.

$$a_{i+1} i(i+1) - a_i i + (2l+1)a_{i+1}(i+1) + (\gamma - l - 1)a_i = 0 \quad (137c)$$

or
$$a_{i+1} \{(2l+2)(i+1) + i(i+1)\} + (\gamma - l - 1 - i)a_i = 0 \quad (137d)$$

$$a_{i+1} = \frac{i+1+l-\gamma}{(i+1)(2l+i+2)} a_i \quad (137e)$$

Equation (137e) is called recursion formula. For different values of γ and l , $A(\beta)$ consists of infinite series of terms. Hence, the wavefunction is not satisfactory. The series shows diverging behaviour, i.e. r increases as β increases. Hence, some restrictions should be introduced to find a satisfactory wavefunction.

4.7.2 Energy Values for the Hydrogen Atom

If we set $a_{i+1} = 0$, then from Eqn. (137e)

$$i+1+l-\gamma = 0 \quad [\text{The series will break after } \beta_k.]$$

$$\gamma = i+l+1 = n \quad (138a)$$

Here i is called radial quantum number and n is called the total quantum number that can have values 1, 2, 3, ...

Now

$$\begin{aligned} \gamma^2 &= \frac{m^2 Z^2 e^4}{\hbar^4 \alpha^2} = \frac{m^2 Z^2 e^4}{\hbar^4 \left[\frac{-2Em}{\hbar^2} \right]} \\ \gamma^2 &= \frac{m^2 Z^2 e^4}{-2Em\hbar^2} \\ E_n &= -\frac{mZ^2 e^4}{2\hbar^2 \gamma^2} \end{aligned} \quad (138b)$$

If $Z = 1$ for hydrogen atom,

$$E_n = -\frac{me^4}{2\hbar^2 \gamma^2} \quad (138c)$$

4.7.3 Radial Wave Function and Complete Wavefunction

Substitute $\gamma = n$ in Eqn. (136a)

$$\beta\rho'' + \{2(l+1) - \beta\}\rho' + (n-l-1)\rho = 0 \quad (138d)$$

Put $2l+1 = \sigma$ (138e)

and $n+l = N$ (138f)

Substituting Eqs (138e) and (138f) in Eqn. (138d), we obtain

$$\beta\rho'' + \{\sigma+1 - \beta\}\rho' + (N - \sigma)\rho = 0 \quad (139a)$$

The solution of this equation is given by Laguerre polynomial multiplied by a constant, that is,

$$\rho(\beta) = C_{nl} L_{n+l}^{2l+1}(\beta) \quad (139b)$$

The value of C_{nl} is obtained after normalization and laguerre polynomial is given by

$$L_{n+l}^{2l+1}(\beta) = \sum_{i=0}^{n-l-1} \frac{(-1)^{i+1} \{(n+l)!\}^2 \beta^i}{(n-l-1-i)! [2l+1+i]! i!} \quad (139c)$$

Thus, the total wave function can be given as follows:

$$R_{nl}(r) = e^{-\beta/2} \beta^l \rho(\beta) = C_{nl} e^{-\beta/2} \beta^l L_{n+l}^{2l+1}(\beta) \quad (139d)$$

The normalization condition is given by

$$\int_0^{\infty} R(r) R^*(r) r^2 dr = 1 \quad [r^2 \text{ converts the length } dr \text{ into volume.}] \quad (139e)$$

$$\begin{aligned} \beta &= 2\alpha r \\ &= \frac{2mZe^2 r}{\hbar^2 \gamma} \quad [\gamma = n \text{ from Eqn. (138a)}] \\ \beta &= \frac{2mZe^2 r}{\hbar^2 n} \end{aligned} \quad (140a)$$

$$\begin{aligned} \beta &= \frac{2r}{n} \frac{mZe^2}{\hbar^2} = \frac{2Zr}{n} \left[\frac{me^2 4\pi^2}{h^2} \right] \\ \beta &= \frac{2Zr}{n} \cdot \frac{1}{a_0} \end{aligned} \quad (140b)$$

where

$$a_0 = \frac{h^2}{4\pi^2 me^2} \quad (140c)$$

a_0 is known as Bohr's radius. Hence from Eqn. (140b), we obtain

$$r = \frac{\beta n a_0}{2Z} \quad (140d)$$

Differentiating Eqn. (140d), we obtain

$$dr = \frac{n a_0}{2Z} d\beta \quad (140e)$$

Substitute $R(r)$, $R^*(r)$, r , and dr in Eqn. (139e),

$$C_{nl}^2 \int_0^\infty e^{-\beta} \beta^{2l} \left[L_{n+l}^{2n+l}(\beta) \right]^2 \left[\frac{n a_0}{2Z} \beta \right]^2 \left[\frac{n a_0}{2Z} \right] d\beta = 1$$

That is,

After solving the above equation, the following result is obtained

$$C_{nl}^2 \left(\frac{n a_0}{2Z} \right)^3 \int_0^\infty e^{-\beta} \beta^{2l} \left[L_{n+l}^{2n+l}(\beta) \right]^2 \beta^2 d\beta = 1$$

$$C_{nl}^2 = \sqrt{\left(\frac{2Z}{n a_0} \right)^3 \frac{(n-l-1)!}{2n \{(n+l)!\}^3}} \quad (140f)$$

Put C_{nl} in Eqn. (139d),

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{n a_0} \right)^3 \frac{(n-l-1)!}{2n \{(n+l)!\}^3}} e^{-(Zr/n a_0)} \left(\frac{2Zr}{n a_0} \right)^l L_{n+l}^{2n+l} \left(\frac{2Zr}{n a_0} \right) \quad (141b)$$

The first two radial functions are

$$R_{10}(r) = \left(\frac{Z}{a_0} \right)^{3/2} 2 e^{-Zr/a_0}$$

and

$$R_{20}(r) = \left(\frac{Z}{2a_0} \right)^{3/2} \left(2 - \frac{Zr}{a_0} \right) e^{-Zr/a_0}$$

Similarly, we can obtain radial equations for different n and l values.

Hence, the complete wavefunction for hydrogen-like atom is given as follows:

$$\varphi_{nlm_l}(r, \theta, \phi) = R_{nl}(r) \Theta_{m_l l}(\theta) \Phi(\phi) \quad (142)$$

$$\begin{aligned} \varphi_{nlm_l}(r, \theta, \phi) = & \left[\sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^2}} \right] e^{-Zr/na_0} \left(\frac{2Zr}{na_0}\right)^l L_{n+l}^{2l+1}\left(\frac{2Zr}{na_0}\right) \\ & \times \sqrt{\frac{(l+1)(l-|m_l|)!}{2(l+|m_l|)!}} P_l^{m_l}(\cos\theta) \times \frac{1}{\sqrt{2\pi}} e^{im_l\phi} \end{aligned} \quad (143)$$

Equation (143) represents complete solution.

4.8 Spherical Harmonics

The product of Φ_{m_l} and Θ_{m_l} is known as spherical harmonic and the harmonic function is denoted by $Y_l^{m_l}(\theta, \phi)$

$$Y_l^{m_l}(\theta, \phi) = \Phi_{m_l} \Theta_{m_l} \quad (144a)$$

$$Y_l^{m_l}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} e^{im_l\phi} \sqrt{\frac{(2l+1)(l-m_l)!}{2(l+m_l)!}} P_l^{m_l}(\cos\theta) \quad (144b)$$

4.9 Three-Dimensional Harmonic Oscillator

4.9.1 In Rectangular Coordinates

A 3-D harmonic oscillator represents a particle experiencing force along x , y , and z axes such that

$$V(r) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 + \frac{1}{2}k_z z^2 \quad (145a)$$

where $-k_x x$, $-k_y y$, $-k_z z$ are the complete components of force along the x , y , and z axes, respectively. k_x, k_y, k_z are the force constants in respective directions. The SWE for this system is

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \frac{2m}{\hbar^2} [E - V(r)] \varphi = 0 \quad (145b)$$

Substitute Eqn. (145a) in Eqn. (145b)

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2}k_x x^2 - \frac{1}{2}k_y y^2 - \frac{1}{2}k_z z^2 \right] \varphi = 0 \quad (145c)$$

Put $\alpha = \frac{2mE}{\hbar^2}$, $\beta_x^2 = \frac{mk_x}{\hbar^2}$, $\beta_y^2 = \frac{mk_y}{\hbar^2}$, $\beta_z^2 = \frac{mk_z}{\hbar^2}$

Substitute $\alpha, \beta_x^2, \beta_y^2, \beta_z^2$ in Eqn. (145c)

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \left[\alpha - (\beta_x^2 x^2 + \beta_y^2 y^2 + \beta_z^2 z^2) \right] \varphi = 0 \quad (145d)$$

Let
$$\varphi(x, y, z) = X(x)Y(y)Z(z) \quad (146a)$$

From Eqn. (145a) and Eqn. (145d),

$$YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} + \left[\alpha - \left[\beta_x^2 x^2 + \beta_y^2 y^2 + \beta_z^2 z^2 \right] \right] XYZ = 0$$

Divide the above equation by XYZ and convert it into full derivative

$$\begin{aligned} \frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} + \left[\alpha - \left(\beta_x^2 x^2 + \beta_y^2 y^2 + \beta_z^2 z^2 \right) \right] &= 0 \\ \left[\frac{1}{X} \frac{d^2 X}{dx^2} - \beta_x^2 x^2 \right] + \left[\frac{1}{Y} \frac{d^2 Y}{dy^2} - \beta_y^2 y^2 \right] + \left[\frac{1}{Z} \frac{d^2 Z}{dz^2} - \beta_z^2 z^2 \right] + \alpha &= 0 \end{aligned} \quad (146b)$$

Function of x
Function of y
Function of z

The above condition is possible only when each factor is equal to a constant. such that the following conditions are satisfied:

$$\left[\frac{1}{X} \frac{d^2 X}{dx^2} - \beta_x^2 x^2 \right] + \alpha_x = 0 \quad (146c)$$

$$\left[\frac{1}{Y} \frac{d^2 Y}{dy^2} - \beta_y^2 y^2 \right] + \alpha_y = 0 \quad (146d)$$

$$\left[\frac{1}{Z} \frac{d^2 Z}{dz^2} - \beta_z^2 z^2 \right] + \alpha_z = 0 \quad (146e)$$

where
$$\alpha = \alpha_x + \alpha_y + \alpha_z \quad (146f)$$

Rearranging Eqs (146c) through (146e), we obtain

$$\frac{d^2 X}{dx^2} + \left(\alpha_x - \beta_x^2 x^2 \right) X = 0 \quad (147a)$$

$$\frac{d^2 Y}{dy^2} + \left(\alpha_y - \beta_y^2 y^2 \right) Y = 0 \quad (147b)$$

$$\frac{d^2 Z}{dz^2} + \left(\alpha_z - \beta_z^2 z^2 \right) Z = 0 \quad (147c)$$

The eigenvalues and eigenfunctions are listed below for Eqs (147a) through (147c)

For Eqn. (147a)

$$E_x = \left(n_x + \frac{1}{2} \right) \hbar w_x \quad (148a)$$

$$X(x) = A_{n_x} \exp \left[\frac{-\beta_x x^2}{2} \right] H_{n_x} \left\{ \sqrt{\beta_x} x \right\} \quad (148b)$$

For Eqn. (147b),

$$E_y = \left(n_y + \frac{1}{2} \right) \hbar \omega_y \quad (149a)$$

$$Y(y) = A_{n_y} \exp \left[\frac{-\beta_y y^2}{2} \right] H_{n_y} \left\{ \sqrt{\beta_y} y \right\} \quad (149b)$$

For Eqn. (147c),

$$E_z = \left(n_z + \frac{1}{2} \right) \hbar \omega_z \quad (150a)$$

$$Z(z) = A_{n_z} \exp \left[\frac{-\beta_z z^2}{2} \right] H_{n_z} \left\{ \sqrt{\beta_z} z \right\} \quad (150b)$$

Complete wave function can be given by

$$\begin{aligned} \varphi_{n_x, n_y, n_z} &= A_{n_x} A_{n_y} A_{n_z} \exp \left[-\frac{1}{2} \left[\beta_x x^2 + \beta_y y^2 + \beta_z z^2 \right] \right] \\ &H_{n_x} \left(\sqrt{\beta_x} x \right) H_{n_y} \left(\sqrt{\beta_y} y \right) H_{n_z} \left(\sqrt{\beta_z} z \right) \end{aligned} \quad (151)$$

where the normalizing factor has the value

$$A_{n_x} A_{n_y} A_{n_z} = \left[\frac{\sqrt{\beta_x} \sqrt{\beta_y} \sqrt{\beta_z}}{\left(n_x + n_y + n_z \right)^{3/2} 2^{(n_x + n_y + n_z)} (n_x!) (n_y!) (n_z!)} \right]^{1/2} \quad (152)$$

The energy of 3-D harmonic oscillator is given by

$$E_{n_x, n_y, n_z} = \hbar \left(n_x + \frac{1}{2} \right) \omega_x + \hbar \left[n_y + \frac{1}{2} \right] \omega_y + \hbar \left[n_z + \frac{1}{2} \right] \omega_z \quad (153a)$$

For the isotropic oscillator, $\omega_x = \omega_y = \omega_z$ and $\beta_x = \beta_y = \beta_z$.

Hence, from Eqn. (153a)

$$\begin{aligned} E &= \left(n_x + n_y + n_z + \frac{3}{2} \right) \hbar \omega \\ E &= \left(n + \frac{3}{2} \right) \hbar \omega \end{aligned} \quad (153b)$$

where $n = n_x + n_y + n_z$ is the total quantum number. The n_x , n_y and n_z must satisfy eqn (153b)

The energy for the system depends on the sum of the quantum numbers, therefore all the energy levels for the isotropic oscillator, are degenerate and the degree of degeneracy is given by $\frac{1}{2}(n+1)(n+2)$. The energy levels and degree of degeneracy for 3-D isotropic harmonic oscillator are shown in Figure 4.11.

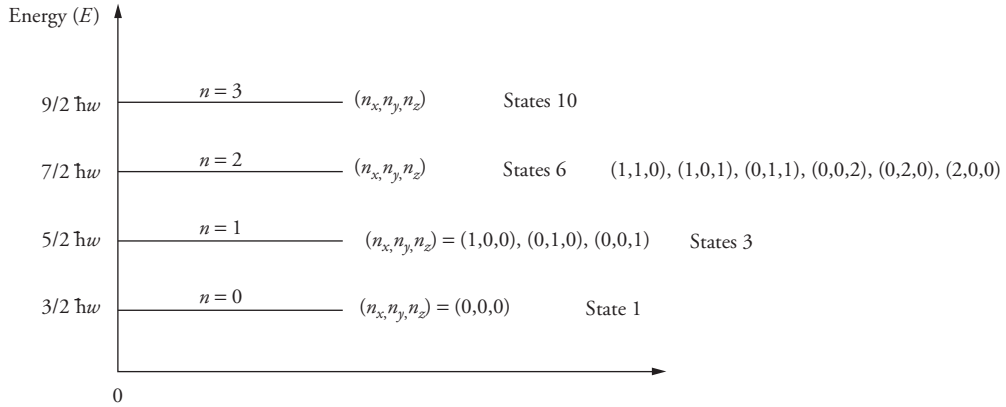


Figure 4.11 Energy-level diagram for 3-D oscillator

4.9.2 In Spherical Coordinates

In spherical coordinates, the time independent SWE is given by

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \varphi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \varphi}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2 \varphi}{\partial \phi^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} kr^2 \right) \varphi = 0 \quad (154)$$

for $V(r) = (1/2) kr^2$

The solution of Eqn. (154) is given by (in terms of spherical harmonics)

$$\varphi(r, \theta, \phi) = R_{nl}(r) Y_l^{m_l}(\theta, \phi) \quad (155a)$$

From Eqn. (132a), the radial equation is given by (in terms of spherical harmonics)

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} kr^2 \right] R - \frac{l(l+1)}{r^2} R = 0 \quad (155b)$$

The solution for Eqn. (155b) is given as

$$R = \exp \left[-\frac{r^2}{2} \right] A(r) \quad (155c)$$

$$\frac{dR}{dr} = -r \exp \left[-\frac{r^2}{2} \right] A(r) + \exp \left[-\frac{r^2}{2} \right] A'(r) \quad (155d)$$

$$\begin{aligned} \frac{d^2 R}{dr^2} &= -\exp \left[-\frac{r^2}{2} \right] A(r) + r^2 \exp \left[-\frac{r^2}{2} \right] A(r) \\ &\quad - r \exp \left[-\frac{r^2}{2} \right] A'(r) + \exp \left[-\frac{r^2}{2} \right] A''(r) - r \exp \left[-\frac{r^2}{2} \right] A'(r) \\ \Rightarrow \frac{d^2 R}{dr^2} &= \exp \left[-\frac{r^2}{2} \right] A'' - 2r \exp \left[-\frac{r^2}{2} \right] A'(r) + (r^2 - 1) \exp \left[-\frac{r^2}{2} \right] A(r) \end{aligned} \quad (156a)$$

Put $R, \frac{dR}{dr}, \frac{d^2R}{dr^2}$ in Eqn. (155b), and we will obtain

$$\begin{aligned} A''(r) \exp\left[-\frac{r^2}{2}\right] - 2r \exp\left[-\frac{r^2}{2}\right] A'(r) + (r^2 - 1) \exp\left[-\frac{r^2}{2}\right] A(r) - 2 \exp\left[-\frac{r^2}{2}\right] A(r) \\ + \frac{2}{r} \exp\left[-\frac{r^2}{2}\right] A'(r) + \frac{2m}{\hbar^2} \left[E - \frac{1}{2}kr^2\right] \exp\left[-\frac{r^2}{2}\right] A(r) \\ - \frac{l(l+1)}{r^2} \exp\left[-\frac{r^2}{2}\right] A(r) = 0 \end{aligned} \quad (156b)$$

$$\begin{aligned} A''(r) - 2r A'(r) + (r^2 - 1) A(r) - 2A(r) + \frac{2}{r} A'(r) + \frac{2m}{\hbar^2} \left[E - \frac{1}{2}kr^2\right] A(r) - \frac{l(l+1)}{r^2} A(r) = 0 \\ A''(r) + \left(\frac{2}{r} - 2r\right) A'(r) + \left[r^2 - 3 + \frac{2m}{\hbar^2} \left(E - \frac{1}{2}kr^2\right) - \frac{l(l+1)}{r^2}\right] A(r) = 0 \end{aligned} \quad (156c)$$

$$\text{Put } \frac{2mE}{\hbar^2} = \alpha \text{ and } \frac{mk}{\hbar^2} = 1 \quad (156d)$$

Eqn. (156c) becomes

$$\begin{aligned} A''(r) + \left[\frac{2}{r} - 2r\right] A'(r) + \left[r^2 - 3 + \alpha - r^2 - \frac{l(l+1)}{r^2}\right] A(r) = 0 \\ A''(r) + \left[\frac{2}{r} - 2r\right] A'(r) + \left[\alpha - 3 - \frac{l(l+1)}{r^2}\right] A(r) = 0 \end{aligned} \quad (157a)$$

As done in Eqs (134c), (136c), and (136d) by power series, we will proceed

$$\begin{aligned} A(r) = r^S \Delta(r) \\ \Delta(r) = \sum a_U r^U \quad \Rightarrow \quad A(r) = \sum a_U r^{S+U} \end{aligned} \quad (157b)$$

$$A'(r) = \sum a_U (U + S) r^{S+U-1} \quad (157c)$$

$$A''(r) = \sum a_U (S + U)(S + U - 1) r^{S+U-2} \quad (157d)$$

Put Eqs (157b), (157c), and (157d) in Eqn. (157a)

$$\begin{aligned} \sum a_U (S + U)(S + U - 1) r^{S+U-2} + \left[\frac{2}{r} - 2r\right] \sum a_U (S + U) r^{S+U-1} \\ + \left[\alpha - 3 - \frac{l(l+1)}{r^2}\right] \sum a_U r^{S+U} = 0 \\ \sum a_U (S + U)(S + U - 1) r^{S+U-2} + 2 \sum a_U (S + U) r^{S+U-2} - 2 \sum a_U (S + U) r^{S+U} \\ + (\alpha - 3) \sum a_U r^{S+U} - l(l+1) \sum a_U r^{S+U-2} = 0 \end{aligned} \quad (158)$$

Comparing the coefficient of r^{S-2} , (put $U = 0$), we obtain

$$\begin{aligned} [S(S-1) + 2S - l(l+1)]a_U &= 0 \\ S(S-1) + 2S - l(l+1) &= 0 \\ S^2 - S + 2S - l^2 - l &= 0 \\ S^2 + S &= l(l+1) \\ S(S+1) &= l(l+1) \\ S &= l \text{ or } S = -(l+1) \end{aligned} \quad (159a)$$

Again comparing the coefficients of r^{S+U} on both the sides of Eqn. (158),

$$\begin{aligned} (S+U+2)(S+U+1) - l(l+1) + 2(S+U+2)a_{U+2} + [\alpha - 3 - 2(S+U)]a_U &= 0 \\ a_{U+2} &= \frac{(2(S+U) + 3 - \alpha)a_U}{(S+U+2)(S+U+1) - l(l+1) + 2(S+U+2)} \end{aligned} \quad (159b)$$

Eqn. (159b) is known as recurrence relation. The condition $a_{U+2} = 0$ should be satisfied for acceptable solution:

$$\begin{aligned} 2(S+U) + 3 - \alpha &= 0 \\ \alpha &= 2S + 2U + 3 \end{aligned} \quad (159c)$$

$$\text{From } \alpha = \frac{2mE}{\hbar^2} = 2S + 2U + 3$$

$$\Rightarrow E = \frac{\hbar^2}{2m}(2S + 2U + 3) = \frac{\hbar^2}{m} \left[S + U + \frac{3}{2} \right]$$

$$\left[\begin{array}{l} as \frac{mk}{\hbar^2} = 1 \\ \frac{\hbar^2}{m} = k \end{array} \right]$$

$$\text{or } E = \hbar w \left[N + \frac{3}{2} \right] \quad (160a)$$

The energy eigenvalues are obtained exactly in correlation with rectangular coordinates

$$\varphi_{nlm_l} = C_{n_l} e^{-r^2/l^2} R_{n_l}(r) Y_l^{m_l}(\theta, \phi) \quad (160b)$$

where C_{n_l} is a normalization constant.

SUMMARY

Chapter 3 provided an insight of matterwaves, as well as time dependent/independent Schrödinger wave equations. This chapter gives a description of behavior of Schrödinger equations under different potentials. Under the potential effects, the Schrödinger equation has been given classical and quantum-mechanical treatment. The wave function of a particle has been described in one-dimensional infinite potential well. Ideally, the minimum energy of a particle is zero. Inside the box, the particle can take any value. But quantum-mechanically there is always some minimum value of energy that is not zero. This value of energy is known as zero-point energy and is given by $\pi^2 \hbar^2 / 2mL^2$. Under the steppotential, the energy E of a particle may be more than the potential barrier height or can be less than barrier height. For a finite potential barrier, there is tunnel

effect. Ideally, the particle with energy E less than barrier height cannot penetrate the barrier. Quantum-mechanically there is always a finite probability of penetration of particle into the barrier region. This effect is known as tunneling effect. Potential has been described for scattered and bound state. Hydrogen value problem has been described using radial, azimuthal, and angular wave function. The analysis of 3-D Harmonic oscillator has also been discussed. The hydrogen value solution has been obtained using separation of variables in polar coordinates.

SOLVED PROBLEMS

Q.1: Obtain the lowest energy for an electron in one-dimensional force free region of width 6 \AA .

Ans: Energy $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$

For lowest energy, $n = 1$

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad \left[\begin{array}{l} L = 6 \times 10^{-10} \text{ m} \\ m = 9.1 \times 10^{-31} \text{ kg} \end{array} \right]$$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (6 \times 10^{-10})^2}$$

$$E_1 = \frac{43.96 \times 10^{-68}}{2620.8 \times 10^{-31} \times 10^{-20}}$$

$$E_1 = \frac{43.96 \times 10^{-68} \times 10^{51}}{2620.8}$$

$$E_1 = 0.01677 \times 10^{-17}$$

$$E_1 = 1.677 \times 10^{-19} \text{ J}$$

Q.2: Find out the energy of an electron having wavelength 2 \AA for $n = 4$.

Ans: $E_n = \frac{n^2 h^2}{8mL^2}$

$$E_4 = \frac{(4)^2 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2 \times 10^{-10})^2}$$

$$E_4 = \frac{16 \times 43.96 \times 10^{-68}}{291.2 \times 10^{-31} \times 10^{-20}}$$

$$E_1 = \frac{703.36 \times 10^{-68}}{291.2 \times 10^{-51}}$$

$$E_4 = 2.415 \times 10^{-17} \text{ J}$$

Q.3: Obtain the momentum of an electron having wavelength 5 \AA for $n = 3$.

Ans:
$$E_n = \frac{p_n^2}{2m}$$

$$p_n^2 = 2m E_n$$

$$p_n^2 = \frac{2m n^2 h^2}{8mL^2}$$

$$p_n^2 = \frac{n^2 h^2}{4L^2}$$

$$p_n = \frac{nh}{4L}$$

Here, $L = 5 \times 10^{-10} \text{ m}$ and $n = 3$

$$p_n = \frac{3 \times 6.63 \times 10^{-34}}{4 \times 5 \times 10^{-10}}$$

$$p_n = 0.994 \times 10^{-24}$$

$$p_n = 9.94 \times 10^{-25} \text{ kg m/s}$$

Q.4: A particle of mass 10^{-4} kg and speed 10^{-5} m/s inside a cubical box of dimension 10^{-6} m . If, it is one-dimensional square-well potential, obtain the value of n .

Ans: Energy
$$E_n = \frac{n^2 h^2}{8mL^2}$$

Also the kinetic energy
$$= \frac{1}{2} mv^2$$

$$\frac{1}{2} mv^2 = \frac{n^2 h^2}{8mL^2}$$

$$n^2 = \frac{1}{2} mv^2 \frac{(8mL^2)}{h^2}$$

$$n^2 = \frac{4m^2 v^2 L^2}{h^2}$$

$$n = \frac{2mvL}{h}$$

Here, $v = 10^{-5}$ m/s, $L = 10^{-6}$ m, $m = 10^{-4}$ kg

$$n = \frac{2 \times 10^{-4} \times 10^{-5} \times 10^{-6}}{6.63 \times 10^{-34}}$$

$$n = \frac{2 \times 10^{-15} \times 10^{34}}{6.63}$$

$$n = 0.301 \times 10^{19}$$

$$n = 3.01 \times 10^{18}$$

$$n = 3 \times 10^{18}$$

Q.5 For one-dimensional rigid box, obtain the expectation value for kinetic energy in n th quantum state.

Ans: The wavefunction is given by the following expression:

$$\varphi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Expectation value is

$$\langle E \rangle = \int_{-\infty}^{\infty} \varphi^* E \varphi dx$$

$$\langle E \rangle = \int_{-\infty}^{\infty} \varphi^* \frac{p^2}{2m} \varphi dx$$

$$\langle E \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} \varphi^* (-i\hbar)^2 \frac{\partial^2}{\partial x^2} \varphi dx$$

$$\langle E \rangle = \frac{-1}{2m} \int_{-\infty}^{\infty} \varphi^* \hbar^2 \frac{\partial^2 \varphi}{\partial x^2} dx$$

$$\langle E \rangle = \frac{-\hbar^2}{2m} \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \frac{\partial^2}{\partial x^2} \left[\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \right] dx$$

$$\langle E \rangle = \frac{\hbar^2}{mL} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \left(\frac{+n^2 \pi^2}{L^2} \right) \sin\left(\frac{n\pi x}{L}\right) dx$$

$$\langle E \rangle = \frac{n^2 \pi^2 \hbar^2}{mL^3} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$\langle E \rangle = \frac{n^2 \pi^2 \hbar^2}{mL^3} \left[\int_0^L \frac{1}{2} dx - \int_0^L \frac{1}{2} \cos \frac{2n\pi x}{L} dx \right]$$

$$\langle E \rangle = \frac{n^2 \pi^2 \hbar^2 L}{2mL^3}$$

$$\langle E \rangle = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

Q.6: Obtain the expectation value of particle in ground state when the particle is confined inside the infinite square-potential well.

Ans:
$$\varphi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

For ground state, $n = 1$

$$\varphi = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \varphi^* p \varphi dx$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \left(-i\hbar \frac{\partial}{\partial x}\right) \varphi dx$$

$$\langle p \rangle = (-i\hbar) \int_0^L \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right) \left(\frac{\pi}{L}\right) dx$$

$$\langle p \rangle = \frac{-i\hbar 2}{L} \left(\frac{\pi}{L}\right) \int_0^L \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right) dx$$

$$\langle p \rangle = \frac{-i\pi\hbar}{L^2} \int_0^L \sin\left(\frac{2\pi x}{L}\right) dx$$

$$\langle p \rangle = \frac{-i\hbar\pi}{L^2} \left(\frac{L}{2\pi}\right) \left[\cos \frac{2\pi x}{L}\right]_0^L$$

$$\langle p \rangle = \frac{-i\hbar}{2L} [\cos 2\pi - \cos 0]$$

$$\langle p \rangle = 0$$

Q.7: Obtain the barrier penetration factor for electrons through a barrier of thickness 3 \AA , width of 15 eV , and the given the kinetic energy of electrons is 10 eV .

Ans: The barrier penetration factor is given by the following equation:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sin^2 b^2 \frac{\sqrt{2m(V_0 - E)}L}{\hbar}} \quad (\text{a})$$

Here, $V_0 = 15 \text{ eV}$, $E = 10 \text{ eV}$, $L = 3 \times 10^{-10} \text{ m}$

Here,

$$\begin{aligned} \frac{V_0^2}{4E(V_0 - E)} &= \frac{(15 \times 1.6 \times 10^{-19})^2}{4 \times 10 \times 1.6 \times 10^{-19} \times 5 \times 1.6 \times 10^{-19}} \\ &= \frac{576 \times 10^{-38}}{512 \times 10^{-38}} = 1.125 \end{aligned}$$

And

$$\begin{aligned} \frac{\sqrt{2m(V_0 - E)}L}{\hbar} &= \frac{\sqrt{2 \times 9.1 \times 10^{-31} \times 5 \times 1.6 \times 10^{-19}}}{1.055 \times 10^{-34}} \times 3 \times 10^{-10} \\ &= \frac{\sqrt{145.6 \times 10^{-50}}}{1.055 \times 10^{-34}} \times 3 \times 10^{-10} \\ &= \frac{12.06 \times 10^{-25} \times 3 \times 10^{-10}}{1.055 \times 10^{-34}} \\ &= \frac{36.18 \times 10^{-35}}{1.055 \times 10^{-34}} = 34.29 \times 10^{-1} \\ &= 3.429 \end{aligned}$$

$$\sin b(3.429) = 15.406$$

Substituting all the values in Eqn. (a)

$$T = \frac{1}{1 + 1.125(15.406)^2}$$

$$T = \frac{1}{238.344} = 4.195 \times 10^{-3}$$

Q.8: The transmission probability is given by 60 percent, what should be the ratio $\frac{E}{V_0}$ which is required for a one-dimensional step potential?

Ans: $T = 60\% = \frac{60}{100} = \frac{3}{5}$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad (\text{a})$$

$$k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \quad (\text{b})$$

$$\text{Put } T = \frac{3}{5}$$

$$\frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{3}{5}$$

$$3(k_1^2 + k_2^2 + 2k_1k_2) = 20k_1k_2$$

$$3k_1^2 + 3k_2^2 = 14k_1k_2 \quad (\text{c})$$

Substitute Eqs (a) and (b) in Eqn. (c)

$$3\left(\frac{2mE}{\hbar^2}\right) + 3\left(\frac{2m(E - V_0)}{\hbar^2}\right) = 14\left(\frac{2mE}{\hbar^2}\right)^{1/2}\left(\frac{2m(E - V_0)}{\hbar^2}\right)^{1/2}$$

$$\frac{6mE}{\hbar^2} + \frac{6m(E - V_0)}{\hbar^2} = 14\left(\frac{2mE}{\hbar^2}\right)\left(1 - \frac{V_0}{E}\right)^{1/2}$$

$$\frac{6mE}{\hbar^2} + \frac{6mE}{\hbar^2}\left[1 - \frac{V_0}{E}\right] = 14\left(\frac{2mE}{\hbar^2}\right)\left(1 - \frac{V_0}{E}\right)^{1/2}$$

$$3 + 3\left[1 - \frac{V_0}{E}\right] = 14\left[1 - \frac{V_0}{E}\right]^{1/2}$$

Squaring both sides,

$$9 + 9\left(1 - \frac{V_0}{E}\right)^2 + 18\left[1 - \frac{V_0}{E}\right] = 196\left[1 - \frac{V_0}{E}\right]$$

$$9 + 9\left[1 - \frac{V_0}{E}\right]^2 = 178\left[1 - \frac{V_0}{E}\right]$$

$$9 + 9\left[1 + \frac{V_0^2}{E^2} - \frac{2V_0}{E}\right] = 178 - 178\frac{V_0}{E}$$

$$9\frac{V_0^2}{E^2} - 18\frac{V_0}{E} + 18 + 178\frac{V_0}{E} - 178 = 0$$

$$9\frac{V_0^2}{E^2} + 160\frac{V_0}{E} - 160 = 0$$

The roots of $\frac{V_0}{E}$ are given by the following equation:

$$\frac{V_o}{E} = \frac{-160 + \sqrt{(160)^2 + 4(9)(160)}}{18}$$

$$\frac{V_o}{E} = \frac{-160 + \sqrt{31360}}{18}$$

$$\frac{V_o}{E} = \frac{-160 + 177.087}{18} = 0.949$$

Similarly, the second root for $\frac{V_o}{E}$ is

$$\frac{V_o}{E} = \frac{-160 - 177.087}{18} = -18.727$$

Negative value of $\frac{V_o}{E}$ are not possible. Hence,

$$\frac{V_o}{E} = 0.949$$

$$\frac{E}{V_o} = \frac{1}{0.949} = 1.054$$

Q.9: Obtain the condition when particle travels through barrier without any reflection.

Ans:

$$T = \frac{1}{1 + \frac{V_o^2}{4E(V_o - E)} \sin^2 b^2 \frac{\sqrt{2m(V_o - E)}}{\hbar} L}$$

For no reflection to occur, $T = 1$

$$\frac{1}{1 + \frac{V_o^2}{4E(V_o - E)} \sin^2 b^2 k_2 L} = 1$$

$$\frac{V_o^2}{4E(V_o - E)} \sin^2 b^2 k_2 L = 0$$

From the above equation,

$$\frac{V_o^2}{4E(V_o - E)} \neq 0$$

Hence,

$$\sin b^2 k_2 L = 0$$

$$k_2 L = n\pi$$

$$L = \frac{n\pi}{k_2}$$

(a)

In addition, the propagation constant is related to de-Broglie wavelength as follows:

$$k_2 = \frac{2\pi}{\lambda_2} \quad (\lambda_2 \text{ is de-Broglie wavelength}) \quad (b)$$

Hence,
$$L = \frac{n\pi}{2\pi/\lambda_2} = \frac{n\lambda_2}{2}$$

Hence, the barrier length must be equal to half-integral number of de-Broglie wavelength.

Q.10: Normalize the wave function $\phi_{m_1} = Ae^{im_1\phi}$

Ans: Condition for normalization is $\int_0^{2\pi} \phi_{m_1}^* \phi_{m_1} d\phi = 1$

$$\int_0^{2\pi} Ae^{-im_1\phi} Ae^{im_1\phi} d\phi = 1$$

$$A^2 \int_0^{2\pi} d\phi = 1$$

$$A^2 (2\pi) = 1$$

Hence $\phi_{m_1} = \frac{1}{\sqrt{2\pi}} e^{im_1\phi} \quad A = \frac{1}{\sqrt{2\pi}}$

OBJECTIVE QUESTIONS

1. Energy of a particle in 1-D box of width L varies as

(a) $E \propto n^2$ (b) $E \propto \frac{1}{n^2}$

(c) $E \propto n$ (d) $E \propto \frac{1}{n}$

2. The zero-point energy for 1-D closed box is

(a) $\frac{h^2}{2mL^2}$ (b) $h^2(2mL^2)$

(c) $\frac{h^2}{8mL^2}$ (d) $h/8mL$

3. The normalization constant for 1-D closed box is

(a) $\sqrt{2L}$ (b) $\sqrt{\frac{2}{L}}$

(c) $\frac{2}{L}$ (d) $2L$

4. The boundary conditions states

- (a) Wave function is discontinuous.
- (b) Derivative of wave function is discontinuous.
- (c) Wave function and its derivative are continuous.
- (d) Both wave function and its derivative are discontinuous.

5. Probability density current is defined as the

- (a) sum of probability density and current.
- (b) product of velocity of particle and its probability density.
- (c) product of current and probability density.
- (d) sum of current and probability density.

6. For a step potential, the value of k_2 is

- (a) $\sqrt{2m/\hbar^2}$
- (b) $\sqrt{2m\hbar^2}$
- (c) $\sqrt{\frac{2mE}{\hbar^2}}$
- (d) None of the above

7. For step potential, the value of K_2 is given by

- (a) $\sqrt{\frac{2m(E - V_0)}{\hbar^2}}$
- (b) $\sqrt{\frac{2mV_0}{\hbar^2}}$
- (c) $\sqrt{\frac{2mE}{\hbar^2}}$
- (d) 0

8. For step potential, e^{iK_1x} represents

- (a) reflected wave
- (b) incident wave
- (c) transmitted wave
- (d) None of the above

9. For step potential, the reflection coefficient is

- (a) $\frac{1 - k_1}{k_2}$
- (b) $\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$
- (c) $\frac{k_2 - k_1}{k_2}$
- (d) 0

10. The transmission coefficient for step potential is

- (a) $\frac{4k_1k_2}{k_1 - k_2}$
- (b) $\frac{(4k_1k_2)^2}{k_1 - k_2}$
- (c) $\frac{2k_1k_2}{k_1 + k_2}$
- (d) $\frac{4k_1k_2}{(k_1 - k_2)^2}$

11. For step potential when energy is less than step height,

- (a) $T = 1$ (b) $T = \frac{1}{2}$
 (c) $R = 0$ (d) $R = 1$

12. According to tunnel effect,

- (a) there is 100 percent probability to penetrate the barrier.
 (b) there is zero probability to penetrate the barrier.
 (c) there is 100 percent probability for reflection.
 (d) There is finite probability for penetration of potential barrier.

13. For the bound state of potential well, K_2 is given by

- (a) $\frac{2m}{\hbar^2}(V_0 - E)$ (b) $\sqrt{\frac{2m}{\hbar^2}(V_0 - W)}$
 (c) $\frac{2m(V_0 - W)}{\hbar^2}$ (d) 0

14. According to transcendental equation,

- (a) W can be obtained from argument of sine
 (b) W can be obtained from argument of cotangent
 (c) E can be obtained from W .
 (d) K_1 can be obtained from argument of cosecant

15. For bound state, the parameter y is given by

- (a) $\alpha/2$ (b) $\alpha/3$
 (c) $\gamma\beta$ (d) $n\pi + \gamma$

16. For scattered case of potential well,

- (a) $T_{\max} = 0.25$ (b) $T_{\max} = 0.5$
 (c) $T_{\max} = 0.75$ (d) $T_{\max} = 1$

17. T_{\min} for scattered state is given by

- (a) $\frac{4k_1^2 k_2^2}{(k_1^2 + k_2^2)^2}$ (b) $\frac{2k_1^2 k_2^2}{(k_1 - k_2)^2}$
 (c) 1 (d) $\frac{k_1 k_2}{4k_1 k_2}$

18. The total energy of hydrogen atom depends on

- (a) l and m_l (b) n
 (c) n and l (d) l

19. The degeneracy for first excited state of hydrogen is

- (a) 2 (b) 6
(c) 1 (d) 4

20. The wave function of hydrogen is dependent on

- (a) n , l , and m (b) n
(c) l (d) m

ANSWERS

- | | | | |
|--------|---------|---------|---------|
| 1. (a) | 6. (c) | 11. (d) | 16. (d) |
| 2. (c) | 7. (a) | 12. (d) | 17. (a) |
| 3. (b) | 8. (b) | 13. (a) | 18. (b) |
| 4. (c) | 9. (b) | 14. (b) | 19. (d) |
| 5. (b) | 10. (d) | 15. (c) | 20. (a) |

Micro-Assessment Questions

1. What is tunneling effect?
2. What do you understand by zero-point energy?
3. What will be the energy of a particle in a box for $n = 3$?
4. Explain the meaning of degeneracy.
5. Write the boundary conditions for step potential.
6. Explain the term “reflection coefficient.”
7. What do you understand by transmission coefficient?
8. Write down the transcendental equation for bound state.
9. What is separation of variables?
10. Write down ground state of hydrogen atom.
11. Give the range of spherical polar coordinates.
12. How many degrees of freedom does hydrogen atom have?
13. Give the relation between spherical polar coordinates and Cartesian coordinates.
14. Give the physical significance of principal quantum number.

Critical Thinking Questions

1. What are the various laws for operators?
2. Write down an eigenvalue equation. Explain eigenfunctions and eigenvalues.
3. What is the physical significance of zero-point energy?
4. Obtain the energy levels for particle inside a box of finite width.
5. Consider a particle of step height V_0 such that it is less than energy E . Calculate the reflection coefficient.
6. Calculate the reflection and transmission coefficient when energy E is greater than V_0 .
7. Show that energy levels are discrete and does not follow a continuum for a particle inside a box.
8. Use Schrödinger wave equation to explain the tunneling phenomena. How does it differ from the classical explanation?
9. What do you understand by scattered state of potential well? Obtain the minimum and maximum transmission in this case.
10. Show that for the bound state of a potential well; the particle can take only discrete energy values.

Graded Questions

1. State the Schrödinger equation in three dimensions for hydrogen problem.
2. Prove that operator d/dx is non-Hermitian.
3. Obtain the energy levels after solving the radial equation for hydrogen atom.
4. State the azimuthal component for hydrogen atom problem and determine its solution.
5. Solve Schrödinger equation for three-dimensional harmonic oscillator in spherical coordinates.
6. Show that the average value of $1/r$ is $1/a_0$ in ground state and normalized wave function.
7. Find the expectation value of kinetic energy, potential energy, and total energy of hydrogen atom

in the ground state. Take $\psi_0 = \frac{e^{-r/a_0}}{(\pi a_0^3)^{1/2}}$, where $a_0 =$ Bohr's radius..

8. Consider the time-independent Schrödinger equation in three dimensions

$$\left[\left(-\frac{\hbar^2}{2m} \right) \nabla^2 + V(r) \right] \psi = E\psi. \text{ In spherical coordinates,}$$

$$\nabla^2 = \left(\frac{1}{r^2} \right) \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \left(\frac{1}{r^2 \sin \theta} \right) \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \left(\frac{1}{r^2 \sin^2 \theta} \right) \frac{\partial^2}{\partial \varphi^2}$$

- (a) Write $\psi(r, \theta, \varphi) = \psi_r(r)Y(\theta, \varphi)$ as a separable solution and split Schrödinger's equation into two independent differential equations: one depending on r and the other depending on θ and φ .
- (b) Further separate the angular equation into θ and φ parts.
9. For a particle in cubic box of dimension L , prove that the normalizing factor is $A = (2/L)^{3/2}$. How will the result change if the box has different edge lengths L_1 , L_2 , and L_3 ?
10. An electron moves in a cube with side length of 0.1 nm. Find the values for the energy of (a) the ground state and (b) the first excited state of the electron.
11. Calculate the average potential and kinetic energies for the electron in the ground state of hydrogen.
12. Prove that the n th energy level of an atom has degeneracy equal to n^2 .

Remember and Understand

1. There is some minimum energy in the ground state of a particle inside a box, which is known as zero-point energy.
2. Classically, the particle inside the box can have any arbitrary value of energy.
3. Reflection coefficient is the ratio of reflected probability density current to incident probability density current.
4. Transmission coefficient is the ratio of transmitted probability density current to incident probability density current.
5. When energy of a particle is greater than the potential step, then $R + T = 1$.
6. When the particle has energy less than potential barrier, then classically there is no penetration inside the region 3, but quantum mechanically the particle always have finite probability of tunneling and can go over another region. This is known as tunneling phenomena.

Atomic and Molecular Structures

Keywords: Bohr model, Rutherford model, spectral lines, spin-orbit interaction, LS coupling, JJ coupling, Zeeman effect, Stark effect

Learning Objectives

- ◆ To study the Thomson's model of atomic structure
- ◆ To understand the failures of Thomson's model and hence rise of Rutherford's model
- ◆ To study the failure of Rutherford's model
- ◆ To understand the postulates of Bohr's model
- ◆ To learn the interpretation of spectra by Bohr's model
- ◆ To learn about the correspondence principle stating that when quantum number approaches infinity, quantum mechanics turns to classical regime
- ◆ To analyze Sommerfeld model
- ◆ To understand the results of vector atom model
- ◆ To learn the orbital and spin magnetic moment along with gyromagnetic ratio
- ◆ To gain insight into LS coupling, fine structure, and multielectron system
- ◆ To learn the splitting of spectral lines in the presence of magnetic field (Zeeman effect)
- ◆ To differentiate between anomalous and normal Zeeman effect
- ◆ To understand the splitting of spectral lines in the presence of electric field (Stark effect)

By the end of the twentieth century, many phenomena such as photoelectric effect, Compton effect, blackbody radiation, and wave particle duality were explained successfully. But the absorption and emission spectra were still to be addressed. In this chapter, we will discuss various models that helped in interpreting the atomic structure.

5.1 Thomson and Rutherford Models

The first model that could show some picture of atom was given by J.J. Thomson (1904). His model was named as "Thomson pudding model." He postulated the following points:

- (i) Atom on the whole is electrically neutral.
- (ii) Positive charges are uniformly distributed inside an atom whereas the electrons are positioned as rotating ring corpuscles defined by Thomson.

This model considers that electrons are free to move within the cloud of positive charges. Electrons were also considered to rotate in rings. The energy spectra was supposed to be due to difference of these electron rings. But this model failed to describe the spectrum of multi-electron atoms. Hence, there was a need to correct atomic model as this model could not explain the precise wavelength patterns being emitted by some elements.

In 1911, Ernest Rutherford, scientist from New Zealand, was doing some experiments on radioactivity. He proved that when atoms emit certain radiations, they are converted to an element of different composition. Hence, his further investigations led him to probe that the nucleus is a dense mass of positive charges concentrated inside the atom. He bombarded α -particles (${}_2\text{He}^4$) on a thin gold foil. Gold foil has high malleability, due to which it could be beaten into thin foils. The scattered α -particles were observed on ZnS screen. ZnS screen produces scintillations (flash of light) when α -particles strike on it. Coulomb's repulsive force was responsible for the scattering of α -particles, that is, the repulsion between positive charge of α -particles and gold target as shown in Figure 5.1.

Rutherford made the following observations:

- (i) Many of the α -particles were not deflected and they passed without any deviation. This indicated that atom is having lots of empty space inside it.
- (ii) Some of the atoms suffered small deflections.
- (iii) Some atoms suffered very large deflections.
- (iv) A few atoms were even scattered in backward direction.

Sir Joseph John Thomson was born to Scottish bookseller in 1856 in Cheetham Hill near Manchester, England. He won a scholarship to Trinity College, Cambridge, in 1876. He received his BA in 1880 in mathematics and MA in 1883. J.J. Thomson was appointed the Master of Trinity College, Cambridge, in 1918 and he remained there until his death on August 30, 1940, at the age of 83 years. Thomson was buried in Westminster Abbey (close to the grave of Isaac Newton).

J.J. Thomson was appointed as a Fellow of the Royal Society in 1865. His favorite student Ernst Rutherford later succeeded him in 1919. Thomson was a successor to Lord Rayleigh as Cavendish Professor of Experimental Physics. The early theoretical work of Thomson helped broadening the electromagnetic theories of James Clerk Maxwell.

Sir Joseph John Thomson was an English physicist who stormed the world of nuclear physics with his 1897 discovery of the electron, as well as isotopes. He invented mass spectrometer and received the Nobel Prize for Physics in 1906. He was knighted two years later in 1908.



The difficulties which would have to be overcome to make several of the preceding experiments conclusive are so great as to be almost insurmountable.

J. J. Thomson

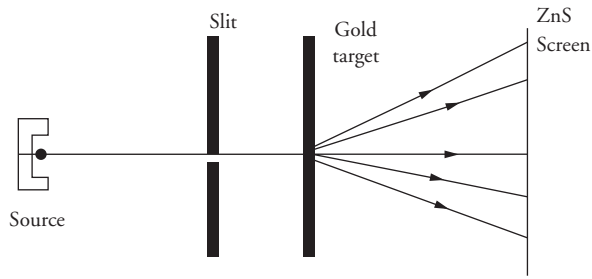


Figure 5.1 Rutherford's scattering experiment set-up.

All these deflections were explained by Rutherford as follows: He proposed that atom consists of a tiny nucleus that contains all the positive charge of atom and electrons are arranged around that nucleus. The undeflected α -particle was due to large empty spaces inside the atom as shown in Figure 5.2. The α -atoms that had direct head-on collision with gold nucleus suffered backward 180° deflection due to strong coulombic repulsions. The α -particles that passed through the atom at a distance from nucleus went undeflected. The atoms that passed at a very small distance from the nucleus suffered very large deflections. Rutherford obtained the following formula:

$$N = \frac{Cnd (Ze)^2 e^2}{r^2 m^2 v^2 \sin^4 \theta/2} \quad (1)$$

where

- C total number of α -particles reaching the screen
- n number of atoms/volume in foil
- Ze nuclear charge of Au atom
- d the thickness of gold foil
- r distance from scattered

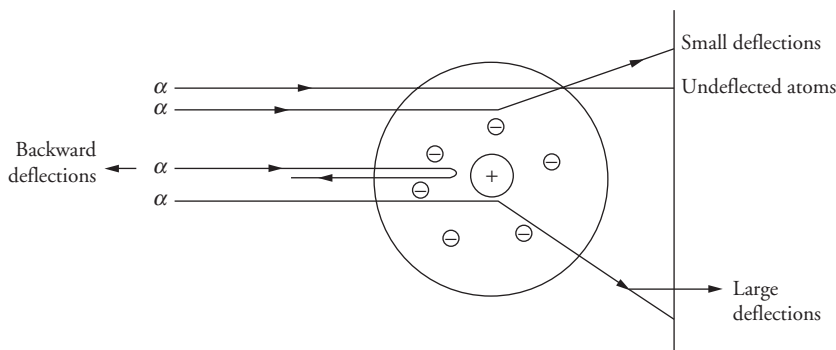


Figure 5.2 Deflection of α -atoms while passing through gold atom.

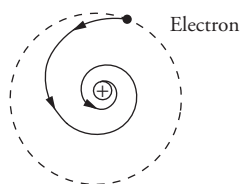


Figure 5.3 Collapsing of electron into nucleus.

v velocity of particles

θ scattering angle

N number of α -particles that are scattered through angle θ .

Rutherford model gave a satisfactory explanation regarding structure and distribution of charges inside the atom. But the main drawback of this model was stability of atom. If we consider an atom having two positive and two negative charges, and they are separated by distance r from each other, then the force of attraction between them is given by $2e^2/r^2$. The force of repulsion between the electrons is given by $e^2/4r^2$. This leads to the conclusion that the force of attraction is eight times higher than the force of repulsion. Hence, on account of high force of attraction, the electrons will start falling on the nucleus (Figure 5.3). This would ultimately lead to the collapse of atomic structure. Furthermore, Rutherford assumed that the electrons may revolve around the nucleus, where the centrifugal force could balance the excess electrostatic attraction. But the electromagnetic theory says that any accelerated charge would produce electromagnetic radiations continuously. Hence, the atoms will keep on losing energy continuously, as all the electrons will be moving emitting electromagnetic radiations. Ultimately, the electron will fall inside the nucleus, following a spiral path. The frequency of orbiting electron will increase continuously. Therefore, the stability of atom cannot be defined using Rutherford's model.

In 1898, Rutherford went to work with Henri Becquerel, a scientist researching on the process of radioactivity. Becquerel first discovered radioactivity and performed the first α -scattering experiment while studying the passage of α -particles through magnetic fields. Rutherford proved one of Becquerel's theories to be wrong and did not get along well. At McGill, Rutherford was accompanied by a young chemist, Frederick Soddy, and they investigated three groups of radioactive elements—radium, actinium, and thorium. In 1902, they



ERNEST RUTHERFORD

concluded radioactivity to be a course of action during which atoms of one element spontaneously disintegrate into atoms of a completely different element, though the new element also remained radioactive. However, this view was not accepted by contemporary chemists who strongly believed that matter can neither be destroyed nor created.

5.2 Bohr's Model

In 1913, Niels Bohr applied quantum theory to Rutherford model to solve the stability problem of atom. This model was quite successful in explaining the spectral lines of atoms. Bohr made an assumption that the angular momentum was quantized. This implies that electrons define their position in certain orbits. These electrons are characterized by particular quantum number. His theory comprised of following basic postulates:

- (i) Electrons revolve in certain orbits which are stationary states. Electrons revolve in these stationary orbits without radiating energy.
- (ii) The energy is lost by electron only when it jumps from higher level to lower level.
- (iii) The angular momentum of electrons revolving in stationary orbits is given by $\frac{nh}{2\pi}$.

Consider an electrons of charge e revolving around nuclei of charge Ze . The Coulomb force is given by (Figure 5.4)

$$F_c = \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r^2} \quad (2)$$

The force that is required to keep the electron in orbit is centrifugal force and is given by

$$F_c = \frac{mv^2}{r} \quad (3)$$

(where " v " is the velocity of revolving electron)
In equilibrium,

$$F_e = F_c$$

$$\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r^2} = \frac{mv^2}{r}$$

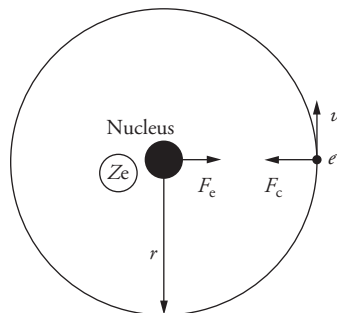


Figure 5.4 Atom as visualized by Bohr.

$$v = \frac{e\sqrt{Z}}{\sqrt{4\pi\epsilon_0 mr}} \quad (4)$$

For hydrogen atom, $Z = 1$, $r = 0.529 \text{ \AA}$

$$v = \frac{(1.6 \times 10^{-19})}{\sqrt{(9.11 \times 10^{-31})(4 \times 3.14)(0.5 \times 10^{-10})(8.85 \times 10^{-12})}}$$

$$v = 2.18 \times 10^6 \text{ m/s} \quad (5)$$

The velocity of electron is less than the velocity of light and hence the electron moves in nonrelativistic regime. We can also obtain the value of velocity from angular momentum equation.

$$\text{We know } L = \frac{nh}{2\pi} \quad (n \text{ is principal quantum number})$$

$$\text{Also } L = mvr$$

$$\text{Hence } mvr = \frac{nh}{2\pi}$$

$$v = \frac{nh}{2\pi mr} \quad (6)$$

From Eqs (4) and (6)

$$r = \frac{n^2 \hbar^2 4\pi\epsilon_0}{e^2 m} = n^2 a_0 \quad (7)$$

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad (8)$$

Put $\epsilon_0 = 8.85 \times 10^{-12} \text{ C}^2/\text{Nm}^2$, $m = 9.1 \times 10^{-31} \text{ kg}$, $e = 1.6 \times 10^{-19} \text{ C}$ and $\hbar = 6.63 \times 10^{-34} \text{ Js}$ in Eqn. (8)

$$a_0 = 0.529 \times 10^{-10} \text{ m} \quad (9)$$

For atoms with atomic number Z ,

$$r = \frac{n^2 a_0}{Z} \quad (10)$$

Hence, radius r is directly proportional to n^2 . 0.529 \AA is the radius of first orbit of hydrogen atom and is known as Bohr's radius. We can calculate the total energy of the system as follows:

Total energy = kinetic energy + potential energy

$$\text{Total energy} = \frac{mv^2}{r} - \frac{Ze^2}{r}$$

$$E_n = \frac{Ze^2}{2r} - \frac{Ze^2}{r} = -\frac{Ze^2}{r}$$

$$E_n = -\frac{Ze^2}{r} \quad (11)$$

From Eqs (7) and (11),

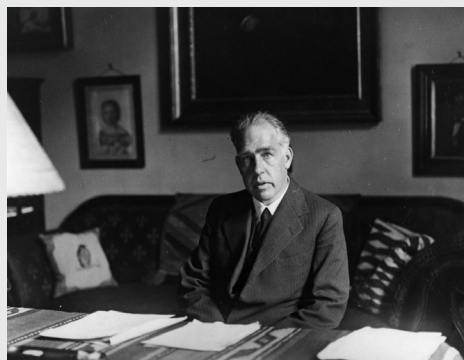
$$E_n = -\frac{2\pi^2 me^4}{n^2 h^2} \quad (12)$$

where E_n is the total energy of n th orbit. As the principal quantum number increases, the energy decreases. But as Eqn. (12) has negative sign, it implies that the energy increases for outer levels. Hence, for $n = 1$, and atomic number Z ,

$$E_1 = -\frac{2\pi^2 me^4 Z^2}{h^2} \quad (13)$$

where $n = 1$ is the level having minimum energy. Hence, E_n is the energy that should be supplied to the atom to get the electron separated from the atom. Thus, E_n also signifies that the binding energy or the attractive energy between the nucleus and electron.

Bohr's atomic model was not successful at first. After a period of about 10 years, "success" was achieved with the hydrogen atom. Bohr's atomic model attributes a planetary motion to electrons, which means that electrons move around the nucleus in defined circular orbits. But according to modern view, the electron distribution around the nucleus of an atom is described by a probability distribution. Hence, the "electron clouds" give rise to discrete circular orbits.



NIELS BOHR

5.3 Interpretation of Spectra using Bohr's Model

The atomic spectra are considered to be very complex. If electric current is passed through gas, then discrete emission spectra is obtained. But for solid/liquid, the spectrum is continuous. Wavelength in the spectrum are separated using diffraction gratings. The spectral lines emitted can be grouped into principal, sharp, diffuse, and fundamental series. Several investigators, especially Balmer, Rydberg, Paschan, and Ritz, gave empirical relations to define these spectral lines.

In 1885, Balmer outlined a relationship for the emission lines obtained for hydrogen. He obtained the following relation:

$$\frac{1}{\lambda} = B \left[\frac{m^2}{m^2 - n^2} \right] \quad (14)$$

where B is constant with value 3.64×10^{-7} m and m is greater than n .

In 1888, Johannes Rydberg generalized the Balmer equation as follows:

$$\frac{1}{\lambda} = R_H \left[\frac{1}{2^2} - \frac{1}{n^2} \right] \quad (15)$$

$$(n = 3, 4, 5, 6, 7, \dots)$$

where R_H is the Rydberg constant and the value of R is $109,737 \text{ cm}^{-1}$.

In 1908, Walter Ritz along with Rydberg provided a Rydberg–Ritz combination principle. This principle states that the spectral lines of elements including frequencies are either the difference or sum of two other lines. For optical and X-ray region, this principle maintained its accuracy. In the previous section, it was proved that outer levels are of high energy and innermost levels have lower energy. Electron loses energy only when it jumps from higher level to lower level. Let E_1 be the energy of level with principal quantum number n_1 and E_2 be the energy of level with principal quantum number n_2 . This implies that

$$E_2 - E_1 = hf$$

Equation (12) in previous section is given as

$$E_n = -\frac{2\pi^2 m e^4 Z}{n^2 h^2}$$

Hence, from the above two equations we conclude

$$hf = -\frac{2\pi^2 m e^4 Z}{n^2 h^2}$$

$$f = -\frac{2\pi^2 m e^4 Z}{h^3} \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

$$f = -\frac{2\pi^2 m e^4 Z}{h^3} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (16)$$

Converting (16) to wavenumbers,

$$\text{wavenumber } \bar{f} = \frac{f}{c} = \frac{2\pi^2 mZ^2 e^4}{cb^3} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (17)$$

In Eqn. (17), $\frac{2\pi^2 mZ^2 e^4}{cb^3}$ is constant with value $109,738 \text{ cm}^{-1}$, which is in agreement with the value obtained for Rydberg constant. Hence, Bohr's model could successfully explain the stability of atom. Along with this, the model successfully explained the origin of different spectral lines. The following is a list of different series, which arise due to different transitions:

(i) Lyman Series

$$\bar{f} = R \left[\frac{1}{1^2} - \frac{1}{n^2} \right] \quad n = 2, 3, 4, \dots \quad (18a)$$

(ii) Balmer Series

$$\bar{f} = R \left[\frac{1}{2^2} - \frac{1}{n^2} \right] \quad n = 3, 4, 5, \dots \quad (18b)$$

(iii) Paschen Series

$$\bar{f} = R \left[\frac{1}{3^2} - \frac{1}{n^2} \right] \quad n = 4, 5, 6, 7, \dots \quad (18c)$$

(iv) Brackett Series

$$\bar{f} = R \left[\frac{1}{4^2} - \frac{1}{n^2} \right] \quad n = 5, 6, 7, 8, \dots \quad (18d)$$

(v) Pfund Series

$$\bar{f} = R \left[\frac{1}{5^2} - \frac{1}{n^2} \right] \quad n = 6, 7, 8, 9, \dots \quad (18e)$$

All these series are depicted in Figure 5.5.

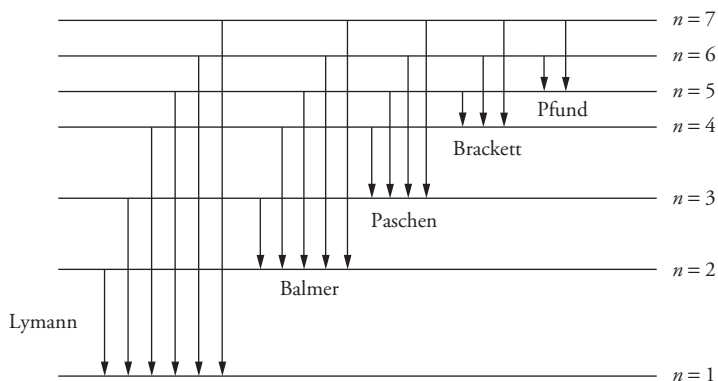


Figure 5.5 Hydrogen spectrum indicating different transitions.

5.4 Correspondence Principle

This principle was put forward by Niels Bohr in 1913. He argued that this principle is replacement of old quantum theory by the new quantum theory. The old quantum theory was given as an interim theory between newtonian mechanics and electrodynamics. But certain empirical relations, especially related to atomic spectra, could not be explained on the basis of old quantum theory. The old quantum theory was subsequently replaced by Heisenberg and Schrodinger when they developed matrix representation and wave mechanics, respectively.

The classical model states that the orbital frequency of electron and spectral line is same. For large principal quantum numbers, this frequency could be same; but at low quantum numbers, there is considerable difference between two frequencies.

According to Bohr theory, the orbital frequency is given as

$$f_B = \frac{f}{2\pi r} = \frac{2\pi Ze^2}{nh} \cdot \frac{1}{2\pi r}$$

$$f_B = \frac{Ze^2}{nhr}$$

$$f_B = \frac{4\pi^2 Z^2 e^4 m}{n^3 h^3} \quad (\text{after using radius from Eqn. (7)})$$

$$f_B = \frac{2Rc}{n^3} \quad (19)$$

where R is Rydberg constant

From Eqn. (17), the frequency is

$$f = Rc \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

Let $n_1 = n$ and $n_2 = n + \Delta n$

$$f = Rc \left[\frac{1}{n^2} - \frac{1}{(n + \Delta n)^2} \right] \quad [\Delta n \ll n]$$

If $\Delta n = 1$

$$f = \frac{2Rc}{n^3} = f_B \quad (20)$$

Hence, it can be concluded that at very large quantum numbers (n_1 and n_2), which are separated by unity, the frequency of spectral line becomes equal to the orbital frequency (classical frequency). Hence, in the limit of large quantum numbers quantum mechanics yield the result of classical mechanics.

Quantum mechanics usually is applied on a microscopic regime, whereas classical mechanics is apt on a macroscopic regime. The limit at which quantum and classical physics unite is called correspondence

limit. Hence, the correspondence principle states that “The behavior of atom tends asymptotically from quantum to classical region for large quantum numbers.”

Bohr stated that

“The aim of regarding the quantum theory as a rational generalisation of classical theories led to the formulation of so-called correspondence principle. The utilization of this principle for the interpretation of spectroscopic results was based on a symbolical application of classical electrodynamics, in which the individual transition processes were each associated with a harmonic in the motion of atomic particle to be expected according to ordinary mechanics.”

5.5 Sommerfeld Model

Bohr atomic model explained many things successfully but could not explain successfully the fine lines in the spectra. Each spectral line was accompanied by many fine spectral lines. Then, Sommerfeld modified Bohr's theory in 1915 by introducing the following two main postulates:

- (i) The electron revolves around the nucleus in elliptical path with nucleus at one of loci of ellipse.
- (ii) The electron possesses different velocity at different points of ellipse.

Elliptical orbit for hydrogen atom as described by Sommerfeld is shown in Figure 5.6.

The above-mentioned model is explained in detail as follows: Sommerfeld assumed that the electrons revolve around nucleus in the same way the planets revolve around the sun. Hence, polar coordinates are used to explain position of electrons: r and ϕ are used to describe the position, where r is radius vector and ϕ is vectorial angle which the radius vector makes a major elliptical axis. \vec{v} is the tangential velocity of electron. This tangential velocity can be resolved into the following two components:

- (i) Radial velocity \rightarrow It is along the radius vector and its magnitude is given by dr/dt .
- (ii) Transverse velocity \rightarrow It is perpendicular to the radius vector and its magnitude is given by

$$r \cdot \left(\frac{d\phi}{dt} \right).$$

Circular and elliptical orbits satisfy the quantum conditions. Hence, Sommerfeld assumed that these elliptical orbits will also satisfy angular momentum condition as follows:

$$\oint p_r dr = n_r h \quad (21a)$$

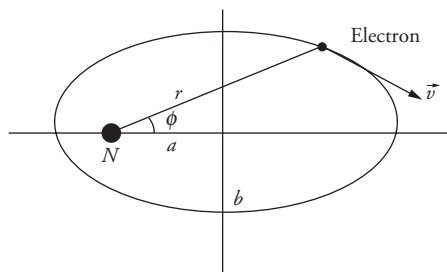


Figure 5.6 Elliptical orbit for hydrogen atom.

$$\oint p_{\phi} d\phi = n_{\phi} h \quad (21b)$$

n_r and n_{ϕ} are related to the principal quantum number by the following equation:

$$n = n_r + n_{\phi} \quad (21c)$$

where n_r is radial quantum number and n_{ϕ} is azimuthal quantum number. Now, the total energy of the system is given by sum of potential and kinetic energy. Here, the kinetic energy is contributed by two parts, that is, radial and angular. Hence, we can write

$$E = PE + KE$$

$$E = -\frac{Ze^2}{r} + \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{1}{2}mr^2\left(\frac{d\phi}{dt}\right)^2 \quad (22)$$

The quantum numbers and eccentricity (ϵ) are related to each other by the following relation:

$$1 - \epsilon^2 = \frac{b^2}{a^2} = \frac{n_{\phi}^2}{(n_{\phi} + n_r)^2} \quad (b \text{ and } a \text{ are semi-major and semi-minor axes})$$

$$(1 - \epsilon^2)^{1/2} = b/a = \frac{n_{\phi}}{n} \quad (23)$$

The following conditions have been deduced on the basis of Eqn. (23):

- (i) n_{ϕ} cannot be zero. If $n_{\phi} = 0$, then the ellipse becomes a straight line that passes through the nucleus.
- (ii) n_{ϕ} is never greater than n . If $n_{\phi} \gg n$, then this implies b to be greater than a , which is impossible.
- (iii) At $n_{\phi} = n$, b is equal to a , and hence the orbit changes from ellipse to circle. Eccentricity also becomes 0 for this condition.
- (iv) There can only be a limited number of elliptical orbits, which have different eccentricities.
- (v) The orbits with same n are degenerate orbits. They may have different shapes due to different eccentricities, but same energy. For example, for $n = 3$, the degenerate levels are shown in Figure 5.7.

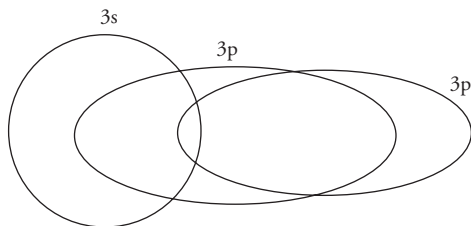


Figure 5.7 Degenerate orbits of $n = 3$ of hydrogen atom.

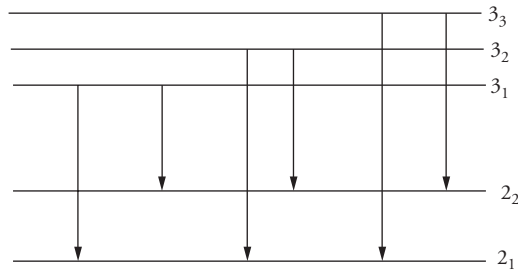


Figure 5.8 Fine structure for H_α lines (For given value of n , n_ϕ has only n values).

The velocity of electron, which moves in elliptical orbit, is different at different positions, that is, the velocity of electron is minimum when it is far from the nucleus, and it is maximum when it is near to the nucleus. But according to Einstein's theory of relativity, the mass varies with the variation of velocity. This theory also considers that the mass effect is very predominant in the regime of high velocities. If mass variation is taken into account, then instead of ellipse, the electron path comes out to be rosette. Sommerfeld showed that the relativistic equation that described the path of electron is

$$\frac{1}{r} = \frac{1 + \varepsilon \cos \phi}{a(1 - \varepsilon^2)} \quad (24a)$$

where

$$\phi^2 = 1 - \frac{Z^2 e^4}{16\pi^2 \varepsilon_0^2 p^2 c^2} \quad [p \text{ is the momentum}] \quad (24b)$$

Equation (24a) represents the path of electron as an ellipse whose major axis processes slowly in the plane of ellipse about an axis passing through nucleus. The total energy of system is given by

$$E_n = \frac{me^4 Z^2}{8\varepsilon_0^2 n^2 h^2} - \frac{me^4 Z^4 \alpha^2}{8\varepsilon_0^2 h^2} \left[\frac{n}{n_\phi} - \frac{3}{4} \right] \frac{1}{n^4} + \dots \quad (25)$$

where

$$\alpha = \frac{e^2}{2\varepsilon_0 ch} \approx \frac{1}{137} \quad (26)$$

α is also called fine-structure constant. From Eqn. (25), it is clear that energy depends on n and n_ϕ . Therefore, relativistic approach leads to splitting of energy level E_n into n -levels. These levels differ slightly from each other as the relativistic mass correction is quite small in magnitude. Hence, this splitting of fine levels gives rise to fine-structure splitting. Figure 5.8 illustrates the fine structure of H_α lines.

However, the fine structure of hydrogen could be explained using Sommerfeld theory. But explaining the spectra of multi-electron system was still complicated process. No idea could be obtained regarding the spectral intensities using Sommerfeld model.

5.6 Vector Atom Model

The orbital angular momentum for an atomic electron can be interpreted in terms of vector model. The precession of angular momentum vector about a direction in space is as shown in Figure 5.9(a).

l is orbital quantum number and it represents the quantization of orbital angular momentum L .

l can have values from 0, 1, 2, ..., $n - 1$, where n is principal quantum number.

Hence, \vec{L} is not fixed in space and changes continuously making same angle with direction of applied magnetic field. In other words, there is magnetic moment associated with orbital angular momentum in some external field. We are familiar that when magnetic moment is placed in magnetic field B , it experiences torque τ . For static case, this torque will orient the magnetic moment along the direction of magnetic field, \vec{B} , as it orients in low-energy configuration. But, when the magnetic moment rises due to motion of electron around the nucleus, then magnetic moment of electron is directly proportional to angular momentum (Moving electron is a source of current and hence magnetic field). Hence, the torque is produced, which tends to change angular momentum in such a way that it is in precession with the direction of magnetic field. This precession is called Larmor precession. There is a characteristic frequency associated with this precession known as Larmor frequency. L has three components and only one component can be along the magnetic field. This process is called space quantization, as the angular momentum vector takes specific values due to specific orientations. Let us suppose that B is along the z -direction, then the component of L along the z -direction is L_z and its

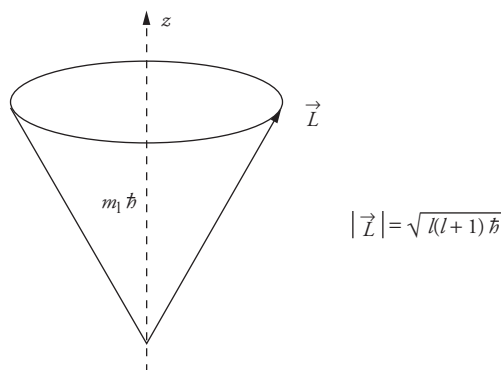


Figure 5.9(a) Precession of angular momentum about z -direction.

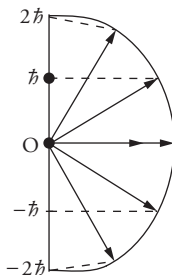


Figure 5.9(b) Space quantization describing the allowed orientations for $l = 2$.

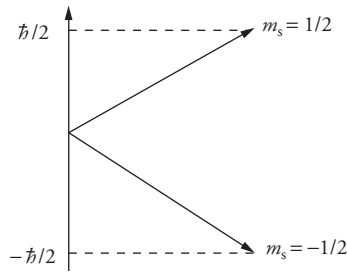


Figure 5.10 Space quantization for electron spin.

value is $L_z = m_l \hbar$, ($m_l = 0, \pm 1$), where m_l is magnetic quantum number. Directions of L_x and L_y keep on changing continuously and hence give average value of zero.

The possible m_l values lie between $+l$ and $-l$ hence, the total possible orientations are $2l + 1$. For $l = 2$, m_l has value $+2, +1, 0, -1, -2$ and total angular momentum is

$$L = \sqrt{l(l+1)} \hbar = \sqrt{6} \hbar$$

Figure 5.9(b) shows the space quantization for $l = 2$.

Hence, there are five orientations for $l = 2$, such that the total magnitude is $\sqrt{6} \hbar$.

In 1925, S. Goudsmit and G. Uhlenbeck proposed that electrons have an intrinsic angular momentum or spin angular momentum which give rise to magnetic field. In 1929, Dirac confirmed the nature of electron spin using relativistic quantum mechanics. s is used to denote the spin angular momentum of electron. S is the magnitude of spin angular momentum and is given by the following equation:

$$S = \sqrt{s(s+1)} \hbar \quad (27)$$

Like orbital momentum, the electron spin is also quantized and the quantum number m_s describes the space quantization of electron. m_s can have $2s + 1$ orientations. For $s = \frac{1}{2}$, $m_s = +\frac{1}{2}$ and $-\frac{1}{2}$ as shown in Figure 5.10.

If magnetic field is along z -axis, then component S_z is along the direction of field and is given by

$$S_z = m_s \hbar \quad (28)$$

$$S_z = \pm \frac{\hbar}{2}$$

5.7 Orbital and Spin Magnetic Moment (μ_l)

Let us consider an electron with mass m and charge $-e$ revolving with velocity v around the nucleus as shown in fig. 5.11. The radius of circular orbit is r . Whenever an electron revolves around in a loop, it generates current and current is always associated with magnetic fields. The current in loop is given by

$$I = -\frac{e}{t} = -\frac{ev}{2\pi r}$$

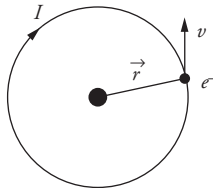


Figure 5.11 Electron revolving around nucleus.

Orbital magnetic moment is given by

$$\begin{aligned}\mu_l &= IA = -\frac{ev}{2\pi r} \times \pi r^2 \\ \mu_l &= -\frac{evr}{2} \\ \mu_l &= -\frac{e mvr}{2m} = -\frac{eL}{2m} \quad (\because L = mvr) \\ \mu_l &= -\frac{eL}{2m}\end{aligned}\quad (29)$$

The “-” sign signifies that orbital magnetic moment and angular momentum are in opposite directions. The above expression is according to classical mechanics, but quantum mechanics introduces a factor g_l (Landau’s factor) and Eqn. 29 becomes

$$\vec{\mu}_l = -g_l \frac{e\vec{L}}{2m} \quad (30a)$$

$$\vec{\mu}_l = -g_l \frac{e\sqrt{l(l+1)}\hbar}{2m} \quad (30b)$$

$$\vec{\mu}_l = -g_l \mu_B \sqrt{l(l+1)} \quad (30c)$$

where $\mu_B = \frac{e\hbar}{2m}$ is Bohr magneton having value of $9.24 \times 10^{-24} \text{ Am}^2$.

The z -component of orbital magnetic moment is given by

$$(\mu_l)_z = -\frac{eL_z}{2m} = -\frac{em_l\hbar}{2m} \quad (31)$$

Equation (31) clearly depicts the quantization of angular magnetic moment.

Similarly, by using quantum theory, we can obtain spin magnetic moment

$$\begin{aligned}\vec{\mu}_s &= -\frac{2e\vec{S}}{2m} = -\frac{2e}{2m} \sqrt{s(s+1)}\hbar \\ &= -g_s \frac{e\hbar}{2m} \sqrt{s(s+1)} \\ &= -g_s \mu_B \sqrt{s(s+1)}\end{aligned}\quad (32)$$

Collectively, we can summarize as

$$\begin{aligned}
 \text{(i)} \quad (\mu_l)_z &= -\frac{eL_z}{2m} & \text{(ii)} \quad (\mu_s)_z &= \frac{2e}{2m} S_z \\
 (\mu_l)_z &= -\frac{em_l\hbar}{2m} & (\mu_s)_z &= -\frac{2em_s\hbar}{2m} \\
 & & &= \pm \frac{e\hbar}{2m} = \pm \mu_B \\
 \text{(iii)} \quad g_l &= 1 & \text{(iv)} \quad g_s &= 2 \\
 \text{(v)} \quad \mu_l &= -g_l \frac{e\vec{L}}{2m} & \text{(vi)} \quad \mu_s &= -g_s \frac{e\vec{S}}{2m}
 \end{aligned}$$

5.8 LS Coupling and Fine Structure

An electron has both spin and orbital angular momentum. The total angular moment (\vec{J}) is the vector sum of these two moments. This is also known as spin-orbit coupling. This coupling is basically due to interaction of two magnetic moments, that is, spin magnetic moment and orbital magnetic moment. This interaction actually explains the fine-structure of lines as it causes the splitting of lines.

The total angular momentum is given by following expression:

$$\vec{J} = \vec{L} + \vec{S} \quad (33a)$$

Like spin and orbital angular momentum, the total angular momentum is also quantized and is given by

$$|\vec{J}| = \sqrt{j(j+1)}\hbar \quad [\text{where } j \text{ is total angular momentum quantum number}] \quad (33b)$$

\vec{J} can also have certain orientations, and its component along the direction of magnetic field is given by

$$J_z = m_j\hbar \quad (m_j \text{ total magnetic quantum number}) \quad (33c)$$

m_j can also take $(2j+1)$ values and varies from $-j$ to $+j$. If we consider only the z -components, then they also follow vector addition rule like Eqn. (33a).

$$\begin{aligned}
 \vec{J}_z &= \vec{L}_z \pm \vec{S}_z \\
 m_j\hbar &= m_l\hbar \pm m_s\hbar \\
 m_j &= m_l \pm m_s
 \end{aligned} \quad (33d)$$

Hence
$$j = l \pm s \quad (33e)$$

When \vec{L} and \vec{S} interact, they exert torque on each other as shown in Figure 5.12. Electron revolves around the field of nucleus along with rotation on its own axis. Hence, the interaction between the two fields gives rise to spin-orbit coupling whose magnitude depends on magnitude of field.

The nucleus of atom is in motion and has charge Ze , and electron is at rest around the nucleus. The mass of electron is m and charge e , the radius of circular orbit is r , and velocity of electron is 0 . As the moving nucleus could be interpreted as a current loop, hence, the current is given by

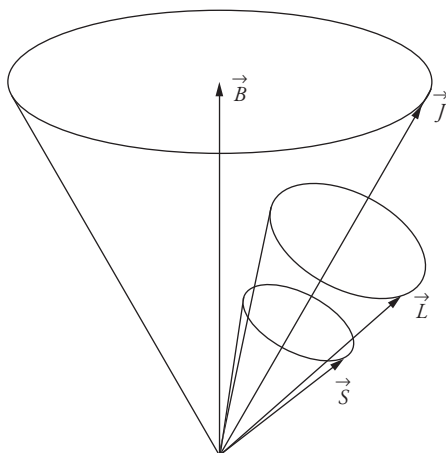


Figure 5.12 \vec{L} and \vec{S} process around total angular momentum \vec{J} and \vec{J} process around magnetic field \vec{B} .

$$I = \frac{Ze}{t} = \frac{Zev}{2\pi r} \quad (34)$$

The magnetic field due to current loop is given by

$$B_o = \frac{\mu_o I}{2r} = \frac{\mu_o Zev}{4\pi r^2} \quad (35)$$

Remember B_o is not the external applied field, but is the internal magnetic field due to the motion of nucleus.

Converting Eqn. (35) to vector form (only tangential component of velocity contribute)

$$B_o = \frac{\mu_o}{4\pi r^2} \frac{(\vec{r} \times \vec{v})}{|\vec{r}|}$$

$$B_o = \frac{\mu_o}{4\pi} \frac{Ze}{mr^3} (\vec{r} \times m\vec{v})$$

$$B_o = \frac{\mu_o}{4\pi} \frac{Ze}{mr^3} \vec{L} \quad (36a)$$

Using

$$c = \frac{1}{\sqrt{\mu_o \epsilon_o}}$$

$$B_o = \frac{Ze\vec{L}}{4\pi \epsilon_o mc^2 r^3} \quad (36b)$$

If we place the dipole of moment $\vec{\mu}_s$ in external magnetic field \vec{B} , then the potential energy of dipole is given as:

$$PE = E = -\vec{\mu}_s \cdot \vec{B}$$

Using this relation to calculate the spin-orbit interaction energy when the dipole is under the influence of internal magnetic fields, that is,

$$PE = E = -\mu_s \cdot \vec{B}_{\text{int.}} \quad (36c)$$

$$E = -\vec{\mu}_s \cdot \frac{Ze}{4\pi\epsilon_0 mc^2 r^3} \vec{L}$$

$$E = +g_s \frac{\mu_B}{\hbar} \vec{S} \cdot \frac{Ze}{4\pi\epsilon_0 mc^2 r^3} \vec{L} \quad [\text{using Eqn. (32)}]$$

$$E = \frac{+g_s \mu_B Ze}{4\pi\epsilon_0 mc^2 r^3 \hbar} \vec{S} \cdot \vec{L}$$

Substituting $\mu_B = \frac{e\hbar}{2m}$ and $g_s = 2$ in above equation.

$$E = \frac{Ze^2 \vec{S} \cdot \vec{L}}{4\pi\epsilon_0 m^2 c^2 r^3} \quad (36d)$$

This equation is obtained when the nucleus is moving and electron is at rest. Therefore, the electron is under the effect of spin motion only (no orbital motion).

By using similar mathematical calculations, when electron is moving and nucleus is at rest, following relation is obtained

$$E = \frac{Ze^2}{8\pi\epsilon_0 m^2 c^2 r^3} \vec{S} \cdot \vec{L} \quad (37)$$

$$E = \frac{Ze^2}{8\pi\epsilon_0 m^2 c^2 r^3} \left[\frac{J^2 - L^2 - S^2}{2} \right] \quad \left[\begin{array}{l} \vec{J} = \vec{L} + \vec{S} \\ \vec{J} \cdot \vec{J} = (\vec{L} + \vec{S})^2 \\ J^2 = L^2 + S^2 + 2\vec{S} \cdot \vec{L} \end{array} \right]$$

$$E = \frac{Ze^2 \hbar^2}{16\pi\epsilon_0 m^2 c^2 r^3} [j(j+1) - l(l+1) - s(s+1)] \quad (38)$$

Hence, Eqn. (38) represents the spin-orbit interaction energy.

Before we proceed further to obtain total magnetic moment of an electron, we should know about the spectroscopic notation of energy level, that is,

$$nl^{2s+1} \quad (39a)$$

where

$n \rightarrow$ principal quantum number

$l \rightarrow$ orbital quantum number

$2s + 1 \rightarrow$ spin multiplicity

$j \rightarrow$ total angular momentum quantum number

For example, take electron in second level or 2s level then $n = 2$, $l = 0, 1$

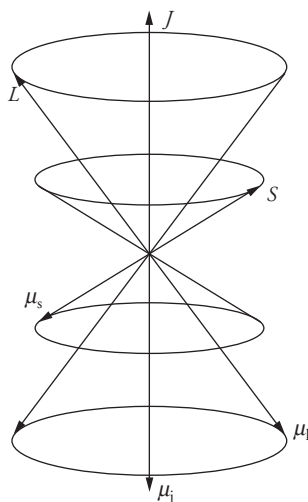


Figure 5.13 Schematic vector diagram showing total angular momentum L , S , and all magnetic moments.

$$\left[s = \frac{1}{2} \right]$$

(i) $n = 2, \quad l = 0 \quad 2S_{\frac{1}{2}}^2$ First term

$$\left[\begin{array}{l} j = l \pm s \\ = 0 \pm \frac{1}{2} \\ = \frac{1}{2} \end{array} \right]$$

(ii) $n = 2, \quad l = 1 \quad 2P_{\frac{1}{2}}^2, 2P_{\frac{3}{2}}^2$ Second term

When the spin-orbit interaction is absent, then all the levels are of same energy or we can say, energy levels are degenerate.

Now, we will proceed further to find out the total magnetic moment for electron. Figure 5.13 shows the schematic of angular momentum and their direction.

As \vec{L} and \vec{S} process around \vec{J} , the component that is along \vec{J} will contribute to the magnetic moment. The components that are perpendicular to \vec{J} will given an average value of zero.

Hence, the magnetic moment along μ_j is given as

$$\begin{aligned} \overline{\mu_j} &= \overline{\mu_l} + \overline{\mu_s} \\ &= -\frac{g_l \mu_B \overline{L}}{\hbar} - \frac{g_s \mu_B \overline{S}}{\hbar} \\ \overline{\mu_j} &= -\frac{\mu_B}{\hbar} [\overline{L} + 2\overline{S}] \end{aligned} \quad (40)$$

$$\mu_j = -\frac{\mu_B}{\hbar} [L \cos \theta_1 + 2S \cos \theta_2] \quad (41)$$

where θ_1 and θ_2 are the angles, which \vec{L} and \vec{S} make with \vec{J} , respectively.

Let us solve two terms of Eqn. (41).

$$\text{Solving for } L \cos \theta_1$$

$$\text{We know } \vec{J} = \vec{L} + \vec{S}$$

$$\vec{S} = \vec{L} - \vec{J}$$

Squaring both sides

$$\begin{aligned} |S|^2 &= |L|^2 + |J|^2 - 2|L||J|\cos\theta_1 \\ L \cos\theta_1 &= \frac{L^2 + J^2 - S^2}{2J} \end{aligned} \quad (42a)$$

$$\text{Similarly, } S \cos\theta_2 = \frac{J^2 + S^2 - L^2}{2J} \quad (42b)$$

Substituting Eqn. 42(a)–(b) into Eqn. (41)

$$\begin{aligned} \mu_j &= -\frac{\mu_B}{\hbar} \left[\frac{L^2 + J^2 - S^2}{2J} + \frac{J^2 + S^2 - L^2}{J} \right] \\ \mu_j &= -\frac{\mu_B}{\hbar} \left[\frac{L^2 + J^2 - S^2 + 2J^2 + 2S^2 - 2L^2}{2J} \right] \\ \mu_j &= -\frac{\mu_B}{\hbar} \left[\frac{3J^2 + S^2 - L^2}{2J} \right] \end{aligned} \quad (43)$$

The term inside the bracket for Eqn. (43) is taken to be g times the total angular momentum vector.

$$\begin{aligned} J \cdot g &= \frac{3J^2 + S^2 - L^2}{2J} \\ g &= \frac{3J^2 + S^2 - L^2}{2J^2} = \left[1 + \frac{J^2 + S^2 - L^2}{2J^2} \right] \\ g &= \left[1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \right] \end{aligned} \quad (44)$$

g in Eqn. (44) is Lande g -splitting factor.

Equation (43) can be written as

$$\mu_j = -\frac{\mu_B}{\hbar} g \vec{J} \quad (45a)$$

$$\mu_j = -\mu_B g \sqrt{j(j+1)} \quad (45b)$$

5.9 LS Coupling For Multi-electron System

For multi-electron system, the total angular momentum \vec{J} is sum total of all individual orbital angular momenta. All the orbital angular momenta L_i couple together to form total orbital angular momentum L ; similarly, the spin of all individual atoms, that is, S_i unite together to produce single spin angular momentum S . Then, both L and S give rise to total angular momentum J via spin-orbit coupling. We can illustrate it through the following example. Let us take two electrons with $l_1 = 2$ and $l_2 = 3$. Then, the following combinations occur:

- (i) L will take value from $l_1 + l_2$ to $|l_1 - l_2|$, that is, 5, 4, 3, 2, 1.
- (ii) S will have values 0 and 1.
- (iii) J will have values from $|L - S|$ to $L + S$.

Hence, for $S = 0, J = 1, 2, 3, 4, 5$, and
for $S = 1, J = 0, 1, 2, 3, 4, 5, 6$.

The LS coupling could be commonly seen in light elements, but for heavier atoms, the nuclear charge is quite high and LS coupling no longer holds good. Then individual total angular momentum of electron J_i adds together to form total angular momentum of atom. This is referred to as JJ coupling. Hence,

$$J_i = L_i + S_i \text{ for individual electron}$$

$$J = \sum J_i \text{ for whole atom}$$

5.10 Zeeman Effect (Normal)

Atomic spectra is influenced by electric and magnetic field, and this phenomena was observed by Zeeman in 1896 and Stark in 1913 respectively.

Zeeman in 1896 found that upon applying magnetic field, the spectral lines are split into multiplets. This phenomenon of splitting the spectral lines under the influence of external applied magnetic field is called Zeeman effect. The experimental set-up used by Zeeman is shown in Figure 5.14(a). Sodium lamp or Hg source could be used as a source of atomic spectra and it is placed between strong magnets.

The spectral lines could be observed in parallel as well as perpendicular direction using some powerful high resolving power spectroscope. The angular velocity (w) of electron moving in circular orbit of radius r and velocity v is given by

$$w = \frac{v}{r} \quad (46)$$

Then the centripetal force experienced by electron is given by

$$F_c = \frac{mv^2}{r} = mrw^2 \quad (47a)$$

When magnetic field B is applied on the electron, then electron also experiences force Bev . The direction of this force depends on the direction of electron. If the force is centripetal, that is, inward direction and the electron is in anticlockwise direction, then the total force on electron is given by (Figure 5.14(b))

$$F = F_c + Bev = m(w + \Delta w)^2 r \quad (47b)$$

$\Delta\omega$ is the small change in angular frequency due to the force produced by magnetic field.

$$mr\omega^2 + Bev = m\omega^2 r + m\Delta\omega^2 r + 2m\omega r \Delta\omega$$

$$Bev = mr\Delta\omega^2 + 2m\omega r \Delta\omega$$

Neglecting the terms with $\Delta\omega^2$

$$Bev = 2m\omega r \Delta\omega$$

$$Bev = 2mv \Delta\omega$$

$$Be = 2m \Delta\omega$$

$$\Delta\omega = \frac{Be}{2m}$$

$$2\pi \Delta f = \frac{Be}{2m}$$

$$\Delta f = \frac{Be}{4\pi m} \quad (47c)$$

This force will cause the acceleration of electrons.

When the magnetic field causes centrifugal action, that is, the direction of force is in outward direction, then the force is given by

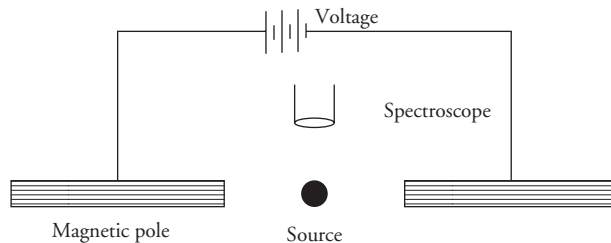


Figure 5.14(a) Experimental set-up for Zeeman effect.

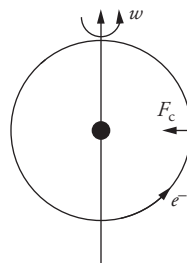


Figure 5.14(b) Electron revolving in anti clockwise direction.

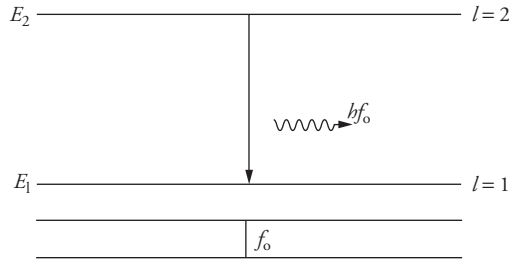


Figure 5.15(a) Frequency line in the absence of Zeeman effect.

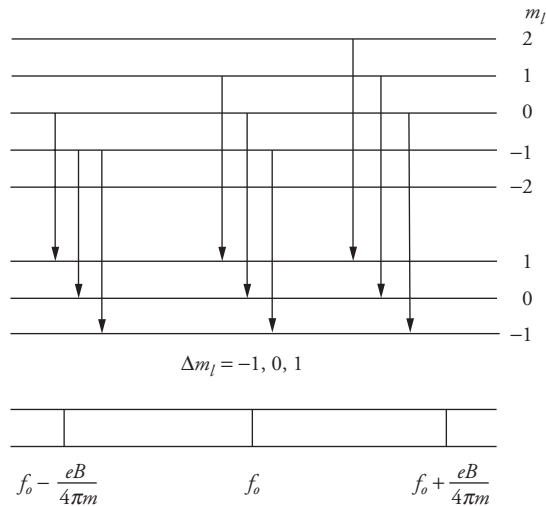


Figure 5.15(b) Zeeman effect in the presence of magnetic field. The transitions showing $\Delta m_l = -1, 0, +1$.

$$\Delta f = -\frac{eB}{4\pi m} \tag{47d}$$

Combining Eqn. 47(c)–(d),

$$\Delta f = \pm \frac{eB}{4\pi m} \tag{48}$$

Hence, the frequency of spectral line changes by Δf . We can conclude:

- (i) If the electron is in anticlockwise direction, then the force increases on electron, which accelerate its motion to $f_0 + \Delta f$.
- (ii) If the electron is in clockwise direction, then the force decreases and the motion of electron decelerates to $f_0 - \Delta f$.

We can demonstrate the Zeeman effect using Figure 5.15. In the absence of magnetic field, the line of frequency is the exact difference of energy of upper and lower energy.

$$E_2 - E_1 = hf_0$$

But, when the magnetic field is tuned on, the splitting of energy levels takes place ($2l + 1$ levels) (Figure 5.15(b)).

We know from Eqn. (29)

$$\mu_l = -\frac{eL}{2m}$$

For the component of L along z -direction, that is,

$$\mu_z = -\frac{e}{2m} L_z = -\frac{em_l \hbar}{2m}$$

The interaction of atom with applied magnetic field depends on the orientation of magnetic moment when an atom is placed inside magnetic field B , and it gives rise to torque (τ)

$$\begin{aligned}\tau &= \bar{\mu} \times \bar{B} \\ \tau &= \mu B \sin\theta\end{aligned}\tag{49a}$$

This torque will tend to rotate the atoms. If dW is the work done to reorient the moment against the torque experienced due to applied force, then it is given by the following expression:

$$dW = \tau \cdot d\theta\tag{49b}$$

where $d\theta$ is the angular displacement produced by torque.

$$dW = \mu B \sin\theta \cdot d\theta$$

This work done is stored in the form of potential energy.

$$-dE = \mu B \sin\theta \cdot d\theta\tag{49c}$$

After integration and mathematical calculations,

$$\Delta E = -\mu \cdot B$$

$$\Delta E = -\frac{eL}{2m} \cdot B$$

$$\Delta E = -\frac{eL_z}{2m} B \quad \text{[Only the } z \text{ component will contribute]}$$

$$\Delta E = -\frac{em_l \hbar B}{2m} \quad \text{[from Eqn. (47c)]}$$

$$\Delta E = m_l \hbar \Delta w\tag{49d}$$

Equation (49d) represents the energy shift of spectral lines, that is, the energies of levels E_1 and E_2 get modified when the atom is under the influence of magnetic field. Let E_{11} and E_{22} be the modified energy levels, such that

$$E_{11} = E_1 + \Delta E = E_1 + \frac{e \hbar m_l B}{2m}\tag{50a}$$

$$E_{22} = E_2 + \Delta E = E_2 + \frac{e \hbar m_l^2 B}{2m} \quad (50b)$$

Subtracting Eqn. (50a) from Eqn. (50b)

$$E_{22} - E_{11} = hf = E_2 - E_1 + \frac{e \hbar B}{2m} (m_l^2 - m_l^1)$$

$$f = f_0 + \frac{eB}{4\pi m} \Delta m_l \quad (51)$$

Allowed transitions are only with $\Delta m_l = 0, \pm 1$

Hence, the following transitions are allowed

(i) $\Delta m = 0$ (Original frequency)

$$f = f_0 \quad (52a)$$

(ii) $\Delta m = -1$

$$f = f_0 - \frac{eB}{4\pi m} = f_0 - \Delta f \quad (52b)$$

(iii) $\Delta m = +1$

$$f = f_0 + \frac{eB}{4\pi m} = f_0 + \Delta f \quad (52c)$$

5.11 Anomalous Zeeman Effect

When the atom is under a strong magnetic field, it gives rise to normal Zeeman effect. But, when the atom is under the influence of weak magnetic field, it gives rise to multiple lines, that is, the spectral line splits into a number of lines. This effect is known as anomalous Zeeman effect. Section 5.8 describes about the Larmor precession. The resultant total angular momentum is given by the vector addition of orbital angular momentum and spin angular momentum, that is, $J = L + S$. Both L and S have precession around J .

From Section 5.8, it is clear that μ_l and μ_s are opposite to \vec{L} and \vec{S} , respectively. This is due to the negative charge on electron. μ_l, μ_s also have precession around J , whereas μ_j cannot have precession around J due to unequal values of $\frac{\mu_l}{L}$ and $\frac{\mu_s}{L}$.

Equation (45b) describes the value of μ_j as

$$\mu_j = -\mu_B g \sqrt{j(j+1)}$$

where

$$g = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \quad (53)$$

As derived in the previous section, according to (49c), the energy is given by

$$\Delta E = -\mu \cdot B$$

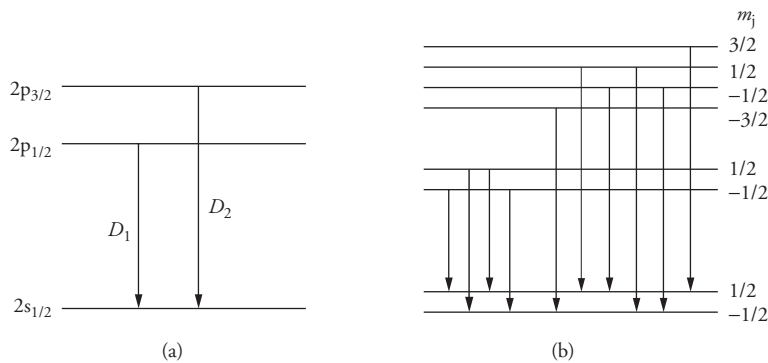


Figure 5.16 Anomalous Zeeman effect (a) in the absence of magnetic field and (b) in the presence of magnetic field.

Here, it can be written as

$$\Delta E = -\mu_j \cdot B$$

$$\Delta E = -\mu_B \cdot g \sqrt{j(j+1)} B$$

$$\Delta E = g B \mu_B \frac{\sqrt{j(j+1)}}{\hbar} \hbar \left[m_j = \frac{J}{\hbar} \right]$$

$$\Delta E = \mu_B g B m_j \quad (54)$$

The allowed transition levels are $m_j = 0, \pm 1$ and total angular momentum J splits for $(2j+1)$ levels. Figure 5.16 illustrates the anomalous Zeeman effect for sodium D_1 and D_2 lines. The allowed transitions are these for which $\Delta l = \pm 1$ and $\Delta m_j = 0, \pm 1$. Hence, according to this rule, D_1 has four splittings and D_2 has six splittings, $\left(\frac{3}{2} \rightarrow -\frac{1}{2}\right)$.

5.12 Stark Effect

In 1913, Stark observed the splitting of spectral lines in an electric field. He observed the splitting of Balmer line in hydrogen spectrum. He used a strong electric field of 10^5 V/cm. Every line was split into many component lines. The number of lines varied as $H_\gamma > H_\beta > H_\alpha$. Hence, the lines increased with higher parent line. Another observation was the linearly polarized s electric component perpendicular to the field. On the contrary, the p components were polarized parallel to the field. The wave number difference between parent line and component line is proportional to the magnitude of electric field. This was directly proportional to electric field up to a field strength of 10^7 V/m and was linear in nature. But as the magnitude of electric field was increased, the difference of parent line and component line was no longer linear in nature.

The Stark effect is responsible for broadening of spectral lines due to charged particle. The splitting of lines is not symmetric in case of stark effect unlike Zeeman effect.

SUMMARY

This chapter deals with the interpretation of atomic structure using different models: Thomson gave pudding model, following which Rutherford performed gold foil experiment. But Rutherford model could not explain the energy spectrum. Later, Bohr postulated that energy is radiated only when electron jumps from higher orbit to lower orbit. Hydrogen spectra could be explained using Bohr's model, but the multi-electron system could not be explained. Furthermore, the correspondence principle demonstrated that at higher quantum numbers, quantum mechanics tends toward classical regime. Sommerfeld modified Bohr's theory in 1955 by postulating that the electrons revolve around nucleus in elliptical orbit. Moreover, electron different velocity at different parts of ellipse vector atom model interpreted orbital angular momentum in terms of vector model along with the space quantization. There are orbital and spin angular momentum for an atom. The total angular momentum (J) is defined as the vector sum of spin and orbital angular momentum. The splitting of spectral lines could be explained on the basis of spin-orbit coupling. The spectroscopic notation of every level is given in terms of term value, that is, $n l_j^{2s+1}$. Lande's g -factor is also explained in terms of angular momentum (spin, orbital, and total). The total angular momentum is also explained for a multielectron system. The influence of magnetic field as spectral lines and the frequency shift was studied using Zeeman effect, whereas the influence of electric field on spectral lines was studied using Stark effect.

SOLVED PROBLEMS

Q.1: Obtain the radius for third orbit of electron in hydrogen atom (given $m = 9.1 \times 10^{-31}$ kg and $h = 6.63 \times 10^{-34}$ Js, charge $e = 1.6 \times 10^{-19}$ C).

Ans: Radius $r_n = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$

For hydrogen, $Z = 1$ and given $n = 3$

$$r_3 = \frac{8.85 \times 10^{-12} \times 9 \times (6.63 \times 10^{-34})^2}{3.14 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^2}$$

$$r_3 = \frac{3501.16 \times 10^{-12} \times 10^{-68}}{73.149 \times 10^{-31} \times 10^{-38}} \Rightarrow r_3 = \frac{3501.16 \times 10^{-80}}{73.149 \times 10^{-69}}$$

$$r_3 = 47.86 \times 10^{-11}$$

$$r_3 = 4.78 \times 10^{-10} \text{ m}$$

$$r_3 = 4.78 \text{ \AA}$$

Q. 2: Obtain the radius for hydrogen atom for second orbit.

Ans: Radius $r_n = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$

For $n = 2$

$$r_2 = \frac{8.85 \times 10^{-12} \times 4 \times (6.63 \times 10^{-34})^2}{3.14 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^2}$$

$$r_2 = \frac{1556.07 \times 10^{-80}}{73.149 \times 10^{-69}}$$

$$r_2 = 21.27 \times 10^{-11} \text{ m} \Rightarrow 2.127 \times 10^{-10} \text{ m}$$

Q. 3: The first member of hydrogen Balmer series has wavelength of 6563 Å. Obtain the wavelength of second member.

Ans:

$$\frac{1}{\lambda_1} = R \left[\frac{1}{2^2} - \frac{1}{3^2} \right] \quad \text{(a)}$$

$$\frac{1}{\lambda_2} = R \left[\frac{1}{2^2} - \frac{1}{4^2} \right] \quad \text{(b)}$$

Dividing Eqn. (a) by (b),

$$\frac{\lambda_2}{\lambda_1} = \frac{20}{27}$$

$$\lambda_2 = \frac{20 \times 6563}{27} \text{ Å} = 4860.2 \text{ Å}$$

Q.4: Obtain the shortest wavelength for principal series of Hydrogen atom.

Ans: $E = hf = \frac{13.6}{n^2}$

For principal series, the electrons should jump from p to $n = 1$.

Hence, $E = hf = 13.6 \text{ eV}$

$$\frac{hc}{\lambda} = 13.6 \text{ eV}$$

$$\lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{13.6 \times 1.6 \times 10^{-19}}$$

$$\lambda = 914 \times 10^{-10} \text{ m}$$

$$\lambda = 914 \text{ Å}$$

Q.5: For Balmer series of hydrogen, the wavelength of first member is given as 6563 Å. Obtain the wavelength for second member of Lyman series for same spectrum.

Ans: For Balmer series,

$$\frac{1}{\lambda_1} = R \left[\frac{1}{2^2} - \frac{1}{3^2} \right] \quad (a)$$

For Lyman series (second member)

$$\frac{1}{\lambda_2} = R \left[\frac{1}{1^2} - \frac{1}{3^2} \right] \quad (b)$$

Dividing Eqs (a) and (b)

$$\frac{\lambda_2}{\lambda_1} = \frac{\frac{5}{36}}{\frac{8}{9}} = \frac{5}{36} \times \frac{9}{8} = \frac{5}{32}$$

$$\lambda_2 = \frac{5}{32} \times \lambda_1 = \frac{5}{32} \times 6563$$

$$\lambda_2 = 1025.46 \text{ \AA}$$

Q.6: The Balmer series wavelength for first member is 6563 Å. Obtain the wavelength for first member of Paschen series in same spectrum.

Ans: For Balmer series,

$$\frac{1}{\lambda_1} = R \left[\frac{1}{2^2} - \frac{1}{3^2} \right] \quad (a)$$

For Paschen series (first member)

$$\frac{1}{\lambda_2} = R \left[\frac{1}{3^2} - \frac{1}{4^2} \right] \quad (b)$$

Dividing Eqs (a) and (b),

$$\frac{\lambda_2}{\lambda_1} = \frac{\frac{5}{36}}{\frac{7}{144}} = \frac{5}{36} \times \frac{144}{7}$$

$$\lambda_2 = \frac{5}{36} \times \frac{144}{7} \times 6563 \text{ \AA}$$

$$\lambda_2 = 18751.42 \text{ \AA}$$

Q. 7: What will be the energy required to excite an electron from the ground state of hydrogen to third level?

Ans: The energy of electron in n th orbit is given by

$$E_n = -\frac{13.6}{n^2}$$

$$E_{n_1} = -\frac{13.6}{1^2} \text{ and } E_{n_3} = -\frac{13.6}{3^2}$$

Hence, energy required = $E_{n_3} - E_{n_1}$

$$E = -\frac{13.6}{3^2} + \frac{13.6}{1^2}$$

$$E = 13.6 \left[\frac{-1+9}{9} \right]$$

$$E = 13.6 \times \frac{8}{9} = 12.08 \text{ eV}$$

Q. 8: For an atom with charge Ze , an electron revolves around the nucleus. 28.4 eV energy is required for an electron to jump from second orbit to third orbit. Obtain the atomic number of atom.

Ans:

$$E_{n_3} - E_{n_2} = 28.4$$

$$28.4 = Z^2 \times 13.6 \left[\frac{1}{2^2} - \frac{1}{3^2} \right]$$

$$\frac{28.4}{13.6} = Z^2 \left[\frac{5}{36} \right]$$

$$Z^2 = \frac{28.4 \times 36}{13.6 \times 5}$$

$$Z \approx 4$$

Q. 9: What would be the energy required to remove the electron from first Bohr's orbit to infinity for helium atom?

Ans: $Z = 2$ for helium

$$E_\infty - E_1 = 13.6 \times Z^2 \left[\frac{1}{1^2} - \frac{1}{\infty^2} \right]$$

$$E_\infty - E_1 = 13.6 \times 4 = 54.4 \text{ eV}$$

Q. 10: What will be the wavelength of electromagnetic radiation required to take out an electron from second Bohr's orbit to ∞ for Beryllium atom?

Ans: $Z = 4$

$$E_\infty - E_2 = 13.6 \times Z^2 \left[\frac{1}{2^2} - \frac{1}{\infty^2} \right]$$

$$E_{\infty} - E_2 = 13.6 \times 4 \text{ eV}$$

$$E_{\infty} - E_2 = hf = 54.4 \text{ eV}$$

$$\frac{hc}{\lambda} = 54.4 \times 1.6 \times 10^{-19} \text{ J}$$

$$\lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{54.4 \times 1.6 \times 10^{-19}}$$

$$\lambda = 0.228 \times 10^{-26} \times 10^{19}$$

$$\lambda = 0.228 \times 10^{-7}$$

$$\lambda = 228 \text{ \AA}$$

Q.11: For hydrogen, an electron is in $2p$ state. Obtain the magnitude of orbital angular momentum and possible z -components of orbital angular momentum \bar{L} .

Ans: The magnitude of orbital angular momentum is

$$L = \sqrt{l(l+1)}\hbar$$

For p state, $l = 1$

$$L = \sqrt{2}\hbar$$

To obtain the possible z -component,

$$L_z = m_l \hbar$$

and m can have values $-1, 0, +1$

Hence,

$$L_z = \hbar, 0, -\hbar$$

Q. 12: If an electron is in $4d$ level for hydrogen, calculate the magnitude of orbital angular momentum along with its possible angular momentum and along with its possible z -components?

Ans:

$$L = \sqrt{l(l+1)}\hbar \quad [l = 2]$$

$$L = \sqrt{2(2+1)}\hbar = \sqrt{6}\hbar$$

$$L = \sqrt{6}\hbar$$

The possible z -components are

$$L_z = m_l \hbar \quad [m_l = +2, +1, 0, -1, -2]$$

$$L_z = 2\hbar, \hbar, 0, -\hbar, -2\hbar$$

Q. 13: For a p -electron for one-electron atom, obtain L , S , and J .

Ans: For a p -electron,

$$l = 1 \quad \text{and} \quad s = \frac{1}{2}$$

Now j can be obtained in the following two ways:

$$(i) \quad j = l + s = 1 + \frac{1}{2} = \frac{3}{2}$$

$$(ii) \quad j = l - s = 1 - \frac{1}{2} = \frac{1}{2}$$

Hence,

$$L = \sqrt{l(l+1)}\hbar$$

$$= \sqrt{1(1+1)}\hbar = \sqrt{2}\hbar$$

$$L = \sqrt{2}\hbar$$

$$S = \sqrt{s(s+1)}\hbar = \sqrt{\frac{1}{2}(\frac{1}{2}+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

$$S = \frac{\sqrt{3}}{2}\hbar$$

$$J = \sqrt{j(j+1)}\hbar$$

For $j = \frac{3}{2}$, $J = \sqrt{\frac{3}{2}(\frac{3}{2}+1)}\hbar = \frac{\sqrt{15}}{2}\hbar$

For $j = \frac{1}{2}$, $J = \sqrt{\frac{1}{2}(\frac{1}{2}+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$

Q. 14: For a d -electron, obtain the values of L , S , and J .

Ans: For a d -electron

$$l = 2 \quad \text{and} \quad s = \frac{1}{2}$$

The values of j can be given in the following two ways:

$$(i) \quad j = l + s = 2 + \frac{1}{2} = \frac{5}{2}$$

$$(ii) \quad j = l - s = 2 - \frac{1}{2} = \frac{3}{2}$$

$$L = \sqrt{l(l+1)}\hbar = \sqrt{6}\hbar$$

$$S = \sqrt{s(s+1)}\hbar = \sqrt{\frac{3}{2}}\hbar$$

$$J = \sqrt{j(j+1)}\hbar$$

For $j = \frac{5}{2}, J = \sqrt{\frac{5}{2}\left(\frac{5}{2} + 1\right)}\hbar = \frac{\sqrt{35}}{2}\hbar$

and $j = \frac{3}{2}, J = \sqrt{\frac{3}{2}\left(\frac{3}{2} + 1\right)}\hbar = \frac{\sqrt{15}}{2}\hbar$

Q.15: For an electron in $p_{3/2}$ state, obtain the values of m_j and J_z .

Ans: $l = 1$ for p -state

and $j = 3/2, s = 1/2$

The values of m_j are $3/2, 1/2, -1/2, -3/2$

and $J_z = m_j\hbar$

$J_z = 3/2\hbar, 1/2\hbar, -1/2\hbar, -3/2\hbar$

Q.16: Obtain the orbital states for $n = 3, s = 1/2$

Ans: $n = 3$ determines $l = 0, 1, 2$

Case I: $l = 0$ (s -state)

$s = 1/2$

$j = l + s = 1/2 \Rightarrow 3s_{1/2}^2$

Case II: $l = 1, s = 1/2$

$j = l \pm s = 3/2, 1/2$

$3p_{3/2}^2, 3p_{1/2}^2$

Case III: $l = 2, s = 1/2$

$j = l \pm s = 5/2, 3/2$

$3d_{5/2}^2, 3d_{3/2}^2$

Orbital state: $n l_j^{2s+1}$ [$2s + 1$ is known as spin multiplicity]

Q. 17: For two electrons with same $l = 2$ and $s = 1/2$, what would be the possible values for quantum number L and spin quantum number S ?

Ans: $l_1 = 2$ and $l_2 = 2$ for both electrons

Hence, $L = l_1 + l_2, l_1 + l_2 - 1, \dots, |l_1 - l_2|$

$L = 4, 3, 2, 0$

$s_1 = 1/2$ and $s_2 = 1/2$ for both electrons

$$S = s_1 + s_2, s_1 + s_2 - 1, \dots, |s_1 - s_2|$$

$$S = 1, 0$$

Q.18: What would be the total quantum number J for two electrons with same $l = 1$ and $s = \frac{1}{2}$?

Ans:

$$l_1 = l_2 = 1$$

$$L = 2, 1, 0$$

$$s_1 = s_2 = \frac{1}{2}$$

$$S = 1, 0$$

The allowed value for J are as follows:

(i) $L = 2, S = 1$
 $J = L + S, L + S - 1, \dots, |L - S|$
 $J = 3, 2, 1$

(ii) $L = 2, S = 0$
 $J = 2$

(iii) $L = 1, S = 1$
 $J = 2, 1, 0$

(iv) $L = 1, S = 0$
 $J = 1$

(v) $L = 0, S = 1$
 $J = 1$

(vi) $L = 0, S = 0$
 $J = 0.$

Q.19: Two electrons have different values of orbital quantum number $l_1 = 1$ and $l_2 = 2$. What will be the values of L, S ?

Ans:

$$l_1 = 1 \quad \text{and} \quad l_2 = 2$$

$$L = l_1 + l_2, l_1 + l_2 - 1, \dots, |l_1 - l_2|$$

$$L = 3, 2, 1$$

$$s_1 = s_2 = \frac{1}{2}$$

$$S = 1, 0$$

Q.20: What would be the total quantum number J for electron with $l_1 = 1$ and $l_2 = 3$?

Ans:

$$l_1 = 1 \quad \text{and} \quad l_2 = 3$$

$$L = 4, 3, 2$$

For $s_1 = s_2 = \frac{1}{2}$

$$S = 1, 0$$

J can have the following values:

(i) $L = 4, S = 1$

$$J = j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2|$$

$$J = 5, 4, 3$$

(ii) $L = 4, S = 0$

$$J = 4$$

(iii) $L = 3, S = 1$

$$J = 4, 3, 2$$

(iv) $L = 3, S = 0$

$$J = 3$$

(v) $L = 2, S = 1$

$$J = 3, 2, 1$$

(vi) $L = 2, S = 0$

$$J = 2$$

Q.21: Obtain the orbital states (term values) for electrons with $l_1 = 1$ and $l_2 = 2$.

Ans:

$$l_1 = 1 \quad \text{and} \quad l_2 = 2$$

$$L = 3, 2, 1$$

$$s_1 = s_2 = \frac{1}{2}$$

$$S = 1, 0$$

The possible values of J are

(i) $L = 3, S = 1$

$$J = 4, 3, 2$$

Term values:

$${}^3F_{4,3,2}$$

(ii) $L = 3, S = 0$

$$J = 3$$

Term values:

$1F_3$

(iii) $L = 2, S = 1$

$$J = 3, 2, 1$$

Term values:

$${}^3D_{3,2,1}$$

(iv) $L = 2, S = 0$

$J = 2$

Term values: 1D_2

(v) $L = 1, S = 1$

$J = 2, 1, 0$

Term values: ${}^3P_{2,1,0}$

(vi) $L = 1, S = 0$

$J = 1$

Term values: 1P_1

Q. 22: Is state ${}^2s_{3/2}$ possible or not?

Ans: $l = 0$ and $2s + 1 = 2$
 $s = 1/2$

Hence, $j = l + s = 1/2$

Therefore, ${}^2s_{3/2}$ cannot exist; but ${}^2s_{1/2}$ can exist.**Q. 23:** Calculate Lande's splitting factor for $l = 1$ and $s = 1/2$.

Ans: $l = 1, s = 1/2$

$$j = l \pm s = 3/2, 1/2$$

$$g_j = 1 + j \frac{(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$$

For $j = 3/2$,

$$g_{3/2} = 1 + \left(\frac{\frac{3}{2} \left(\frac{3}{2} + 1 \right) + \frac{1}{2} \left(\frac{1}{2} + 1 \right) - (1+1)}{2 \times \frac{3}{2} \left(\frac{3}{2} + 1 \right)} \right)$$

$$g_{3/2} = 1 + \left(\frac{\frac{15}{4} + \frac{3}{4} - 2}{15} \right)$$

$$g_{3/2} = 1 + \left(\frac{\frac{18}{4} - 2}{15} \right) = 1 + \frac{10}{4 \times 15}$$

$$g_{\frac{3}{2}} = 1 + \frac{10}{60} = \frac{7}{6} = 1.16$$

For $j = \frac{1}{2}$,

$$g_{\frac{1}{2}} = 1 + \left(\frac{\frac{1}{2} \left(\frac{1}{2} + 1 \right) + \frac{1}{2} \left(\frac{1}{2} + 1 \right) - (1+1)}{2 \times \frac{1}{2} \left(\frac{1}{2} + 1 \right)} \right)$$

$$g_{\frac{1}{2}} = 1 + \left(\frac{\frac{3}{2} - 2}{\frac{3}{2}} \right)$$

$$g_{\frac{1}{2}} = 1 + \left(-\frac{1}{2} \times \frac{2}{3} \right)$$

$$g_{\frac{1}{2}} = 1 - \frac{1}{3} = \frac{2}{3} = 0.66$$

Hence,

$$g_{\frac{3}{2}} = 1.16$$

$$g_{\frac{1}{2}} = 0.66$$

Q. 24: The spectral lines are separated by 0.04 nm. Obtain the magnitude of magnetic field required to a line of 422.7 nm in order to resolve the triplets? (given $e/m = 1.76 \times 10^{11}$ C/kg)

Ans:
$$df = \pm \frac{eB}{4\pi m}$$

$$f = \frac{c}{\lambda}$$

$$df = -\frac{c}{\lambda^2} d\lambda$$

$$-\frac{c}{\lambda^2} d\lambda = \pm \frac{eB}{4\pi m}$$

$$d\lambda = \pm \frac{\lambda^2}{c} \frac{eB}{4\pi m}$$

where $d\lambda$ is Zeeman shift.

Here,
$$d\lambda = \frac{\lambda^2}{c} \frac{eB}{4\pi m}$$

$$B = \frac{d\lambda}{\lambda^2} \frac{c 4\pi m}{e}$$

$$B = \frac{d\lambda}{\lambda^2} \frac{c 4\pi}{(e/m)}$$

$$\lambda = 422.7 \text{ nm}$$

$$d\lambda = 0.04 \times 10^{-9} \text{ m}$$

$$e/m = 1.76 \times 10^{11} \text{ C/kg}$$

$$B = \frac{0.04 \times 10^{-9} \times 4 \times 3.14 \times 3 \times 10^8}{(422.7 \times 10^{-9})^2 \times (1.76 \times 10^{11})}$$

$$B = \frac{1.5072 \times 10^{-1}}{314468.51 \times 10^{-18} \times 10^{11}}$$

$$B = \frac{1.5072 \times 10^{-1} \times 10^7}{314468.51}$$

$$B = \frac{1.5072 \times 10^6}{314468.51}$$

$$B = \frac{1507200}{31446851}$$

$$B = 4.79 \text{ T}$$

Q. 25: If magnetic field of 1 T is applied and Zeeman separation of 0.0116 nm is observed for 500 nm spectral line, obtain charge/mass ratio for electron.

Ans: $B = 1 \text{ T}$, $d\lambda = 0.0116 \text{ nm}$, and $\lambda = 500 \text{ nm}$

$$d\lambda = \frac{\lambda^2}{c} \frac{e}{4\pi m} \cdot B$$

$$\left(\frac{e}{m}\right) = \frac{d\lambda}{\lambda^2} \frac{c(4\pi)}{B}$$

$$\left(\frac{e}{m}\right) = \frac{0.0116}{(500)^2} \times \frac{3 \times 10^8 \times 4 \times 3.14}{1}$$

$$\left(\frac{e}{m}\right) = 1.754 \times 10^{11} \text{ C/kg}$$

OBJECTIVE QUESTIONS

1. According to Thomson's pudding model

- (a) neutrons are uniformly distributed (b) atom is charged
 (c) positive charge is uniformly distributed (d) all of the above

2. Thomson model failed because
- (a) it could not explain energy spectra
 - (b) it could not explain the wavelength pattern
 - (c) it could not explain multi-electron system
 - (d) all of the above
3. Rutherford used the following particle for gold foil experiment:
- (a) Hydrogen
 - (b) Helium
 - (c) Carbon
 - (d) Nitrogen
4. The undeflected α -particles were due to
- (a) empty space inside atom
 - (b) direct head-on collision
 - (c) due to magnetic field
 - (d) none of the above
5. According to Bohr's model,
- (a) energy is lost when electron moves in shell
 - (b) energy is lost even if electron is stationary
 - (c) energy is lost when electron jumps from one orbit to another
 - (d) energy is gained when electron is stationary
6. For $Z = 1$ and $r = 1.129 \text{ \AA}$, the velocity of electron is
- (a) $2.13 \times 10^8 \text{ m/s}$
 - (b) 0
 - (c) $3.148 \times 10^5 \text{ m/s}$
 - (d) $\approx c$
7. The radius of first orbit for hydrogen is
- (a) 0.42 \AA
 - (b) 1.2 \AA
 - (c) 0.63 \AA
 - (d) 0.529 \AA
8. The energy of an electron in orbit is proportional to
- (a) $\frac{1}{n}$
 - (b) n^2
 - (c) n^3
 - (d) $\frac{1}{n^2}$
9. Value of Rydberg constant is
- (a) 102.535 cm^{-1}
 - (b) 109737 cm^{-1}
 - (c) 1097.37 cm^{-1}
 - (d) 10973.7 cm^{-1}
10. For Brackett Series, the transition occurs from n to
- (a) 4
 - (b) 3
 - (c) 2
 - (d) 1

11. According to correspondence principle, the frequency is given by

- (a) $2Rc$ (b) $\frac{2Rc}{n^3}$
(c) $\frac{2R^2c}{n^3}$ (d) $2Rcn^3$

12. At what value of n , the frequency of spectral line tends to the orbital frequency?

- (a) 1 (b) 10
(c) ∞ (d) 0

13. According to Sommerfeld atomic model, the velocity

- (a) changes (b) remains same
(c) zero (d) is infinite

14. The fine structure constant is given by

- (a) 200 (b) $\frac{1}{200}$
(c) 137 (d) $\frac{1}{137}$

15. The magnitude of L is given by

- (a) $l(l+1)\hbar$ (b) $\sqrt{l(l+1)}\hbar$
(c) $(2l+1)\hbar$ (d) $\sqrt{(2l+1)}\hbar$

16. If magnetic field is along z -direction, then S_z is given by

- (a) $(m_s + 1)$ (b) $m_s\hbar$
(c) $\frac{m_s}{\hbar}$ (d) $m_s^2\hbar$

17. The value of Bohr magneton ($\mu_B = \frac{e\hbar}{2m}$) is given by

- (a) $8 \times 10^{-10} \text{ Am}^2$ (b) $9.26 \times 10^{-10} \text{ Am}^2$
(c) $9.24 \times 10^{-24} \text{ Am}^2$ (d) $9.24 \times 10^{-14} \text{ Am}^2$

18. The value of g_l and g_s is

- (a) 1, 2 (b) 2, 1
(c) 0, 2 (d) 2, 0

19. The total angular momentum j is given by

- (a) $j = \frac{l}{s}$ (b) $\frac{s}{l}$
(c) $l \pm s$ (d) $2s + l$

20. Term-value is represented by

(a) $n L_{2s+1}^j$

(b) $n J_{2s+1}^l$

(c) $n S_j^{2l+1}$

(d) $n L_j^{2s+1}$

21. The Lande's g -factor is given by

(a) $\frac{j(j+1) - s(s+1) + l(l+1)}{2j(j+1)}$

(b) $1 + \left[\frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \right]$

(c) $1 - \left[\frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \right]$

(d) $2j(j+1) - l(l+1) + s(s+1)$

22. The frequency shift in Zeeman effect is given by

(a) $\frac{eB}{4\pi m}$

(b) $\frac{4\pi m}{eB}$

(c) eB

(d) $eB4\pi m$

ANSWERS

1. (c)

7. (d)

13. (a)

19. (c)

2. (d)

8. (d)

14. (d)

20. (d)

3. (b)

9. (b)

15. (b)

21. (b)

4. (a)

10. (a)

16. (b)

22. (a)

5. (c)

11. (b)

17. (c)

6. (a)

12. (c)

18. (a)

Micro-Assessment Questions

1. How do we know that a photon has a spin of 1?
2. For a one-electron atom or ion, spin–orbit coupling splits all states except s-states into doublets. Why are s-states exceptions to this rule?
3. Give the postulates of Thomson’s model.
4. Why Rutherford model was not a success?
5. What is the total angular momentum for an atom?
6. Why was the concept of electron spin introduced?
7. What is correspondence principle?
8. What do you understand by symmetric functions?
9. Describe antisymmetric wave functions.
10. Comment on the angular momentum conservation for orbits.
11. What are the postulates of Bohr’s model.
12. What do you understand by Zeeman effect? How it differs from anomalous Zeeman effect?
13. Give the significance of Lande g -factor.
14. Explain LS coupling. Also explain the term value.
15. What do you understand by Larmor precession?
16. Why Zeeman effect occur in the nuclei with even number of electrons?
17. What do you understand by quantization of angular momentum?

Critical Thinking Questions

1. What do you understand by binding energy of an electron?
2. Find out the expression for Bohr’s radius.
3. Categorize the spectral lines in different series according to principal quantum number.
4. Obtain the Rydberg empirical formula for spectral lines in optical spectra.
5. Explain Bohr’s correspondence principle. Show that at high quantum numbers, the behavior of atoms follows classical trend.
6. What do you understand by stationary state? Does it infer the particle at rest in that state?
7. Compare old and new quantum theory.
8. Calculate the velocity of electron in Bohr’s 4th orbit.
9. Calculate the wavelength of Balmer series line originating from 4th shell to 2nd shell.
10. How the shortcomings of Rutherford’s model are overcome by Bohr’s model?
11. Derive the expression for Zeeman shift.
12. Derive an expression for Rydberg constant.
13. Describe the splitting of spectral lines for sodium atom using Zeeman effect.
14. Describe the spin–orbit interaction and obtain the interaction energy.
15. Explain the splitting of spectral lines in the presence of electric field.
16. Give the mathematical proof for Bohr’s correspondence principle.
17. What is the value for spin magnetic moment of free electron?

Graded Questions

1. Calculate the energy required to eject an electron from 2nd shell of the hydrogen atom.
2. Calculate the radius of 4th Bohr orbit of hydrogen atom along with the energy of electron in that orbit.
3. The Balmer series of hydrogen correspond to wavelength of 6563×10^{-10} m. Find out the wavelength for first line of Lyman series.
4. Discuss LS and JJ coupling in detail. Which one holds for lighter particles?
5. Calculate the wavelength of first line in Paschen series and Paschen series limit ($R_H = 1.097 \times 10^7/\text{m}$).
6. Derive the expression for Larmor frequency for an atom with magnetic moment μ , under the influence of external magnetic field H .
7. Compute Zeeman components for ${}^2D_{3/2}$ to ${}^2P_{1/2}$.
8. Derive the expression for Lande g -factor. Using it, explain anomalous Zeeman effect.
9. Calculate the Lande g -factor for an atom with single (a) p electron and (b) d electron.
10. Find out the possible values of L , S , and J under LS coupling for $l_1 = 1$ and $l_2 = 3$.
11. Show that the term values for pd configuration is same for JJ and LS coupling.
12. Derive the spin-orbit coupling for one-electron system.
13. Derive the expression for total magnetic moment of atomic electron.
14. Why the spin and orbital angular momenta show coupling?
15. Calculate the energy between Zeeman levels corresponding to $m_1 = 0, +1$, when the atom is under the influence of 3 T magnetic field.
16. When sodium is in ${}^2P_{3/2}$ state and is placed in magnetic field of 1.5T, the levels split into four levels. Calculate the energy difference between these levels.

Remember and Understand

1. Electrons revolve the nucleus in orbits having a set size and energy.
2. The energy of the orbit is related to its size. The smallest orbit possesses lowest energy. Radiation is absorbed or emitted when an electron jumps from one orbit to another.
3. Bohr model violates the Heisenberg uncertainty principle because it assumes electrons to have known values for both radius and orbit.
4. Bohr model provides an incorrect value for the ground state orbital angular momentum and it cannot predict the spectra of larger atoms. It does not predict the relative intensities of spectral lines.
5. Bohr model fails in explaining fine structure and hyperfine structure in spectral lines. It does not explain the Zeeman effect or Stark effect.
6. For multi-electron atoms, when the spin-orbit coupling is weak, it can be presumed that the orbital angular momenta of the individual electrons add to form a resultant orbital angular momentum L .
7. For heavier elements with larger nuclear charge, the spin-orbit interactions become as strong as the interactions between individual spins or orbital angular momenta. For such cases, the spin and orbital angular momenta of individual electrons tend to couple to form individual angular momenta.

8. Pieter Zeeman observed that the splitting of spectral lines in the presence of magnetic field is attributed to the interaction between the magnetic field and the magnetic dipole moment associated with the orbital angular momentum. However, in the absence of the magnetic field, the hydrogen energies depend only on the principal quantum number n .
9. The splitting of atomic spectral lines as a result of an externally applied electric field was discovered by Stark and is called the Stark effect. The splitting of spectral lines is not symmetric like that of the Zeeman effect.
10. Zeeman effect gives frequency shift by Δf , given by

$$\Delta f = \frac{eB}{4\pi m}$$

11. The Land- g factor is given by

$$g = \left[\frac{1 + j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \right]$$

Nuclear Physics — I

Nuclei and Nuclear Models

Keywords: Nucleus, neutrons, meson-theory, exchange forces, magic numbers, liquid drop model, shell model, nuclear forces, spin dependence, electric quadrupole

Learning Objectives

- ◆ To understand the components of nuclear and nuclear density
- ◆ To learn atomic mass unit as special unit to measure mass
- ◆ To understand the behavior of nuclear forces as short range, spin dependent, charge independent, and strongest forces
- ◆ To understand the various components of tensor forces
- ◆ To gain insight into electric quadrupole moment
- ◆ To understand Wigner, Barlett, Majorana, and Heisenberg force as exchange forces
- ◆ To learn and understand Yukawa theory and its postulates
- ◆ To learn about various nuclear models
- ◆ To understand the tensor and exchange forces
- ◆ To understand the liquid drop model where the nuclei are considered to be incompressible liquid drop of high density
- ◆ To obtain the semi-empirical Weizsacker's formula
- ◆ To explain nuclear fission on the basis of liquid drop model
- ◆ To learn the merits and demerits of liquid drop model
- ◆ To understand the concept of "magic numbers"
- ◆ To learn about shell model, where nucleon is assumed as a particle moving in potential well
- ◆ To gain insight into spin-orbit coupling demonstrating stretch and jackknife case
- ◆ To discuss the success of shell model
- ◆ To learn why shell model failed

Matter in the universe is composed of atoms. The atoms further combine to form molecules. The basic structure of an atom consists of electrons, protons, and neutrons. Electrons are present in the outermost shells and neutrons and protons are present inside the nucleus. Hence, nucleus can be considered as the smallest entity that encloses elementary particles, that is, neutron and proton. The role of nucleus and the various phenomena related to it will be studied in detail in this chapter, as nucleus is the smallest but a very complex entity.

Nuclear physics deals with the study of microscopic phenomena inside nucleus, along with the behavior and characteristic of nucleus. The origin of research on matter started in 4 BC. Furthermore, with the help of Mendeleev Periodic table, the systematic study of matter was done. Rutherford, Marie Curie, Geiger, Marsden, Thomson, etc., are the common names associated with nuclear and atomic physics. Thomson and Rutherford performed studies to determine individual nature of atoms. Atomic physics deals with the study of individual atoms. Atomic physics and chemistry are the foundation of nuclear physics. Furthermore, nuclear physics helped to gain insight into particle physics, that is, study of elementary particles such as electron, proton, and neutron.

6.1 Components of Nucleus

Thomson described the atom to be like a plum pudding. Anyhow Rutherford's gold foil experiment determined lots of empty space inside the atom and positive charge centered at one point. The entity in which all the protons (positive charges) are present is called nucleus; electrons are present outside this positive core. Bohr specified that the electrons revolve around the nucleus in fixed orbits. He also concluded that the revolving electrons lose energy whenever they jump from higher orbit to lower orbit. Hence, the elementary particles play a vital role in determining the properties of nucleus. Some properties are listed below.

6.1.1 Nucleus

It contains neutrons and protons:

	Neutron	Proton
Charge	0	1.6×10^{-19} C
Mass	1.67×10^{-27} kg	1.67×10^{-27} kg

Size of nucleus = 10^{-14} m

Size of atom = 10^{-10} m

The impact parameter can be given by

$$d = \frac{2Ze^2}{4\pi\epsilon_0 E} \quad (1)$$

where E represents energy of incident particle, Z is the atomic number

The nuclear density can be calculated as

$$\begin{aligned} \text{Nuclear density} &= \frac{\text{Mass}}{\text{Volume}} = \frac{\text{Mass}}{\frac{3}{4}\pi R^3} = \frac{M}{\frac{3}{4}\pi (R_0 A^{1/3})^3} \quad \left[\begin{array}{l} R = R_0 A^{1/3}, A = \text{atomic mass} \\ R_0 \approx 1.2 \text{ fermi} \end{array} \right] \\ &= \frac{1.67 \times 10^{-27} A}{\frac{4}{3}\pi R_0^3 A} = 2.29 \times 10^{17} \text{ kg/m}^3 \quad (2) \end{aligned}$$

Ernest Rutherford was an English physicist who is credited with discovering the nucleus in the early 1900s. Rutherford's gold foil experiment is a well-known experiment in which he bombarded α -particles onto a thin sheet of gold foil. This experiment was done at the University of Manchester. Most of the α -particles passed through the atom and some of them got deflected. He concluded a large empty space within the atom. He discovered that the atom consists of positive mass known as nucleus, which is concentrated at the center. He further postulated that nucleus contained a particle with a positive charge known as "proton" from the Greek word "protos," meaning "first." Every element is characterized by different number of protons in their nuclei. Hence, hydrogen nucleus is the fundamental nuclei consisting of one proton. Before the discovery of nucleus, it was believed that positive and negative charges were distributed evenly throughout the atom. Ernest Rutherford also did extensive experimentation to explore radioactivity. He studied radioactivity along with Marie and Pierre Curie and Henri Becquerel. During his career in atomic physics, Rutherford taught many famous physicists.



ERNEST RUTHERFORD

During his career in atomic physics, Rutherford taught many famous physicists.

6.1.2 Electrons

Following are the properties of electron:

Mass of electron = 9.1×10^{-31} kg

Charge of electron = -1.6×10^{-19} C

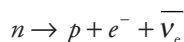
We should now calculate atomic density. From Eqn. (2), it is clear that nuclear density is almost independent of mass number A . The atomic radius is four orders bigger than nuclear radius, hence

$$\text{Atomic density} = \frac{2.29 \times 10^{17}}{(10^4)^3} = 2.29 \times 10^5 \text{ kg/m}^3 \quad (3)$$

Figure 6.1 shows the variation of nuclear density with nuclear radius. It is concluded that the density (nuclear) is almost constant everywhere except the surface. The density on surface is less than the density at center due to the phenomena of surface tension.

Note:

*Free neutron is unstable and decays through weak interaction,



where $t_{1/2} = 12$ min

$\bar{\nu}_e$ = antineutrino

*Bound neutron is stable.

*Free proton is stable whereas bound proton is unstable. Bound proton decays as



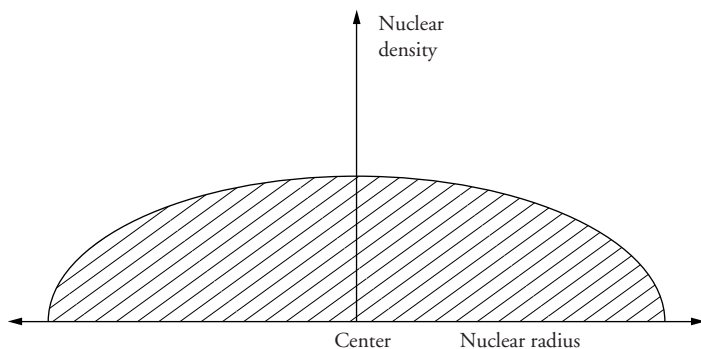
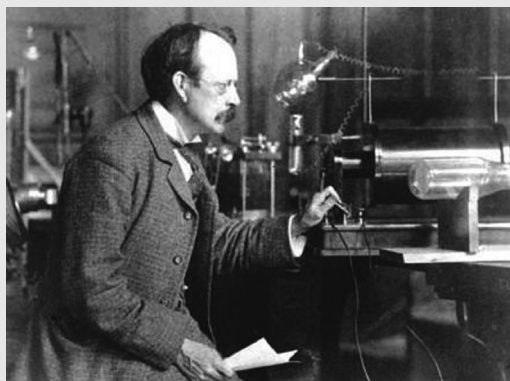


Figure 6.1 Nuclear radius versus nuclear density.

In 1897, the experiments of Dr J.J. Thomson led to the discovery of the basic building block of matter, that is, electron. Thomson was working with currents of electricity inside empty glass tubes at the Cavendish Laboratory at Cambridge University. Along with it, he was also investigating the cathode rays. He found the mysterious particles in cathode rays to be very smaller than the size of atomic nucleus. He coined the term corpuscles for these particles. It was believed that the atom is the most fundamental and indivisible unit of matter. Hence, the scientific community was astonished to imagine more smaller particle occupying some position inside the atom. Thomson did strenuous experimental work to prove the existence of these fundamental particles (corpuscles) and to avoid confusion. He concluded the cathode rays to be made up of electrons, which are negatively charged particles. These electrons are indeed fundamental parts of every atom.



J.J. THOMSON

6.2 Mass of Nucleus

When we talk about atomic mass, it is sum of mass of neutrons, protons, and electrons. The electrons possess very small atomic mass, hence their mass is almost negligible in comparison to protons as well as neutrons. In other words, we can take atomic mass to be “nuclear mass.” For calculating nucleus mass, subtraction of electronic mass from atomic mass is important. The masses are measured in terms of special unit, that is, atomic mass unit or a.m.u., which is defined as the $\frac{1}{12}$ th of mass of single carbon atom (${}_6\text{C}^{12}$) (according to general conference on weight and measures held in 1960).

Twelve grams of carbon correspond to 1 mole atoms of carbon (1 mole = 6.023×10^{23} atoms).

$$1 \text{ a.m.u.} = \frac{1}{12} \times \frac{12}{6.023 \times 10^{23}} = 1.66 \times 10^{-27} \text{ kg}$$

Corresponding to 1 a.m.u., the energy is given by relation $E = mc^2$

$$\text{Energy in 1 a.m.u.} = \frac{(1.66 \times 10^{-27} \text{ kg}) \times (3 \times 10^8 \text{ m/s})^2}{1.6 \times 10^{-19}} \text{ eV} \quad (6a)$$

$$1 \text{ a.m.u.} = 931 \text{ MeV} \quad (6b)$$

The mass defect for nuclues is given by $\Delta m = (Zm_p + Nm_n - M)$ a.m.u where m_p , m_n , and M represent mass of proton, mass of neutron, and mass of atom respectively. Furthermore, the packing fraction can be obtained by dividing mass defect with the total number of nucleons. Z is the atomic number and N is the number of neutrons for an atom.

James Chadwick was an English physicist working with Rutherford. In 1932, while working with Rutherford, he detected neutrons and measured their mass. He bombarded the neutrons onto a block of paraffin wax. The paraffin wax had high concentration of hydrogen, which made it rich in protons. Upon collision of neutrons with protons present in the wax, some protons were knocked out. Chadwick detected the protons and calculated their energy and mass. He further used principles of energy and momentum conservation to obtain the mass of the neutrons. He obtained the mass of neutrons to be slightly more than that of a proton.



JAMES CHADWICK

6.3 Nuclear Forces

Inside nucleus, neutrons and protons exist and electrons revolve around the nucleus. Proton is positively charged, although neutron is a neutral particle. A question arises: If so many protons coexist inside the nucleus, then the electrostatic repulsive forces must be there. Despite strong electrostatic repulsive force, the nucleus behaves as a strong and stable entity. Hence, some other force must be coexisting, which binds the nucleus together. Obviously, these forces must be more strong than Coulomb's forces and gravitational forces. These strong forces that exist inside the nucleus and bind the proton and neutron together are know as nuclear force. Following are the properties of nuclear forces:

- (i) **Strongest forces:** The nuclear forces are 100 times more stronger than the electrostatic Coulombs' repulsive force and 10^{38} times more stronger than the gravitational forces. Indeed, the nuclear forces can be regarded as the strongest forces present in nature.
- (ii) **Charge independent:** Neutrons and protons inside the nucleus interact with each other. The following interactions occur within a nucleus: neutron–neutron, proton–proton, and neutron–proton. These interactions are independent of the electric charge on the nucleons (neutrons and protons are collectively known as nucleons). Hence, n–n, n–p, and p–p interactions posses the same nature. We can illustrate it with the help of an example, that is, consider tritium, ${}_1\text{H}^3$ and ${}_2\text{He}^3$ nuclei,

For tritium, number of protons = 1 = number of neutrons in helium

For helium, number of protons = 2 = number of neutrons in tritium

The binding energy of tritium (${}_1\text{H}^3$) is 8.49 MeV, whereas the isotope of helium (${}_2\text{He}^3$) possesses binding energy of 7.72 MeV. Comparing both the binding energies, it is clear that tritium has higher and strong attractive force inside the nucleus. The lower binding energy in ${}_2\text{He}^3$ could

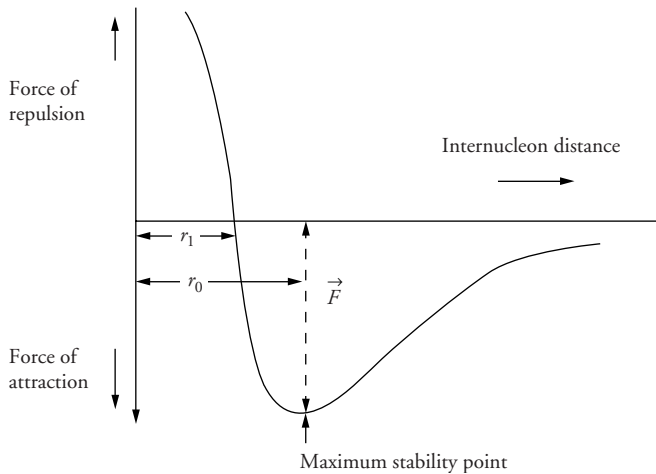


Figure 6.2 Variation of force with internucleon distance.

be due to repulsive force existing between the p–p pair. In lower atomic mass nuclei, n–p pair is the preferred one. As the atomic mass increases, the number of neutrons also increases and it leads to n–n pairing. Hence, n–n forces could also lead to stable nuclei. We can approximate the magnitude of these forces to be same.

- (iii) **Short range:** Figure 6.2 shows nuclear forces exist within certain range. They do not extend upto large distances. The distance between nucleons should be comparable to the size of nucleons for nuclear forces to exist. The range of nuclear forces is approximately 2.2 fm and the forces drop to almost negligible value at a distance of 4.2 fm (1 Fermi = 10^{-15} m). The maximum forces of attraction between nucleons exist at a distance of 1.5×10^{-15} m. If the distance is decreased beyond this, then the nuclear attractive force also decreases. At a distance of 0.5 fm, the nuclear attractive force becomes zero. If the distance is decreased below 0.5 fm, then instead of attractive force, the repulsive forms within nucleons come into action. This repulsive force also plays a very important role, as it stabilizes the nucleus by preventing the collapse of nucleons. At long distances, the nuclear forces are almost zero. Moreover, electrons are totally immune from the nuclear forces, that is, they do not feel the influence of nuclear forces on them.
- (iv) **Spin-dependent and saturated:** The nucleons with same spin have stronger force of attraction than the nucleons with antiparallel spin. Nucleon can satisfy certain coordinate number with its neighbors, that is, there is defined number of bonds that nucleons can make with each other. For atomic number greater than 40 MeV, average binding energy per nucleon is constant. This indicates that the nuclear forces are saturated. If nucleons have interacted with every nucleon, then the binding energy would have been quite large. Hence, the nuclear forces are saturated forces.
- (v) **Non-central:** The forces that donot act along the line joining the centers of nucleons are known as non-central forces. The nuclear forces do not act along the line that joins the centers of two nucleons. Hence, nuclear forces are regarded as non-central forces. The nuclear forces have tensor components that give non-central character to them. Under the effect of tensor forces the angular momentum component is no longer conserved.

- (vi) **Exchange character:** The nuclear forces exhibit exchange character. The nucleons keep on exchanging π -mesons between them (discussed in Meson Theory, Section 6.7).

We will proceed to the theory of nuclear forces, but we should have an understanding of tensor forces and exchange forces first. The following sections describe these forces.

6.4 Tensor Forces

The total magnetic moment is the sum of magnetic moment due to spin and orbital motion of the particle for a two-electron system. With $l = 0$, the possible spin states can be $s = 1$ or 0 . When $l = 0$, it signifies no contribution of orbital momentum. Let us elaborate this concept with the help of neutron problem.

The wave function of deuteron is described by the following equation:

$$\varphi = a_s \varphi_s + a_d \varphi_d \quad (7)$$

Equation 7 gives the wave function divided in two parts φ_s corresponds to s state, that is, $l = 0$ and φ_d corresponds to wave function representing $l = 2$ state or d-state a_s and a_d are scattering constants, which describe extent of scattering. In d -state, the nucleus is distorted in shape and the nuclear force is noncentral. The new force is known as tensor forces that satisfy the following points:

1. It depends on orientation of spin w.r.t. the line that joins nucleons.
2. It depends on distance r (within the nucleons).

The spin orientations are regarded as $\vec{\sigma}_1$ and $\vec{\sigma}_2$. These spin orientations are also responsible for quadrupole moment (deviation from spherical symmetry). The equation of potential under the effect of tensor forces is given by

$$V(r) = V_1(r) + V_2(r) \vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_3(r) S_{12} \quad (8)$$

where $V_1(r)$ is the potential of particle 1 and $V_2(r)$ is the potential of particle 2. Both the potentials are dependent on orbital momentum, and charge. $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are spin orientations that are given in the form of spin matrices. S_{12} is the tensor operator; V_3 gives the interaction potential between the particles 1 and 2.

S_{12} is derived as follows:

$$S_{12} = \frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \quad (9)$$

where $\frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2}$ indicates that the interaction is dependent on the spin angles. The second term $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ in Eqn. (9) is subtracted from the spin-dependent term in order to make average of S_{12} zero along all the directions. Individually, Pauli spin matrices are not invariant but $\vec{\sigma}_1$ and $\vec{\sigma}_2$ is invariant. In contrast, $(\vec{\sigma}_1 \cdot \vec{r})$ and $(\vec{\sigma}_2 \cdot \vec{r})$ are invariant to rotation but not to inversion.

The potential in Eqn. (8) can be interpreted as the sum of three terms. The first term $V_1(r)$ represents central force. $V_2(r)$ is the spin-dependent central force. $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ is 3 for singlet state and

1 for triplet state. The third term $V_{i_3}(r)S_{12}$ represents the interaction potential term that depends on the angles that the spins make with the line that joins two particles and the internuclear separation. Therefore, S_{12} is the most important term that represents non-central character of forces. S_{12} is a scalar quantity and hence potential $V(r)$ is also scalar.

6.5 Shape of Nucleus (Electric Quadrupole Moment)

The shape of nucleus is not spherical. The nucleus gets deviated from the spherical symmetry, and this deviation is given by electric quadrupole moment. Suppose a charge distribution of Ze with volume charge density $\rho(\vec{r}')$ is at a distance \vec{r}' from origin (Figure 6.3). To study the effect of electric field at a point P from Q , the potential can be written as

$$dV' = \frac{1}{4\pi\epsilon_0} \frac{dq}{d} \quad [\text{where } dq \text{ is small charge corresponding to volume } dV] \quad (10)$$

To obtain the total potential, we will have to integrate Eqn. (10),

$$V'(\vec{r}) = \iiint dV' = \frac{1}{4\pi\epsilon_0} \iiint \frac{dq}{d} \quad (11)$$

$$V'(\vec{r}) = \frac{1}{4\pi\epsilon_0} \iiint \frac{\rho(\vec{r}')dV}{d} \quad \left[\rho(\vec{r}') = \frac{dq}{dV} \right] \quad (12)$$

Use the cosine formula in Figure 6.3.

$$\begin{aligned} d^2 &= r^2 + r'^2 - 2rr' \cos \theta \\ d &= (r^2 + r'^2 - 2rr' \cos \theta)^{1/2} \\ d &= r \left[1 + \left(\frac{r'^2}{r^2} - \frac{2r'}{r} \cos \theta \right) \right]^{1/2} \end{aligned} \quad (13)$$

Binomial expansion states that

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \dots \quad (14)$$

Applying binomial expansion to Eqn.13, we obtain

$$\begin{aligned} \frac{1}{d} &= \frac{1}{r} \left[1 + \left(-\frac{1}{2} \right) \left(\frac{r'^2}{r^2} - \frac{2r'}{r} \cos \theta \right) + \frac{3}{8} \left(\frac{r'^2}{r^2} - \frac{2r'}{r} \cos \theta \right)^2 + \dots \right] \\ \frac{1}{d} &= \frac{1}{r} \left[1 + \frac{r'}{r} \cos \theta + \frac{r'^2}{2r^2} (3 \cos^2 - 1) + \dots \right] \end{aligned} \quad (15)$$

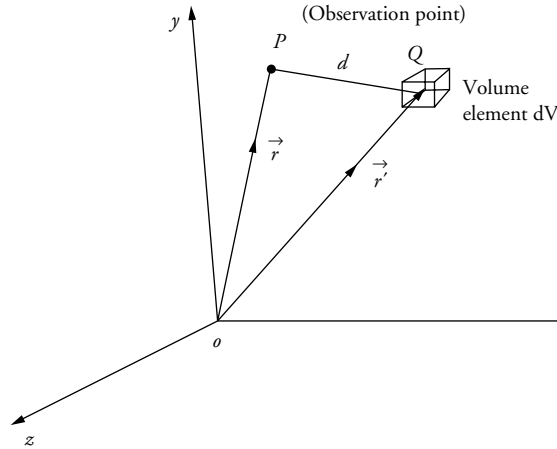


Figure 6.3 Charge distribution and multipole expansions.

In Eqn. (15), we have neglected higher order terms and substituted Eqn. (15) in Eqn. (12).

$$V'(\vec{r}) = \frac{1}{4\pi\epsilon_0} \iiint \rho(\vec{r}') \frac{dV}{r} \left[1 + \frac{r'}{r} \cos\theta + \frac{r'^2}{2r^2} (3\cos^2\theta - 1) \right]$$

$$V'(r) = \frac{1}{4\pi\epsilon_0} \int_{\text{vol}} \frac{\rho(\vec{r}') dV}{r} + \frac{1}{4\pi\epsilon_0 r^2} \int_{\text{vol}} \rho(\vec{r}') r' \cos\theta dV + \frac{1}{4\pi\epsilon_0 r^3} \int_{\text{vol}} \frac{\rho(\vec{r}') r'^2 (3\cos^2\theta - 1)}{2} dV + \dots \quad (16)$$

$$V'(\vec{r}) = V_1 + V_2 + V_3 + \dots \quad (17)$$

From Eqs (16) and (17), it can be concluded that

$$V_1 = \frac{1}{4\pi\epsilon_0 r} \int_{\text{vol}} \rho(\vec{r}') dV$$

↓
Q₁ (potential due to monopole)

$$V_2 = \frac{1}{4\pi\epsilon_0 r^2} \int_{\text{vol}} \rho(\vec{r}') r' \cos\theta dV$$

↓
Q₂ (potential due to dipole)

$$V_3 = \frac{1}{4\pi\epsilon_0 r^3} \int_{\text{vol}} \rho(\vec{r}') r' (3\cos^2\theta - 1) dV$$

↓
Q₃ (potential due to quadrupole)

From Eqn. (16), it is clear that as r increases, the potential decreases. Hence, it represents a converging series. Due to quadrupole moment, the symmetry of nucleus gets changed to oblate ellipsoid or prolate ellipsoid as shown in Figure 6.4 (a)–(b).

The distortion in spherical symmetry may be attributed to the nonuniform charge distribution in the nucleus. When nucleus is treated as an ellipsoid, then quadrupole moment Q_3 (Q_1 represent monopole and Q_2 is dipole moment), is given by

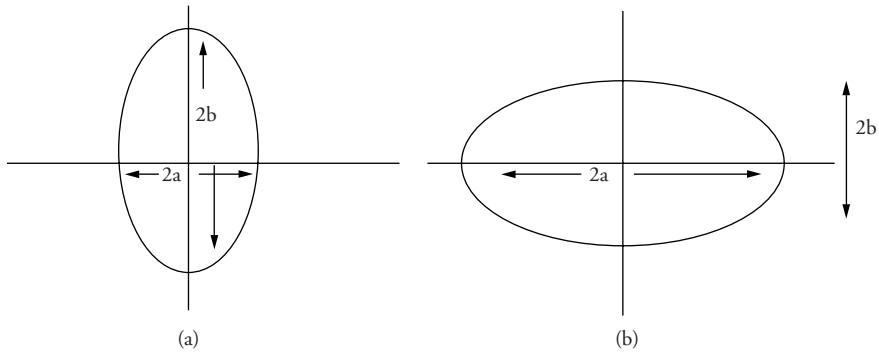


Figure 6.4 (a) Elongated prolate ellipsoid ($b > a$) and (b) flattened oblate ellipsoid ($a > b$).

$$Q_3 = \frac{2}{5} Z (b^2 - a^2) \quad (18)$$

As shown in Figure 6.4(a), $b > a$ makes Q positive. For Figure 6.4(b), $b < a$, hence quadrupole moment Q is negative. For $b = a$, the quadrupole moment vanishes and the shape of nucleus is spherical. Quadrupole moment plays a vital role during the theory of nuclear models especially collective model. Q also defines the extent of deviation from spherical symmetry, nucleus size as well as nuclear charge.

6.6 Exchange Forces

We have discussed that the nuclear density is of the order of 10^{17} kg/m^3 . This density is almost constant for all the nuclei. The binding energy of nuclei with mass number greater than 40 is almost saturated. The saturated binding energy is almost 8 MeV for nuclei. Nuclear forces act between pair of nucleons. The neighboring nucleons do not influence the force between other pair of nucleons. The nature of nucleons, that is, whether they are p or n , do not influence nuclear forces. Nuclear forces are attractive in nature and velocity independent.

The saturation of nuclear forces was explained by Heisenberg in 1932. Quantum mechanics was introduced in the twentieth century. With the introduction of quantum mechanics, many questions could be explained. Up to the nineteenth century, the concept of fields in space around an object could be generated. The interaction of an object with another object under the influence of some field was also studied in the nineteenth century. Quantum mechanics describes the exchange of energy in discrete packets known as quanta. Hence, quantum mechanics describe the energy to be discrete rather than continuous. Therefore, when one object emits field quanta, the second object may absorb the field quanta. Hence, the two objects can exchange field indirectly without establishing any field around its vicinity.

The neutron and proton inside the nuclear are under effect of such fields. For example, a proton may emit some exchange particle. If the emitted exchange particle is in the vicinity of neutron, then the neutron may absorb it after exerting force on it. After some time the neutron may emit the particle that later on is absorbed by the proton. Hence, such cycle of absorption and emission of exchange particles continues. These exchange particles are known as mesons. Basically, mesons are of two types: π^+ and π^- which can be obtained through following reaction mechanisms:

$$\begin{aligned}
 n &\rightarrow p + \pi^- \\
 p &\rightarrow n + \pi^+
 \end{aligned}
 \tag{19}$$

The forces between nucleons, which involve exchange of particles, are known as exchange forces. Exchange forces are of the following types:

- (i) **Wigner force:** Alternatively, this force is known as no exchange force. The wave equation for central force for two bodies is given by the following equation:

$$\left(\frac{\hbar^2}{M} \nabla^2 + E \right) \varphi(r, \sigma) = V_w(r) \varphi(r, \sigma)
 \tag{20}$$

M is the reduced mass for two-body problem. The spin(σ) and space (r) coordinates are not exchanged under the effect of these forces:

- (ii) **Bartlett force:** Under the influence of Bartlett force, only the spin coordinates are exchanged and not the position coordinates, for two nucleons. Hence, these forces are known as spin exchange forces.

$$\begin{aligned}
 \bar{P}_\sigma \varphi(\bar{r}_1, \bar{\sigma}_1, \bar{r}_2, \bar{\sigma}_2) \\
 = \varphi(\bar{r}_1, \bar{\sigma}_2, \bar{r}_2, \bar{\sigma}_1)
 \end{aligned}
 \tag{21}$$

The eigenvalue of \bar{P}_σ is given by $(-1)^{s+1}$ and P_σ is the Bartlett exchange operator. Consider the wave equation under Bartlett force,

$$\left(\frac{\hbar^2}{M} \nabla^2 + E \right) \varphi(r, \sigma) = (-1)^{s+1} V_B(r) \varphi(r, \sigma)
 \tag{22}$$

From Eqn. (22), the wave function is said to be antisymmetric if $s = 0$. The wave function is said to be symmetric if $s = 1$. For symmetric wave function, the force between nucleons is attractive.

- (iii) **Majorana force:** Majorana force changes the position coordinates leaving spin coordinates same. These forces are also known as position exchange forces. \bar{P}_r is the Majorana exchange operator and it operates in as follows:

$$\bar{P}_r \varphi(\bar{r}_1, \bar{\sigma}_1, \bar{r}_2, \bar{\sigma}_2) = \varphi(\bar{r}_2, \bar{\sigma}_1, \bar{r}_1, \bar{\sigma}_2)
 \tag{23}$$

The Eigen value of \bar{P}_r is $(-1)^l$. Consider the wave equation under Majorana force:

$$\left(\frac{\hbar^2}{M} \nabla^2 + E \right) \varphi(r, \sigma) = (-1)^l V_M(r) \varphi(r, \sigma)
 \tag{24}$$

If l is even, then the wave function is symmetric and nucleons in system attract each other. When l is negative, then the wave function is anti-symmetric and nucleons repel each other.

- (iv) **Heisenberg force:** Both the spin and space coordinates get exchanged under the effect of Heisenberg forces. Hence, Heisenberg force is also known as spin–space exchange force. $\bar{P}_{r\sigma}$ is the Heisenberg operator and the equation of operation is given by

$$\bar{P}_{r\sigma} \varphi(\vec{r}_1, \vec{\sigma}_1, \vec{r}_2, \vec{\sigma}_2) = \varphi(\vec{r}_2, \vec{\sigma}_2, \vec{r}_1, \vec{\sigma}_1) \quad (25)$$

The Eigen value of $\bar{P}_{r\sigma}$ is $(-1)^{l+s+1}$.

The equation under Heisenberg force is given by

$$\left(\frac{\hbar^2}{M} \nabla^2 + E \right) \varphi(r, \sigma) = (-1)^{l+s+1} V_H(r) \varphi(r, \sigma) \quad (26)$$

When $l+s$ is even, the wave function is anti-symmetric and repulsive force exists between the nucleons. When $l+s$ is odd, the wave function is symmetric and nucleons attract each other. The relation between exchange operators is given by

$$\bar{P}_{r\sigma} = \bar{P}_r \bar{P}_\sigma \quad (27)$$

and

$$(\bar{P}_{r\sigma})^2 = (\bar{P}_r)^2 = (\bar{P}_\sigma)^2 = 1 \quad (28)$$

The exchange potential can also be expressed in terms of exchange operator as given below:

$$V_{\text{exch}} = V_w(r) + V_M(r) P_r + V_B(r) P_\sigma + V_H(r) P_{r\sigma} \quad (29)$$

Note:

During isotopic spin formalism the proton and neutron are considered as different quantum states of nucleon.

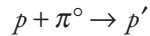
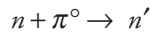
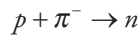
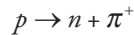
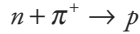
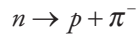
6.7 Yukawa Theory—Theory of Nuclear Forces

Nucleus has a size of 10^{-14} m and it holds nucleons together. Neutrons are natural but protons are positively charged. Hence, a question arises: How can a nucleus be so stable despite the fact that positive charges repel each other. Protons carry positive charge and hence one can expect electrostatic repulsive force—But along with the electrostatic repulsive force, there exists gravitational attractive force, which is due to the mass of protons.

Earlier, it was believed that due to the presence of gravitational attractive force the nucleus is stable. But after the magnitude of forces was calculated, the magnitude of Coulomb's repulsive force was obtained to be almost 10^{36} times the gravitational attractive force. Heisenberg suggested the presence of exchange forces. But the theory of beta-decay proved the magnitude of exchange forces to be extremely small. A new force named as nuclear force was postulated, which was considered the strongest force of nature, that is, almost 10^2 times more than the electrostatic force. These forces are different in nature than weak, Coulomb, and gravitational forces.

Basically, the attractive force between the two particles is considered to be due to exchange of some particles or common field. For example, gravitons are considered as exchange particles of gravitational force. If we consider the case of electrostatic force, then for some molecule and electric field surrounding it, some proton or electron may be the exchange particle, that is, if the molecule is Cl_2^- , then the exchange particle is proton and if the molecule is H_2^+ , then electron is exchange particle. In 1935, a Japanese scientist Yukawa proposed the origin of nuclear forces to be due to some exchange particles, which have some rest mass. The virtual particles were coined as “mesons.” The mass of these particles were found to be 270 times as that of electrons. Mesons are supposed to have negative and positive charge. Neutral mesons also do exist. This theory is known as Yukawa theory of nuclear forces. The Yukawa theory has the following postulates:

1. Mesons can be neutral (π^0) or carry some negative or positive charge.
2. Meson clouds are supposed to be the reason behind different nature of neutron and proton. All nucleons are supposed to consist of identical core, which is surrounded by a pulsating cloud of π -mesons. The meson cloud is shown in Figure 6.5.
3. The protons and neutrons keep on exchanging mesons, which results in attractive force between them. π^0 are responsible for attraction between proton–proton and neutron–neutron.
e.g.



When proton or neutron absorbs π^0 , they are converted to different state and soon they come back to their original state.

4. It is postulated that the nucleons absorb and emit pions all the time. But at the same time, the question arises why all the protons and neutrons are found with same masses. Here the Heisenberg uncertainty principle comes into action. According to Heisenberg uncertainty principle, two simultaneous quantities cannot be measured accurately. Hence, if a nucleon emits meson with no mass, then the law of conservation of mass and energy is violated, although the violation is temporary. In other words, the nucleon should absorb some other pion quickly, so that the mass change is difficult to detect.
5. If the meson is supposed to travel with velocity of light, then the distance traveled by it in time is known as range of pion exchange force.

According to uncertainty principle,

$$\Delta E \Delta t \approx \hbar \quad \left[\begin{array}{l} \Delta E \text{ is uncertainty in energy} \\ \Delta t \text{ is uncertainty in time} \end{array} \right]$$

$$\Delta t = \hbar / \Delta E = \frac{\hbar}{m_\pi c^2} \quad [m_\pi \text{ is mass of meson}] \quad (30)$$

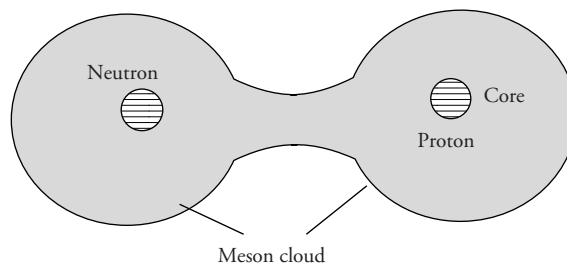


Figure 6.5 Pulsating meson cloud around nucleons.

$$\text{Hence,} \quad \text{Range} = R = c\Delta t = \frac{\hbar}{m_{\pi}c} \quad [c \text{ is velocity of meson}] \quad (31)$$

The range of Yukawa force is obtained to be almost 2×10^{-15} m.

From Eqn. (31),

$$m_{\pi} = 200 m_e \quad [m_e \text{ is mass of electron}] \quad (32)$$

During the discovery of meson, scientists had to face some problems. The meson is not a very stable particle. The average life time of charge meson is about 10^{-8} s and for neutral meson is 10^{-16} s. This very small life time of neutral meson made the detection of meson difficult. Moreover, emission of meson requires large amount of energy.

Note: Nuclear potential is given by
$$V = \frac{-g^2 e^{-\mu r}}{r}$$

where
$$\mu = \frac{m_{\pi}c}{\hbar} \quad (33)$$

and g is the strength of source.

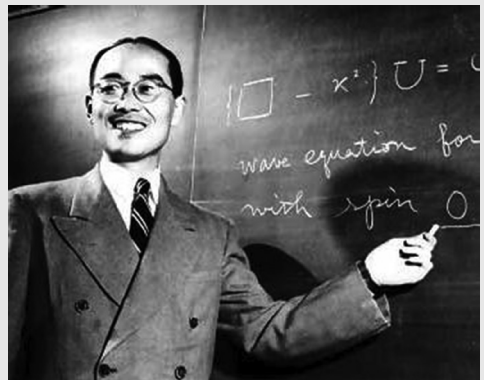
Coulomb potential
$$= \frac{-1}{4\pi\epsilon_0} \frac{Ze}{r} \quad (34)$$

From Eqn. (33) and (34), it is clear that the nuclear potential decreases very rapidly compared with Coulomb's potential. The exponential factor $e^{-\mu r}$ in Eqn. (33) causes the rapid decrease in potential. When $r = \frac{1}{\mu}$, then the potential varies in similar fashion as that of Coulomb's potential.

The meson theory had certain drawbacks like lack of explanation for spin dependence and exchange nature of force, etc. Then it was modified by taking isospin and tensoral character of wave functions into consideration. The coupling constant between the nucleons was also considered.

Yukawa Hideki was born on January 23, 1907, in Tokyo, Japan. He received Nobel Prize for Physics for research on the theory of elementary particles in 1949. Yukawa graduated from Kyoto Imperial University in 1929 and joined lectureship there. In 1933, he moved to Osaka Imperial University and got his doctorate in 1938. From 1939 to 1950, he worked as professor of theoretical physics in Kyoto Imperial University, at the Institute for Advanced Study in Princeton, and at Columbia University. While he was working as a lecturer at Osaka Imperial University, he predicted the existence of mesons, which have masses between those of the electron and the proton. His hypothesis was supported by American physicists in 1937 and his theory became very famous as meson theory.

After the development of meson theory, he worked on comprehensive theory of elementary particles. Then he was the director of the Research Institute for Fundamental Physics in Kyoto from 1953 to 1970. He died on September 8, 1981.



YUKAWA HIDEKI

6.8 Nuclear Models

Till now, we have studied the nucleus and its properties. The exchange forces and nuclear forces have been discussed, but still some questions remain unanswered, for example, how the protons and neutrons are arranged inside the nucleus, what is the reason behind the constant binding energy for atomic mass greater than 40, why some nucleus such as 2, 8, 20, 28, 50, and 82 exhibit higher stability than other nuclei. Later on, it was found that during the radio activity studies, the nuclei emitted α , β , and γ radiations. Hence, it was also of prime concern why some nuclei emit α , β , and γ radiations despite the fact that these particles are not present inside the nucleus. To answer these questions, many models were proposed that could explain the reason behind these questions. The following section describes these models. Every model has some assumptions. No model can explain all the properties and has some drawbacks. Models compare the theoretical observations with experimental observations. A nuclear model is said to be successful if it can predict these properties that are experimentally measurable. With the help of nuclear models, the nuclear interaction involving strong interactions can be studied. In addition, the scattering of nucleons could be studied, which gives rise to collective potential. The two most common models are shell model and liquid drop model.

The shell model assumes independent motion of nucleons whereas the liquid drop model considers the dependent motion of nucleons, that is, the nucleons possess strong interaction and coupling among themselves.

6.8.1 Liquid Drop Model

The binding energy is defined as the energy that holds nucleons together. The binding energy of nucleons is proportional to the number of nucleons. This condition has been interpreted analogous to molecules in liquid drop, that is, the molecules are considered to be nucleons and liquid drop is nucleus. The volume of drop is proportional to the number of molecules present in it in the same way

the volume of nucleus is dependent on number of nucleons $\left[\text{Volume of nucleus} = \frac{4}{3} \pi (R_0 A^{1/3})^3 \right]$.

The molecule in liquid is free to move keeping a fixed intermolecular distance. The analogy of nucleons with solid is not possible because the vibrations of nucleons around the mean position become too large that the nucleus cannot be regarded stable. But if we consider the nucleus to be analogous to liquid drop, then no such problem is posed because the density of liquid drop is constant and independent of size and shape of liquid drop. This condition exactly represents the nucleus. Nuclear density is also independent of size and shape of nucleus. The following are certain assumptions in liquid drop model:

- (i) The nucleus behaves like an incompressible liquid drop of high density.
- (ii) The density of nucleus does not depend on size and shape of nucleus just similar to liquid density, which is independent of size and shape of liquid drop.
- (iii) Liquid drop exhibits surface tension force. This surface tension force is analogous to the nuclear force between nucleons. The liquid drop is spherical due to property of surface tension. In equilibrium state, the shape of nuclei is spherically symmetric due to nuclear forces.
- (iv) Nucleus splits into nucleons when sufficient amount of energy is supplied. This situation is similar to the evaporation of liquid drop.
- (v) The molecules inside liquid move within a spherical enclosure. Similarly, the nucleons move within nuclear potential, which is also spherical.

- (vi) Liquid drops condense when small drops coalesce together. Similarly, when a nucleus absorbs any bombarding particle, it forms compound nucleus.
- (vii) The molecules inside liquid drop exhibit thermal vibrations. Similarly, the nuclei do possess internal energy.

All these points could be understood with the help of semiempirical formula (Weizsacker formula) as demonstrated below.

If ρ is the number of protons and N is number of neutrons, then the mass of nucleus is given by

$$M_{\text{NUC}} = Zm_p + Nm_n - E/c^2 \quad [Z = \text{no of electrons/protons}] \quad (35)$$

Where M_{NUC} = mass of nucleus, $m_p \rightarrow$ mass of proton, m_n = mass of neutron, and E = binding energy of nucleons. The binding energy in Eqn. (35) is not one single term. Rather, it is a combination of different terms. In general, five types of binding energies contribute to the net binding energy, which are given by

$$E = E_v + E_s + E_c + E_a + E_p \quad (36)$$

The significance and contribution of these individual terms is as follows:

- (i) **Volume effect:** There is a finite number of nucleons with which a single nucleon can bond. In other words, there is only a certain number of neighbors for a nucleon. As stated earlier, the volume of nucleus is given by

$$\text{Volume} = \frac{4}{3} \pi R^3 = \frac{4}{3} \pi (R_0 A^{1/3})^3 \quad [A - \text{atomic mass}]$$

$$\text{Volume} = \frac{4}{3} \pi R_0^3 A$$

$$\text{Volume} \propto A \quad (37)$$

Hence, the volume energy term (E_v) varies directly as A

$$E_v \propto A$$

$$E_v = a_v A \quad (38)$$

$$a_v > 0 \quad [\text{Usually } a_v \approx 14.1 - 15.29 \text{ MeV}]$$

The term E_v is also known as exchange energy term.

- (ii) **Surface effect:** Nucleon is considered to be spherical in shape. From Figure 6.6, it is clear that the nucleons are surrounded by equal number of nucleons. It is clear that the nucleons that lie in the interior of nucleus are surrounded by nucleons from all sides; but when it comes to surface nucleons, they do not have same number of nucleons from all sides. The interior nucleons experience higher attractive force from all sides. By contrast, the surface nucleons experience less force. This can also be interpreted in terms of binding energy, i.e. surface nucleons have less binding energy as compared with interior nucleons. Hence, the total binding energy is overestimated, which needs to be corrected.

The surface area is of nucleus given by

$$\text{Surface area} = 4\pi R^2, \text{ where } R \text{ is radius of nuclei}$$

$$\text{Surface area} = 4\pi (R_0 A^{1/3})^2 = 4\pi R_0^2 A^{2/3}$$

$$\text{Surface area} \propto A^{2/3} \quad (39)$$

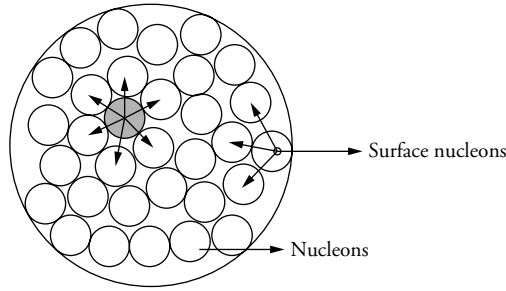


Figure 6.6 Interior nucleons experience force from all direction.

This is extra contribution, hence it should be deducted from total energy. Therefore, surface energy term (E_s) is given by

$$E_s \propto A^{2/3} \quad (40)$$

$$E_s = -a_s A^{2/3}$$

[Usually $a_s \approx 13 - 15.76$ MeV]

For light nuclei, this surface energy term is more significant due to large number of nucleons on the surface. The spherical symmetry has least surface energy, therefore it is the preferred symmetry. Therefore, the natural tendency of the system like nucleus is to attain the spherical symmetry.

- (iii) **Coulomb effect:** Nuclei is having protons, and these protons are positively charged. Hence, there is interprotonic Coulomb repulsive forces. These repulsive forces tend to decrease the binding energy of nucleus. Suppose W is work done to pack Z protons together from infinity into the segregated state, that is, from free state to a bound state. This work done is stored as the Coulomb energy of nucleus. This work is done against the repulsive forces to keep the nucleons together. The charge density for charge distribution of Ze is given by

$$\rho = \frac{Ze}{\frac{4}{3}\pi R^3} = \frac{Ze}{\frac{4}{3}\pi R_0^3 A} \quad (41)$$

Consider a shell of radius r with charge dq and thickness dr (Figure 6.7).
Then

$$\text{Volume} = \frac{\text{charge}}{\text{density}}$$

$$\text{Charge} = \text{volume} \times \text{density}$$

$$dq = 4\pi r^2 dr \times \text{density}$$

$$dq = \frac{Ze}{\left(\frac{4}{3}\pi R_0^3 A\right)} \times 4\pi r^2 dr \quad (42)$$

$$dq = \frac{3Ze}{R_0^3 A} r^2 dr$$

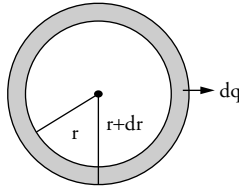


Figure 6.7 Spherical shell carrying charge dq .

The work done in bringing charge dq from infinity to radius is

$$dW = V dq \quad [V \text{ is the potential due to charge } dq]$$

$$dW = \left(\frac{\text{charge}}{4\pi\epsilon_0 r} \right) dq$$

$$dW = \left(\frac{\text{volume} \times \text{density}}{4\pi\epsilon_0 r} \right) dq \quad [\text{from Eqn. (42)}]$$

$$dW = \left(\frac{\frac{4}{3}\pi r^3 \times \rho}{4\pi\epsilon_0 r} \right) \times \frac{3Ze r^2 dr}{R_0^3 A} \quad (43)$$

$$dW = \frac{3}{4} \frac{Z^2 e^2 r^4 dr}{\pi\epsilon_0 R_0^6 A^2} \quad (44)$$

Upon integrating from 0 to radius R ,

$$dW = -\frac{3}{5} \frac{Z^2 e^2}{4\pi\epsilon_0 R_0 A^{1/3}}$$

$$E_c = dW = -a_c \frac{Z^2}{A^{1/3}} \quad (45)$$

[Usually $a_c = 0.69 \text{ MeV}$]

- (iv) **Asymmetry term:** The stable nuclei have $Z = N = \frac{A}{2}$, that is, equal number of protons and

neutrons. Usually neutrons and protons pair up. With the increase in atomic mass, the repulsive forces increase much faster than the attractive nuclear force. As A increases the neutrons increase more than the protons to maintain stability. Therefore, the heavier nuclei possess more number of neutrons ($N > Z$). Such nuclei are asymmetric Hence,

$$\text{excess number of Neutrons is } (N - Z) \quad (46a)$$

$$A = (N + Z)$$

$$N = (A - Z) \quad (46b)$$

Using Eqn. (46b) in (46a),

$$\text{excess neutrons} = A - 2Z \quad (47)$$

The asymmetry energy term is

$$E_a = -a_a \frac{(A - 2Z)^2}{A} \quad (48)$$

Due to excess number of neutrons, the asymmetry energy term should be deducted,

$$(a_a \approx 19 \text{ MeV})$$

- (v) **Pairing term:** In nuclei, pairing may take place between neutron–neutron, proton–proton, and neutron–proton. The pairing term is due to the proton–proton and neutron–neutron pairing. Experimentally, it is proved that even–even nuclei are more stable than odd–odd nuclei. The “odd–even” and “even–odd” nuclei possess intermediate stability. Hence, the nuclei with even A are more stable than the nuclei with odd A . Hence, the nuclei with $A = 2, 8, 12, 16, 20, 48, \text{etc.}$, are more stable. Odd–odd nuclei may have unpaired neutron or unpaired proton. Such nuclei have low binding energy. The pairing energy is taken to be

1. zero for “odd–even” and “even–odd” nuclei
2. positive for “even–even” nuclei
3. negative for “odd–odd” nuclei

The pairing energy is given by

$$E_p = a_p A^{-3/4} \quad (49)$$

$$[a_p \approx 35 \text{ MeV}]$$

The total energy is the sum of all these terms:

$$E = E_v + E_s + E_c + E_a + E_p$$

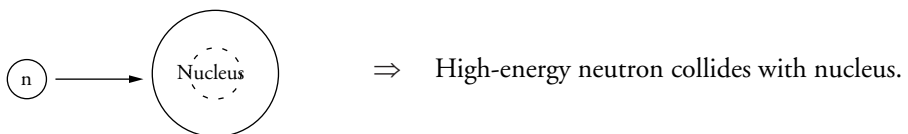
$$E = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - \frac{a_a (A - 2Z)^2}{A} (\pm, 0) \frac{a_p}{A^{3/4}} \quad (50)$$

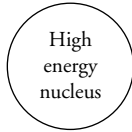
Equation (50) is known as the semiempirical mass formula. Constants are predicted by fitting the known masses. The masses and binding energies of many stable nuclei have been predicted by this relation.

6.8.2 Explanation of Nuclear Fission

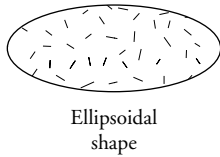
The nuclear fission could be explained on the basis of liquid drop model. The following steps explain the sequential fission process:

STEP 1:

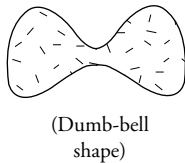


STEP 2:

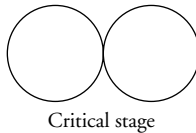
⇒ The binding energy of nucleus increases, and compound nucleus is formed.

STEP 3:

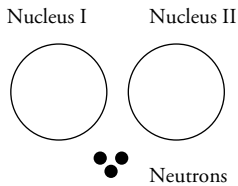
⇒ The increased energy distorts the spherical shape and the nucleus may attain ellipsoidal shape.

STEP 4:

⇒ There is competition between surface tension and excitation energy of compound nucleus. The excitation energy tends to distort the spherical symmetry of nucleus, but the surface tension tends to bring back the original spherical shape of nucleus.

STEP 5:

⇒ The critical stage is reached only when the surface tension force fails to bring back the nucleus in spherical shape, that is, the magnitude of excitation energy increases more than the surface tension.

STEP 6:

⇒ After the magnitude of oscillations increases, the fission of nuclei occurs resulting in breakdown of parent nuclei into daughter nuclei along with emission of three neutrons.

Production of critical stage requires some critical or threshold energy so that the nuclei cannot regain its original spherical shape. Bohr and Wheeler gave a detailed explanation on nuclear fission with the help of Legendre polynomial expansion:

$$r = R \left[1 + \sum_{l=0}^{\infty} \alpha_l P_l(\cos \theta) \right] \quad (51)$$

where $R \rightarrow$ radius of spherical nucleus, r is the deformation radius, α_l is deformation parameter, and $P_l(\cos \theta)$ is Legendre's polynomial.

The center of mass of drop is assumed to be the same, hence the deformative parameter $\alpha_0 = \alpha = 0$.

$$r = R[1 + \alpha_2 P_2(\cos\theta) + \dots] \quad (52)$$

Surface energy is given by

Surface energy (SE) = surface tension (T) \times area of spherical drop (R)

$$SE = E_s = T \times 4\pi R^2 \quad (53)$$

The deformation radius (Figure 6.8) of nucleus with radius R is r .

$$E_s = T \times 4\pi r^2$$

$$E_s = T \times 4\pi R^2 [1 + \alpha_2 P_2(\cos\theta) + \dots]^2 \quad (54)$$

Solving Legendre's polynomial [$R = R_0 A^{1/3}$],

$$E_s = 4\pi R_0^2 A^{2/3} T + 4\pi R_0^2 A^{2/3} T \left[\frac{2}{5} \alpha_2^2 + \dots \right]$$

$$E_s = E_s(\text{sphere}) + E_s(\text{sphere}) \left[\frac{2}{5} \alpha_2^2 + \dots \right] \quad (55)$$

$$\Delta E_s = E_s^{\text{sphere}} \left[\frac{2}{5} \alpha_2^2 + \dots \right]$$

where $\Delta E_s = E_s - E_s(\text{sphere})$

Similarly, the Coulomb energy for spherical drop is given by

$$E_c = \frac{3}{5} \frac{Z^2 e^2}{4\pi\epsilon_0 R} \quad (56)$$

For deformed nuclei, $R \rightarrow r$

$$E_c = \left(\frac{3}{5} \right) \left(\frac{Z^2 e^2}{4\pi\epsilon_0 r} \right)$$

$$E_c = \frac{3}{5} \frac{Z^2 e^2}{4\pi\epsilon_0 R [1 + \alpha_2 P_2(\cos\theta) + \dots]} \quad (57)$$

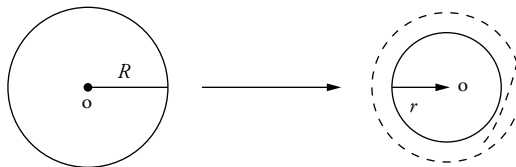


Figure 6.8 Change of radius from R to r upon deformation.

Solving Eqn. (57),

$$E_c = E_c(\text{sphere}) - E_c(\text{sphere}) \left[\frac{1}{5} \alpha_2^2 + \dots \right]$$

$$\Delta E_c = -E_c(\text{sphere}) \left[\frac{1}{5} \alpha_2^2 + \dots \right] \quad (58)$$

$$[\Delta E_c = E_c - E_c(\text{sphere})]$$

The total energy is given by

$$\Delta E = \Delta E_s + \Delta E_c$$

$$\Delta E = \frac{1}{5} \alpha_2^2 [2E_s(\text{sphere}) - E_c(\text{sphere})] \quad (59)$$

Equation (59) gives rise to the following two conditions:

(i) $\Delta E < 0$, then for this case

$$E_c(\text{sphere}) > 2E_s(\text{sphere})$$

Hence, Coulomb energy is greater than the surface energy. This condition is required for nuclear fission.

$$\frac{3}{5} \frac{Z^2 e^2}{4\pi\epsilon_0 R} > 2(4\pi R^2 T)$$

$$\frac{Z^2}{A} > 45 \quad (60)$$

Equation (60) is the condition for nuclear fission. The critical parameter is given by

$$\xi = \frac{E_c(\text{sphere})}{2E_s(\text{sphere})} \quad (61)$$

$\xi < 1$ represents stable nucleus and $\xi > 1$ represents that the nucleus that can undergo fission.

The threshold energy is given by

$$E_{\text{critical}} = 4\pi R^2 T f(\xi)$$

$$E_{\text{critical}} = 17.8 A^{2/3} f(\xi) \text{ MeV} \quad (62)$$

$\xi \approx 1$ represents small deformation in the nuclei. Figure 6.9 represents how the uranium nuclei undergo fission process. For U^{235} , the threshold critical energy is 5.5 MeV and the excitation energy is 6.6 MeV. Therefore, fission occurs easily. The pairing term in semi-empirical mass formula contributes to the difference in excitation energy of U^{235} and U^{239} . A general graphical representation indicating nuclear stability is indicated in Figure 6.10. The table nuclei have equal no of protons and neutrons.

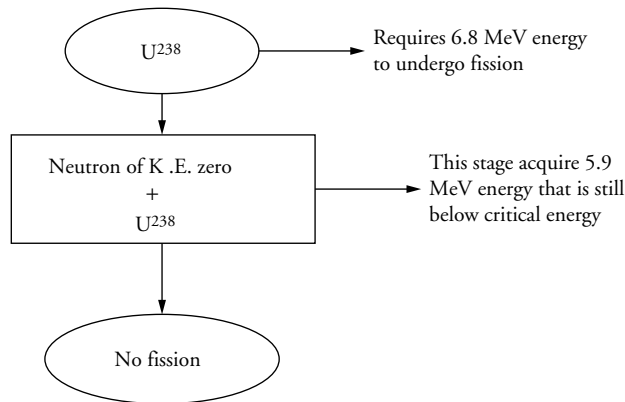


Figure 6.9 Fission process for U^{238} .

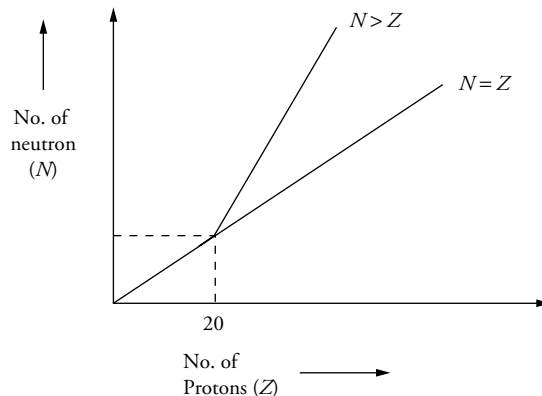


Figure 6.10 Graph indicating nuclear stability.

(ii) $\Delta E > 0$: For this condition $2E_s(\text{sphere}) > E_c(\text{sphere})$ which indicates stable nuclei and hence no fission.

6.8.3 Merits and Demerits of Liquid Drop Model

- (i) **Merits:** The atomic masses and binding energy can be predicted accurately. This model could give an idea about collective model and Bohr's theory of compound nucleus. α and β emission properties could also be predicted.
- (ii) **Demerits:** This model could not describe the actual excited states. The calculation of excited state requires the deformation of spherical shape to oscillating sphere. The model describes Z/A ratio, but many other points could not be explained. The most important point is the quantum character of nucleon and classical character of molecules of liquid. This could be explained as follows: The molecules in liquid possess KE of 0.1 eV, which correspond to de-Broglie wavelength, of, 5×10^{-11} m. Indeed, this is very small than the intermolecular distance. The KE of nucleons is 10 MeV and de-Broglie wavelength $\lambda = 6 \times 10^{-15}$ m. This $\lambda = 6 \times 10^{-15}$ m is of the order of internucleon distance. Hence, they are in contrast to each other.

6.9 Shell Model

Shell model explained the “magic numbers.” It is one of the successful models. Liquid drop model could not explain the existence of magic numbers. Moreover, liquid drop model provided no evidence of quantum-controlled nuclear shells. Furthermore, it was not clear whether the quantum numbers such as n , l , s , and j could be applied to nucleons.

The most striking features of shell model is the explanation of magic nuclei. Certain nuclei exhibit more stable characteristics compared with others. These nuclei have either N or Z equal to (2, 8, 20, 28, 50, 82, 126). Liquid drop model could not explain the behavior of these nuclei. In addition, the shell model also explained the inequivalence of protons and neutrons, although liquid drop mode treats them to be equivalent. Many properties such as spin, magnetic moment, and energy levels could be explained using shell model. Shell model assumes nucleon as a particle moving in potential well. The potential well is produced by all nucleons. Every nucleon inside the nucleus observes almost same rotation. Hence, the nucleons are considered to move independent of each other in the potential well created by them. Before we discuss the shell model, the closed shell structure of nuclei should be discussed. As electrons fill the atom in a systematic pattern, similarly, we expect the filling of nuclear shells systematically. The protons and neutrons also fill the shells according to Pauli exclusion principle. Let us see how potential varies for nuclei and why the need of spin orbit coupling is required:

- (i) **Potential:** Let us consider the average potential to be “square-well” potential. The coulombic repulsion between the nucleons must be ignored so that the nucleons observe equal potential. Second assumption assumes each energy state to occupy maximum four nucleons. Two nucleons are protons with opposite spins and other two are neutrons (with opposite spins). The shell potential has been approximated as Woods–Saxon potential.

$$V(r) = \frac{-V_0}{1 + \exp\left(\frac{\pi - R}{x}\right)} \quad (63)$$

where $V_0 = 1 \text{ MeV}$, $x = 0.65 \times 10^{-15} \text{ m}$, and $R = 1.25 A^{1/3}$

As the distance increases the nuclear force diminishes but the coulombic potential comes into action. For calculating the nuclear orbits time-dependent Schrödinger equation is solved for a particle in potential well, as given below:

$$\nabla^2 \varphi + \frac{2m}{\hbar^2} [E - V(r)] \varphi = 0 \quad (64)$$

When Eqn. (64) was solved, it was observed that the nucleons are characterized by n , l , and m_l but the sequence of magic numbers obtained was not the same. Hence, further correction on Eqn. (64) was applied by M.G. Mayer and J.H.D. Jensen. They applied spin–orbit interaction as an important factor to analyze the sequence of magic numbers.

- (ii) **Spin–orbit coupling:** Atom has interaction among the orbital and spin angular momentum of nucleons. Spin–orbit interaction is proportional to $\vec{L} \cdot \vec{S}$, where \vec{L} is total angular momentum and \vec{S} is the total spin angular momentum. The total angular momentum is the sum of orbital angular momentum and spin angular momentum.

$$\vec{J} = \vec{L} + \vec{S}$$

Spin-orbit interaction is almost 20 times more stronger than the individual spin or orbital interaction. This interaction is also inverted in nature, which means positive $\vec{L} \cdot \vec{S}$ corresponds to decrease in energy (Figure 6.11).

The vector J can combine with spin in two possible ways, that is,

$$\vec{J} = \vec{L} \pm \vec{S} \tag{65}$$

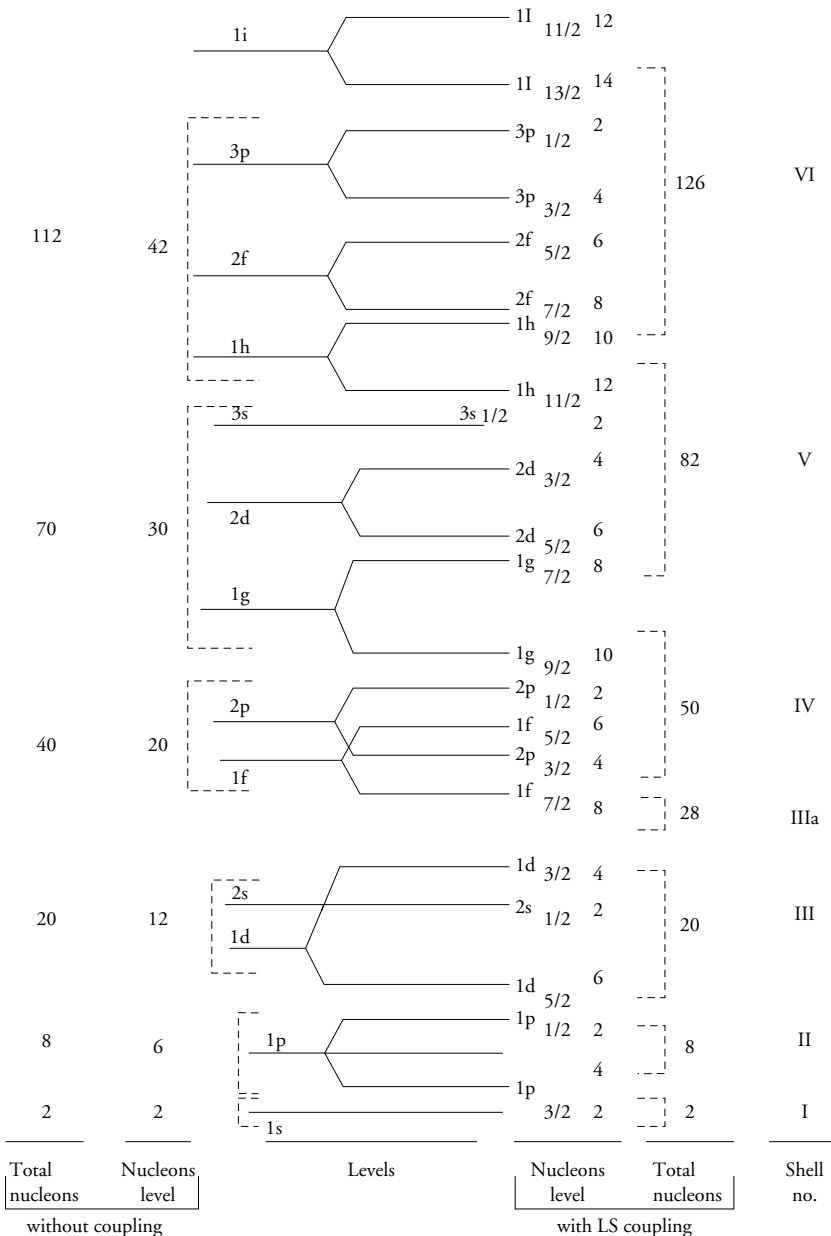


Figure 6.11 LS coupling (left side without coupling and right side with coupling).

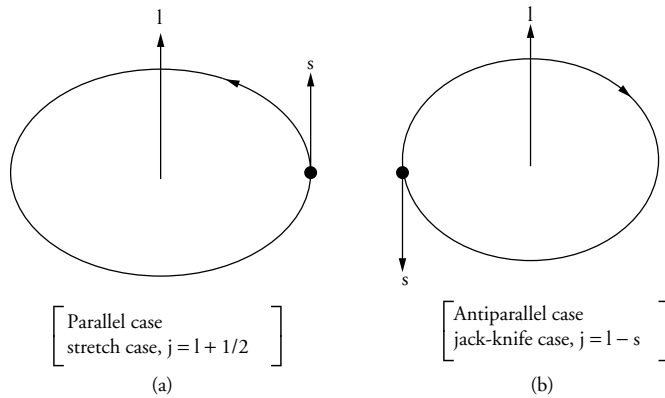


Figure 6.12 Spin and angular momentum can interact in two ways: (a) stretch case and (b) Jack-knife case.

Two sublevels are formed corresponding to $s = \pm \frac{1}{2}$

$$j = l + \frac{1}{2}, j = l - \frac{1}{2} \quad (66)$$

$(2j+l)$ nucleons could be accommodated in every sublevel (Figure 6.12). Higher value of l represents higher splitting of levels. The coupling can result in the following two cases:

- (i) When l and s are parallel, the angular momentum is $j = l + s = l + \frac{1}{2}$. The levels with higher value of j represent lightly bound nucleons. These nucleons lie in lower level, that is, higher j values means lower levels are occupied first. This case is also known as stretch case.
- (ii) When l and s are antiparallel, the angular momentum is $j = l - s = l - \frac{1}{2}$. These levels have lower j value. This case is known as Jack-knife case.

Haxel, Mayer, and Jensen concluded that “Nucleons are subjected to strong spin–orbit interactions. These strong interactions couple their own spin and orbital angular momentum, which is also known as jj coupling. Parallel \vec{L} and \vec{S} decrease the energy and vice versa. Hence, parallel \vec{L} and \vec{S} represent lower energy state, which is more stable. A gap between the levels is proportional to l -value. The splitting between degenerate levels is wider and wider with increasing l -value.

Magnetic field is also associated with moving nucleon, which give rise to interaction energy $W = -\vec{\mu} \cdot \vec{B}$.

We know that

$$\langle \vec{l} \cdot \vec{s} \rangle = \frac{j(j+1) - l(l+1) - s(s+1)}{2} \quad (67)$$

Mayer and Jensen also suggested spin–orbit interaction must be added to the centrally symmetric potential in order to obtain magic numbers. The energy shift can be written as

$$\Delta E \left(j = l + \frac{1}{2} \right) = -\frac{1}{2} l \int |\varphi_{nl}(r)|^2 f(r) dr \quad (68a)$$

$$\Delta E \left(j = l - \frac{1}{2} \right) = \frac{1}{2} (l+1) \int |\varphi_{nl}(r)|^2 f(r) dr \quad (68b)$$

where $f(r)$ is a potential function.

6.10 Discussion on Magic Numbers/Success of Shell Model

Shell model gives a clear-cut explanation for the existence of energy shells inside the nucleus and magic numbers. The following points explain the existence of magic numbers:

- (i) The nuclides with magic numbers are more abundant in nature and possess high stability. For example, relative abundance of barium, strontium, and lead is more than other elements.
- (ii) The nuclides with the neutron number equal to one of the magic number have most stable isotones. For example, when $N = 50$, the number of isotones is 6, whereas for $N = 49$ and 51 , the number of isotones is 1. Similarly, the magic number nuclei also have more stable isotopes. If either number of proton or neutron is equal to magic number, then the nuclei is doubly magic nuclei if both proton and neutron numbers are magic numbers, for example, ${}^4_2\text{He}$, ${}^{16}_8\text{O}$, ${}^{208}_{82}\text{Pb}$. The magic number nuclei with number of protons equal to 50 have 10 isotopes; whereas for $Z = 49$ or 51 , the number of isotopes is 2. The binding energy of magic number nuclei is high, as can be seen from Figure 6.13. Obviously, this is due to increased stability of magic number nuclei.
- (iii) A neutron can be captured by a nucleus to form a compound nucleus. The factor that decides the capturing tendency of nuclei is effective cross-sectional area. The magic nuclei have very low effective cross-sectional area, which indicates no vacancy for additional neutrons as the shells are closed due to stability of nuclei; for example, the magic nuclei with $Z = 50$ have cross-sectional area of 0.64 mb (millibarn), whereas $Z = 49$ and 51 have cross-sectional area of 19 and 6.4 mb, respectively.
- (iv) Krypton (${}^{87}_{51}\text{Kr}$) and Xenon (${}^{137}_{54}\text{Xe}$) contain one extra nucleon above the magic number. This extra nucleon is emitted spontaneously as it possesses very small binding energy. This goes in accordance with the shell model.
- (v) Whenever a nucleus emits α or β particle, the mass number changes. It has been observed experimentally that whenever the parent nuclei emits α or β particle, such that the daughter nuclei is a magic number, the energy of α and β particles is quite large, for example, polonium, ${}^{212}_{84}\text{Po}$, has 128 neutrons. When it emits α -particles it has $N = 126$, which is a magic number. These α -particles are very energetic.

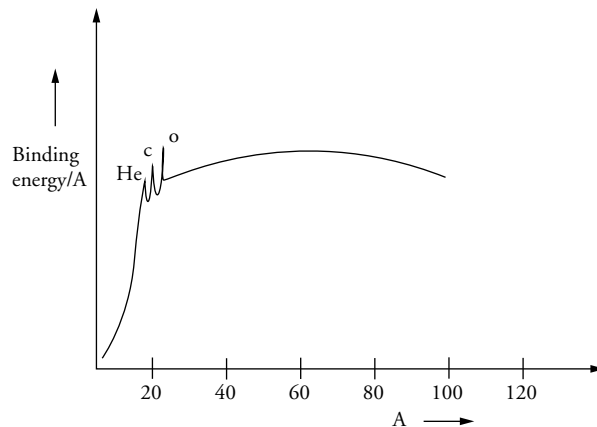


Figure 6.13 Binding energy variation versus the atomic mass.

6.11 Failure of Shell Model

1. The value of total angular momentum for some nuclides could not be obtained, for example, sodium, manganese, selenium, etc.
2. ${}^1_1\text{H}^2$, ${}^{13}_3\text{Li}^6$, ${}^{10}_5\text{B}^{10}$, ${}^{14}_7\text{N}^{14}$, etc., are very stable nuclei. But these are odd-odd nuclei. The shell model could not explain the reason behind it.

SUMMARY

This chapter deals with the study of nucleus and its properties. The nuclear density and atomic density have been obtained for the atom. Nuclear forces have been described as the strongest forces within the nucleons that are short range, charge independent, spin dependent, noncentral, and saturated in nature. The tensor forces are responsible for distorting the nucleus from its spherical shape. σ_1 and σ_2 are spin orientation represented in the form of spin matrices. It is also shown that due to quadrupole moment, the symmetry of nucleus gets changed to oblate ellipsoid or prolate ellipsoid. Furthermore, exchange forces are explained for the nucleus under the effect of which the nucleons exchange particles known as meson particles (π^+ and π^-). There are four types of exchange forces: Wigner, Barlett, Majorana, and Heisenberg. The Yukawa theory of nuclear forces has been explained, which demonstrates the stability of nuclei despite the fact that charged particles do exhibit electrostatic repulsion. This chapter dealt with two important models to interpret the nuclear behavior; liquid drop model considered the nuclei as an incompressible liquid drop of high density. The binding energy is given as the sum of five individual binding energies yielding semiempirical formula. This model could explain the nuclear fission but failed to explain the quantum character of nucleon. Hence, shell model was proposed, which could explain the existence of magic numbers and the issues that could not be addressed by liquid drop model.

SOLVED PROBLEMS

Q. 1: Calculate the nuclear and atomic density (given $R_0 = 1.2f$).

Ans:

$$\text{Nuclear density} = \frac{\text{Mass}}{\text{Volume}} = \frac{M}{\frac{4}{3}\pi R^3}$$

$$\rho = \frac{M}{\frac{4}{3}\pi (R_0 A^{1/3})^3} = \frac{M}{\frac{4}{3}\pi R_0^3 A}$$

$\left[\begin{array}{l} \text{Nuclear mass} = \text{mass of nucleon} \times \\ \text{number of nucleons} \end{array} \right]$

$$\rho = \frac{1.67 \times 10^{-27} \times A}{\frac{4}{3}\pi R_0^3 A} \quad [R_0 = 1.2 \times 10^{-15} \text{ m}]$$

$$\rho = 2.29 \times 10^{17} \text{ kg/m}^3$$

For atomic density, we have to consider the point that atomic radius is four orders higher than nuclear radius. Therefore,

$$\text{Atomic density} = \frac{2.29 \times 10^{17}}{(10^4)^3}$$

$$\text{Atomic density} = 2.29 \times 10^5 \text{ kg/m}^3$$

Q. 2: Obtain the energy of 1 a.m.u. in MeV.

Ans: Velocity of light $c = 3 \times 10^8 \text{ m/s}$

$$\text{Mass of proton} = 1.67 \times 10^{-27} \text{ kg}$$

According to Einstein's relation,

$$E = mc^2$$

$$E = 1.67 \times 10^{-27} \times (3 \times 10^8)^2 \text{ J}$$

$$E = \frac{1.67 \times 10^{-27} \times (3 \times 10^8)^2}{1.6 \times 10^{-13}} \text{ MeV}$$

$$E = 931 \text{ MeV.}$$

Q. 3: What would be the energy equivalent of 1 g in 1 kWh?

Ans: $1 \text{ kWh} = 36 \times 10^5 \text{ J}$

Also,

$$E = mc^2$$

$$[m = 10^{-3} \text{ kg}$$

$$c = 3 \times 10^8 \text{ m/s}]$$

$$E = 10^{-3} \times 9 \times 10^{16}$$

$$E = 9 \times 10^{13} \text{ J}$$

Energy equivalence of 1 g

$$= \frac{9 \times 10^{13}}{36 \times 10^5} = 2.5 \times 10^7 \text{ kWh}$$

Q. 4: What would be the radii for N^{14} nucleus, if $R_0 = 1.2 \text{ fm}$?

Ans: $R = R_0 A^{1/3}$ [$A = 14$, $R_0 = 1.2 \text{ fm}$]

$$R = 1.2 \times (14)^{1/3}$$

$$R = 1.2 \times 2.41 = 2.89 \text{ fm}$$

Q. 5: Obtain the radius for Pb^{206} nucleus for $R_0 = 1.2 \text{ fm}$.

Ans: $R = R_0 A^{1/3}$ [$A = 206$, $R_0 = 1.2 \text{ fm}$]

$$R = 1.2 \times (206)^{1/3}$$

$$R = 7.08 \text{ fm}$$

Q. 6: A nucleus with $A = 235$ splits into two fragments with mass numbers in ratio 2:1. Find the radii of new nuclei and distance between the nucleons.

Ans: $A = 235$

Hence, A_1 and A_2 are the new mass numbers such that

$$A_1 = 235 \times \frac{1}{3}$$

and

$$A_2 = 235 \times \frac{2}{3} \quad [R_0 = 1.2 \text{ fm}]$$

$$R_1 = R_0 A_1^{1/3} = R_0 \left[\frac{235}{3} \right]^{1/3}$$

$$R_1 = 5.13 \text{ fm}$$

Similarly

$$R_2 = R_0 A_2^{1/3} = R_0 \left[235 \times \frac{2}{3} \right]^{1/3}$$

$$R_2 = 1.2 \times 5.39$$

$$R_2 = 6.46 \text{ fm}$$

Hence, the radii of the nuclei are 5.13 and 6.46 fm. The separation distance between the nuclei is given by

$$R = R_1 + R_2$$

$$R = 5.13 + 6.46$$

$$R = 11.59 \text{ fm}$$

Q. 7: Obtain the binding energy for ${}_{26}\text{Fe}^{56}$. Also, calculate binding energy/nucleon.

Ans: Given $m_p = 1.007825 \text{ a.m.u.}$

$$m_n = 1.008665 \text{ a.m.u.}$$

$$\text{Mass of Fe nuclei} = 55.934939 \text{ a.m.u.}$$

$$\text{Binding energy of nuclei} = [Zm_p + Nm_n - M_{\text{nucleus}}]c^2$$

Here

$$Z = 26, \quad A = 56$$

$$N = A - Z = 30$$

$$\text{Binding energy of nuclei} = [(26 \times 1.007825 + 30 \times 1.008665) - 55.934939] \times 931 \text{ MeV}$$

$$\text{Binding energy of nuclei} = 492.2 \text{ MeV}$$

$$\text{Hence, binding energy} = 492.2 \text{ MeV}$$

$$\begin{aligned} \text{Binding energy per nucleon} &= \frac{\text{Binding energy}}{\text{Number of nucleons}} \\ &= \frac{492.2}{56} \approx 8.8 \text{ MeV} \end{aligned}$$

Q. 8: Obtain the binding energy of a nucleon for α -nucleus.

Ans:

$$\text{Binding energy} = [Zm_p + Nm_n - M]c^2$$

α nucleus, ${}_2\text{He}^4$

$$A = 4, Z = 2 \text{ and } N = A - Z = 2$$

$$\text{Binding energy} = [2m_p + 2m_n - M]c^2$$

The Mass M of ${}_2\text{He}^4$ is 4.00 2603 a.m.u.

$$m_p = 1.007825 \qquad m_n = 1.008665$$

$$\text{Binding energy} = [2(1.007825) + 2(1.008665) - 4.002603]c^2$$

$$\text{Binding energy} = (0.030377) \times 931 \text{ MeV}$$

$$\text{Binding energy} = 28.3 \text{ MeV}$$

$$\text{New binding energy/nucleon} = \frac{\text{Binding energy}}{\text{Number of nucleons}}$$

$$\frac{\text{Binding energy}}{A} = \frac{28.3}{4} = 7.075 \text{ MeV}$$

Q. 9: Obtain the rest mass energy of an electron.

Ans:

$$E = m_0 c^2$$

For electron,

$$m_0 = 9.1 \times 10^{-31} \text{ kg}$$

$$c = 3 \times 10^8 \text{ m/s}$$

$$E = m_0 c^2$$

$$E = 9.1 \times 10^{-31} \times (3 \times 10^8)^2 \text{ J}$$

$$E = \frac{9.1 \times 10^{-31} \times 9 \times 10^{16}}{1.6 \times 10^{-13}} \text{ MeV}$$

$$E = 0.511 \text{ MeV}$$

Q. 10: Obtain the binding energy and packing fraction for deuteron nucleus.

Given:

Mass of deuteron = 2.013553 a.m.u.

Mass of proton = 1.007825 a.m.u.

Mass of neutron = 1.008665 a.m.u.

Ans:

$$\text{Mass defect} = [Zm_p + Nm_n - M] = \Delta m$$

For deuteron, ${}_1\text{H}^2$, $A = 2$, $Z = 1$, and $N = 1$

$$\Delta m = (1.007825 + 1.008665 - 2.013553) \text{ a.m.u.}$$

$$\Delta m = 0.002937 \text{ a.m.u.}$$

$$\text{Binding energy} = \text{Mass defect} \times 931 \text{ MeV}$$

$$= 0.002937 \times 931 \text{ MeV}$$

$$= 2.73 \text{ MeV}$$

$$\begin{aligned} \text{Packing fraction} &= \frac{\text{Mass defect}}{\text{Number of nucleons}} = \frac{0.002937}{2} \\ &= 0.0014685 \text{ a.m.u.} \end{aligned}$$

Q. 11: What is the packing fraction for ${}_{28}\text{Ni}^{64}$ with mass 63.928 a.m.u.?

Ans: Mass defect is given by

$$\Delta m = [Z m_p + N m_n - M] \text{ a.m.u.}$$

$$\text{For } {}_{28}\text{Ni}^{64}, A = 64, Z = 28, \text{ and } N = 36$$

Given

$$m_p = 1.007825 \text{ a.m.u.}$$

$$m_n = 1.008665 \text{ a.m.u.}$$

$$M = 63.928 \text{ a.m.u.}$$

$$\Delta m = [28(1.007825) + 36(1.008665) - 63.928]$$

$$\Delta m = [28.2191 + 36.31194 - 63.928] \text{ a.m.u.}$$

$$\Delta m = 0.60304 \text{ a.m.u.}$$

$$\text{Packing fraction} = \frac{\text{Mass defect}}{\text{Number of nucleons}} = \frac{0.60304 \text{ a.m.u.}}{64}$$

$$\text{Packing fraction} = 0.0094225 \text{ a.m.u.}$$

Q. 12: For Neon, ${}_{10}\text{Ne}^{20}$, the binding energy is given by 160.64 MeV. Obtain the atomic mass for ${}_{10}\text{Ne}^{20}$

Ans:

Given

$$m_p = 1.007825 \text{ a.m.u.}$$

$$m_n = 1.008665 \text{ a.m.u.}$$

$$\text{Binding energy} = 160.64 \text{ MeV}$$

$$\text{Binding energy} = [Z m_p + N m_n - M] \times 931 \frac{\text{MeV}}{\text{a.m.u.}}$$

$$Z = 10, A = 20, N = 10$$

$$160.64 \text{ MeV} = [10(1.007825) + 10(1.008665) - M] \times 931 \frac{\text{MeV}}{\text{a.m.u.}}$$

$$\frac{160.64}{931} = [10.07825 + 10.08665 - M] \frac{1}{\text{a.m.u.}}$$

$$0.1726 = [20.165 - M] \frac{1}{\text{a.m.u.}}$$

$$0.1726 = 20.165 - M$$

$$M = 19.9924 \text{ a.m.u.}$$

OBJECTIVE QUESTIONS

1. Size of nucleus and atom is, respectively,
(a) 10^{-14} , 10^{-12} m (b) 10^{-12} , 10^{-14} m
(c) 10^{-10} , 10^{-8} m (d) 10^{-8} , 10^{-10} m
2. The atomic density is approximately
(a) 2.29×10^{17} kg/m³ (b) 2.29×10^{15} kg/m³
(c) 2.29×10^5 kg/m³ (d) 2.29×10^{10} kg/m³
3. The free neutron
(a) decays through weak interaction (b) has life-time of 12 minutes.
(c) is unstable (d) all of the above
4. 1 a.m.u. equals
(a) 0.511 MeV (b) 931 MeV
(c) 511 MeV (d) 0.931 MeV
5. Nuclear forces are _____ times stronger than the gravitational force.
(a) 10^{36} (b) 10^{14}
(c) 10^{38} (d) 10
6. The maximum force of attraction between nucleus exists at a distance of _____.
(a) 1.5×10^{-15} m (b) 1.5×10^{-10} m
(c) 1×10^{-10} m (d) 1.5×10^{-20} m
7. The noncentral character of nucleus is due to
(a) electrostatic force (b) weak interaction
(c) tensor component (d) all of the above
8. The tensor forces are
(a) dependent on r (b) independent of r
(c) independent of spin (d) none of the above
9. For quadrupole moment, when $b > a$, is
(a) circular (b) flattened oblate ellipsoid
(c) spherical (d) elongated prolate ellipsoid
10. For quadrupole moment, when $a > b$, is
(a) spherical (b) flattened oblate ellipsoid
(c) circular (d) elongated prolate ellipsoid

11. The quadrupole moment is given by

(a) $\frac{2}{3}Z(b^2 - a^2)$

(b) $\frac{2}{5}Z(b^2 - a^2)$

(c) $\frac{3}{2}Z(b^2 - a^2)$

(d) $2Z(b^2 - a^2)$

12. For Barlett forces acting on nuclei

- (a) position coordinates are exchanged
- (b) position and spin coordinates are exchanged
- (c) neither spin nor position coordinates are exchanged
- (d) spin coordinates are exchanged

13. For Majorana forces acting on nuclei

- (a) position coordinates are exchanged
- (b) position and spin coordinates are exchanged
- (c) neither spin nor position coordinates are exchanged
- (d) spin coordinates are exchanged

14. For Heisenberg forces acting on nuclei

- (a) position coordinates are exchanged
- (b) position and spin coordinates are exchanged
- (c) neither spin nor position coordinates are exchanged
- (d) spin coordinates are exchanged

15. The range of Yukawa force is

- (a) 1 Å
- (b) 1 nm
- (c) 1 fm
- (d) 1 pm

16. Meson theory could not explain

- (a) spin dependence
- (b) exchange character of forces
- (c) none of these
- (d) both (a) and (b)

17. According to liquid drop model

- (a) nuclei is incompressible liquid drop of high density
- (b) liquid drop have surface tension force
- (c) the molecules inside liquid drop Posen thermal vibrations
- (d) all of the above

18. The value of a_v is volume energy term is

- (a) ≈ 10 MeV
- (b) $14 - 15$ MeV
- (c) ≈ 30 MeV
- (d) < 5 MeV

19. In Coulomb energy, a_c is equal to
 (a) 1 MeV (b) 2 MeV
 (c) 0.69 MeV (d) 10 MeV
20. The condition required for nuclear fission is
 (a) $\frac{Z^2}{A} > 45$ (b) $\frac{A}{Z^2} > 45$
 (c) $\frac{Z}{A} \geq 30$ (d) $\frac{Z}{A} > 45$
21. The magic numbers are
 (a) 2, 8, 20, 28, 50 (b) 121, 119, 117
 (c) 1, 3, 5, 7 (d) none of the above
22. Shell model could explain
 (a) magnetic moment (b) spin
 (c) energy (d) all of the above
23. For stretch case in LS coupling
 (a) $j = l - s$ (b) $j = l + s$
 (c) $j = l \pm s$ (d) $j = 0$
24. For Jack-knife case in LS coupling
 (a) $j = l + s$ (b) $j = l \pm s$
 (c) $j = l - s$ (d) $j > l / 2$
25. Shell model could not explain
 (a) total spin (b) total energy
 (c) magic numbers (d) total angular momentum

ANSWERS

- | | | | |
|--------|---------|---------|---------|
| 1. (a) | 8. (a) | 15. (c) | 22. (d) |
| 2. (c) | 9. (d) | 16. (d) | 23. (b) |
| 3. (d) | 10. (b) | 17. (d) | 24. (c) |
| 4. (b) | 11. (b) | 18. (b) | 25. (d) |
| 5. (c) | 12. (d) | 19. (c) | |
| 6. (a) | 13. (a) | 20. (a) | |
| 7. (c) | 14. (b) | 21. (a) | |

Microassessment Questions

1. What is atomic mass unit?
2. Write down the energy associated with 1 a.m.u.
3. What are the constituents of nucleus?
4. Explain whether proton is stable or not.
5. Is free or bound neutron stable? Explain.
6. Give the size of atom and nuclei.
7. What do you understand by nuclear charge?
8. Explain binding energy of a nucleus.
9. Calculate energy of electron in MeV.
10. Describe the noncentral behavior of nuclear forces.
11. Atomic binding energy is smaller than nuclear binding energy. Explain.
12. Write down the relation between mass number and nuclear radius.
13. What is electric quadrupole moment?
14. What are nuclear forces?
15. Why nuclear models are necessary?
16. What are magic numbers?
17. Krypton and xenon emit nucleon easily. Why?
18. What do you understand by meson clouds?
19. Obtain the range of Yukawa force.
20. What do you understand by short-range forces?
21. Find out the nuclear density for U^{235} .
22. Calculate the binding energy for α -particle in joules.

Critical Thinking Questions

1. What are the forces that exist within the nucleons?
2. How do nuclear forces differ from gravitational and electrostatic forces?
3. Write short note on nuclear density.
4. Do nuclear forces depend on charge of neutron and proton?
5. Explain the saturation of nuclear forces.
6. What are the tensor forces? On which factors do they depend?
7. Explain exchange forces.
8. Write down the basic forces, which exist in nature.
9. How do Majorana forces differ from Heisenberg force?
10. Describe the four types of exchange forces.
11. Give the wave equation under the effect of Barlett forces.
12. Why stable nuclei have more neutrons than the protons?
13. How does binding energy affect the stability of nucleus?
14. What is Wigner force? Why is it known as no exchange force?
15. What are the drawbacks of meson theory?
16. Write down the assumptions made using liquid drop model.
17. Atom is considered as incompressible liquid. Explain.
18. Write down the merits and demerits of liquid drop model.

19. How does asymmetry and pairing effect the nuclear stability?
20. Why even–even nuclei are more common than odd–odd nuclei?
21. Explain spin–orbit coupling. How would you explain stretch and jackknife case?
22. Give the variation of binding energy versus atomic mass indicating stability of magic nuclei.
23. Why are lighter nuclei stable than heavier nuclei?
24. What is the theoretical basis of shell model?
25. What do you understand by isotopes and isotones?

Graded Questions

1. Show that due to quadrupole moment the symmetry of nucleus gets changed.
2. State and explain Yukawa's meson theory.
3. Write down the postulates of meson theory.
4. State and explain all the postulates of liquid drop model.
5. Derive the semi-empirical mass formula indicating the significance of each term.
6. How could nuclear fission be explained on the basis of liquid drop model?
7. Explain critical parameter using Bohr and Wheeler theory. Show the variation indicating the nuclear stability.
8. Explain shell model in detail using potential and spin–orbit coupling.
9. Give the schematic energy level diagram upto nucleon number 126.
10. What are the limitations of shell model?
11. Discuss briefly the experimental evidence for existence of magic numbers.
12. Write down the achievements of shell models.
13. How does shell model differ from liquid drop model? How shell model succeeds in explaining the existence of shell model?
14. Discuss the contribution of Meyer and Jensen to shell model.

Remember and Understand

1. Atoms were thought to be indivisible particles.
2. Nucleus is made up of neutrons and protons, whereas electrons orbit around the nucleus.
3. The nuclear density is almost constant everywhere except at the surface. The surface density is less than the density at the center.
4. Free neutron is unstable, whereas free proton is stable.
5. The nuclear masses are measured in terms of atomic mass unit. 1 atomic mass unit is defined as the 1/12th of mass of single carbon atom.
6. Nuclear forces are the strongest forces in nature. These forces are charge independent and spin dependent. These forces are also saturated and exhibit exchange character.
7. The nucleus is not spherical and gets distorted, which could be due to the non-uniform charge distribution in the nucleus.
8. There are four types of exchange forces, that is, Wigner, Barlett, Heisenberg, and Majorana forces.
9. Meson theory explains the existence of nuclear forces.
10. The interaction between nucleons can be studied using different nuclear models. The two important models are shell model and liquid drop model.

11. Liquid drop model treats atomic nucleus as a drop of liquid. This model was successful in explaining radioactivity, fission, and nuclear stability but could not explain the existence of magic numbers.
12. The time-dependent Schrödinger wave equation was solved using interaction potential.
13. Shell model explains the existence of magic numbers. Magic numbers represent the closed shells of protons and neutrons.
14. The Weizsacker's formula is given by $E = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - \frac{a_a (A - 2Z)^2}{A} (\pm, 0) \frac{a_p}{A^{3/4}}$
15. The potential due to quadrupole moment is $V_3 = \frac{1}{4\pi\epsilon_0 r^3} \int \rho(\vec{r}') r' (3 \cos^2 \theta - 1) dV$
16. The quadrupole moment Q_3 is given by $Q_3 = \frac{2}{5} Z(b^2 - a^2)$
17. The potential under the effect of tensor forces is given by $V(r) = V_{l_1}(r) + V_{l_2}(r) \vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_{l_3}(r) S_{12}$

Nuclear Physics — II

Decay Process and Radiation Detectors

Keywords: Radioactivity, α -decay, β -decay, γ -decay, internal conversion, radiation detectors, Geiger Muller counters, scintillation counters, proportional counters, Ionization counters

Learning Objectives

- ◆ To understand the phenomena of disintegration of heavy nuclei into smaller nuclei, that is, radioactivity
- ◆ To study the emission of α -, β -, and γ -rays from radioactive nuclei
- ◆ To get insight into laws of radioactivity
- ◆ To know about units of measurement of radioactivity
- ◆ To understand Geiger–Nuttall law, that is, most energetic α -particles are emitted by shortest lived nuclides
- ◆ To learn the Gamow's theory of α -decay considering particle in nuclear potential barrier under constant motion
- ◆ To understand the β -decay with the help of negatron emission, positron emission, and electron capture
- ◆ To learn about Fermi's theory of β -decay and conservation of energy and angular momentum during the process
- ◆ To get insight into γ -decay using multipole expansions
- ◆ To learn and understand the phenomena of internal pair creation and internal conversion
- ◆ To understand the importance of detection of particles using radiation detectors
- ◆ To study the principle, working, and theory of ionization chamber
- ◆ To learn the principle, working, and theory of proportional counter
- ◆ To understand the principle and working of Scintillation counter
- ◆ To understand the behavior of ionization current versus voltage

The most important contribution of “modern physics” is the discovery of “radioactivity” by a French scientist Henri Becquerel in 1896. He observed a particular property for the uranium salt. He found that photographic plate gets affected by some kind of radiations emitted. These radiations were termed Becquerel rays. Later on, it was found that not only uranium emitted these kinds of radiations, but many other elements too emitted these radiations, for example, radium, actinium, thorium, etc. Hence, such materials are said to be radioactive.

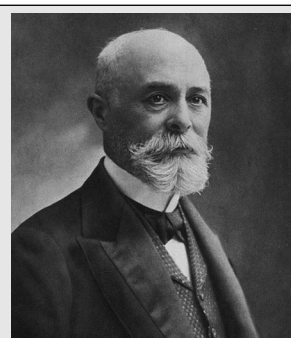
7.1 Radioactivity

The phenomena of disintegration of heavy nuclei into smaller nuclei in the absence of any external force is called radioactivity. The elements endowed with this property are called radioactive elements. The nuclei of radioactive elements are unstable. The elements with atomic number greater than 82 are radioactive. There is nuclear force acting within the nucleus, which holds the nucleons together. Despite the fact that the nuclear force maintains stability, some nuclei do emit radiations. Temperature, pressure, etc., do not affect radioactivity. After Becquerel discovered radioactivity, Rutherford in 1899 confirmed the emission of two types of radioactivity, that is, α - and β -rays. In 1909, γ -rays were discovered as neutral radiations with very high penetration power. α - and β -rays consist of particles, hence they are not necessarily considered as corpuscles.

Antoine Henri Becquerel was born on December 15, 1852, in Paris. His family consisted of scholars and scientists. He won the Nobel Prize in Physics in 1903 for discovering radioactivity. His father, Alexander Edmond Becquerel, was a professor of Applied Physics. Alexander did his research on phosphorescence and solar radiation. Henri joined the Polytechnic in 1872 and became a professor of Applied Physics. His initial research was on optics and the rotation of plane-polarized light by magnetic fields. He then studied phosphorescent crystals under infrared illumination and absorption of light in those crystals. Becquerel got his doctorate in 1888 from the Faculty of Sciences of Paris.

Becquerel investigated any connection between X-rays and naturally occurring phosphorescence. He found that the plate was discovered to be fogged, when uranium salts were placed near to a photographic plate covered with opaque paper. All uranium atoms exhibited this property (later on this property was known as radioactivity). Furthermore, Becquerel demonstrated that the rays emitted from uranium atoms ionized the gases. These rays could be deflected using electric and magnetic fields unlike X-rays. He worked on different radioactive stones, so he developed many skin problems. Becquerel also did extensive studies of the physical properties of ozone, cobalt, and nickel. The basic unit of radioactivity used in the international system of radiation units is "Becquerel."

Besides being a Nobel Laureate, Becquerel was a member of the Academe des Sciences de France, Accademia dei Lincei, and the Royal Academy of Berlin. He was appointed as an Officer of the Legion of Honour. He died in 1908 in Brittany and is still remembered by the entire world.



A.H. BECQUEREL

7.1.1 Description of α -, β -, and γ -Rays

A small hole is drilled inside a block of lead and the radioactive material is placed at the bottom of the hole. These radiations are studied under the effect of electric and magnetic fields (Figure 7.1(a)–(b)).

As can be seen from Figure 7.1(a), the α -rays get deflected toward the negative plate and the β -rays get deflected toward the positive plate. Under the influence of magnetic field (Figure 7.1(b)), α - and β -rays get deflected, whereas γ -rays did not deflect toward any electric plate and magnetic field. Hence, the following conclusions are drawn:

- (i) The α -particles get deflected toward negative plate, hence they are positively charged particles (${}_2\text{He}^4$).

- (ii) The β -particles get deflected toward positive plate, hence they are negatively charged particles (electrons).
- (iii) γ -rays did not get deflected along any plate, hence they are stream of neutral particles.

Marie Curie was born on November 7, 1867, in Warsaw. She was the youngest daughter and her childhood was difficult as her mother and sister passed away. Her primary education was from local school though her father taught her mathematics and physics. She left Warsaw at the age of 24 years and moved to Paris for higher education. Marie Curie was a chemist and a physicist. She met Pierre Curie in 1894 who was an instructor in the School of Physics and Chemistry. They got close to each other due to their common interests and got married. Curie was very much inspired from the work of Henri Becquerel on radioactivity and she decided to study uranium rays for her thesis. She was the first person in the scientific history to receive two Nobel Prizes in different fields of science, that is, chemistry and physics. The Royal Swedish Academy of Sciences honored Pierre Curie and Marie Curie in 1903 with the Nobel Prize in Physics. Marie Curie gave the theory of radioactivity, radioactive isotopes, and the discovery of polonium and radium. Pierre Curie died in 1906 and she took his place as professor of General Physics in the Faculty of Sciences. She continued to develop methods for obtaining pure radium from radioactive residues and was successful in 1910 in doing so. She was also appointed as the director at the Curie Laboratory in the Radium Institute of the University of Paris. In 1911, she was awarded with second Nobel Prize, but this time in Chemistry for her work in the field of radioactivity. The great scientist Marie Curie died due to aplastic anemia on July 4, 1934, at the Sancellemoz Sanatorium in Passy, in Haute-Savoie.



MARIE CURIE

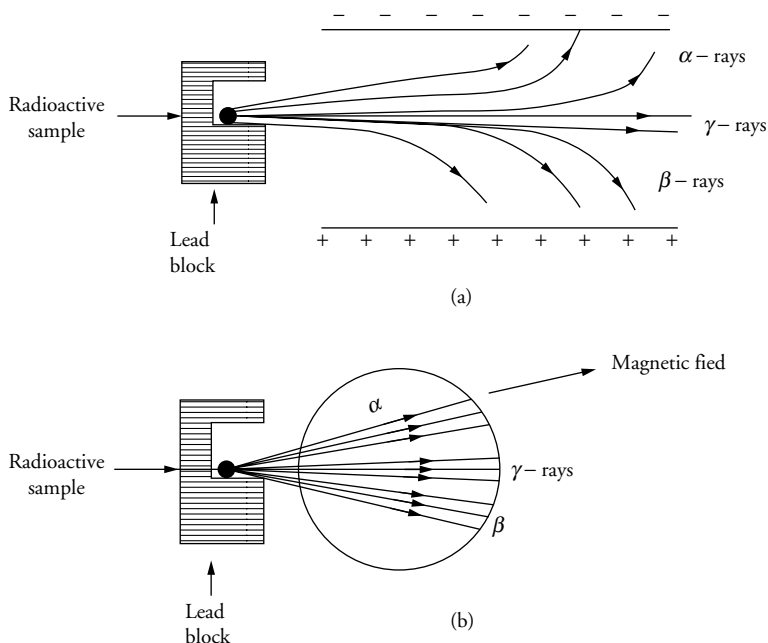


Figure 7.1 Deflection of α - and β -rays under the effect of (a) electric field and (b) magnetic field.

Table 7.1 Comparison of α -, β -, and γ -rays and their properties

	α -rays	β -rays	γ -rays
Charge	It is equivalent to that of Helium	Charge is $1.6 \times 10^{-19} C$	Charge is zero
Velocity	1.4×10^7 m/s 2.1×10^7 m/s	Can go upto 99% of velocity of light	3×10^8 m/s
Penetration power	Very small	Large	Very large
Ionizing power	Large ionizing power	$\frac{1}{100}$ times that of α -particles	Very small
Fluorescence	Can produce fluorescence	Can cause fluorescence	Can cause fluorescence
Deflection	Deflected by electric and magnetic field	Deflected by electric and magnetic fields	Are not deflected by any field
Scattering power	Get scattered while passing through mica, gold foil, etc.	Scattered through the matter	Scattered from crystals

7.2 Laws of Radioactivity

Soddy and Fajan stated the following laws which are known as laws of radioactivity:

- During radioactive transformation, α - or β -particles are emitted. Both the particles are not emitted together.
- After emission of α -particle, the atomic number is reduced by 2 units and atomic mass is reduced by 4 units. Hence, the nuclei has a position that is shifted by two groups on the left.

For example,



For example,



- When a nuclei emits β -particle, the atomic number is increased by 1 unit. The daughter nuclei position gets shifted by one group on the right.

That is,



7.3 Units of Radioactivity

The radioactivity is described as atoms disintegrating per unit time. The unit of radioactivity is given by curie, which is activity of 1 g of radium. Curie can be defined as the activity of radioactivity material that produces 3.7×10^{10} disintegrations/sec. Due to the confusion over the units, Rutherford is given as a unit of radioactivity. Rutherford is defined as the activity of radioactive material that produces 10^6 disintegrations/sec. Hence,

$$1 \text{ curie} = 3.7 \times 10^{10} \text{ disintegrations/sec}$$

$$1 \text{ Rutherford} = 10^6 \text{ disintegrations/sec}$$

7.4 Radioactive Decays (α , β , and γ Decays)

The radioactive decay is defined as the process when nucleus disintegrates by emitting α , β , or γ radiations or when the nucleus captures an electron from the atomic shell. All the three decays have been discussed in following sections.

7.4.1 Alpha Decay

α -particles can be detected by cloud chambers, scintillation counters, nuclear emulsions, and ionization chamber. For measuring energy of α -particles, techniques such as spectrography, deflection method, calorimetric measurements, and range measurements are used. Nucleons comprise of neutrons and protons. The protons have repulsive force within them which is proportional to Z^2 (Z is the atomic number). The binding energy inside the nucleons is proportional to atomic mass (A). When the number of nucleons increases, the electrostatic repulsion dominates over the attractive nuclear forces within the nucleons. Hence, mostly for nuclei with $Z > 82$, α decay occurs in order to reduce the number of nucleons which helps in stabilizing the nuclei. Here, the main concern is why α -particle is emitted despite any other nuclear particles such as deuterium and tritium. It can be explained as follows: The nucleus of α -particle is made up of 2 neutrons and 2 protons. The nuclei of α -particle have very high binding energy. The disintegration energy Q is given by

$$Q = [M_i - (M_f + M_\alpha)]c^2 \quad (5)$$

where M_i is mass of initial parent nuclei

M_f is mass of final daughter nuclei

M_α is mass of the α -particle emitted

When the particle is formed inside nucleus, the kinetic energy is sufficient to make α -particle free from the nuclei. The α -decay makes the nuclei energetically and structurally stable. For example, uranium nuclei (${}_{92}\text{U}^{238}$) becomes stable due to loss of 5.4 MeV of energy after releasing α -particle. Furthermore, if ${}_{2}\text{He}^3$ or proton is emitted from the nuclei, then 9.6 and 6.1 MeV energy is required, respectively and is difficult to attain. However, the kinetic energy of α -particle is a bit different from the disintegration energy and given by the following relation:

$$\text{K.E} \approx \frac{A-4}{A}Q \quad (6)$$

This difference in KE and Q can be explained as follows:

- (i) The nucleus gets recoiled by taking small amount of kinetic energy in order to conserve energy and momentum.

- (ii) The linear momentum is conserved during α -decay. As initially the nuclei is at rest, hence initial momentum is zero. If final daughter nuclei have velocity v_f and alpha nucleus (mass M_α) have velocity v_α , then according to conservation of linear momentum,

$$0 = M_f v_f + M_\alpha v_\alpha$$

$$M_f v_f = -M_\alpha v_\alpha \quad (7)$$

Therefore, final daughter nuclei and alpha nuclei move opposite to each other.

- (iii) The mass energy is also conserved during the process of α -emission. Let E_α be the energy of ejection of α -particle and E_f be the kinetic energy of final daughter nuclei. Then, the total energy of initial parent nuclei can be written as

$$M_i c^2 = M_f c^2 + M_\alpha c^2 + E_f + E_\alpha \quad (8)$$

Comparing Eqs (5) and (8),

$$Q = E_f + E_\alpha$$

$$Q = \frac{1}{2} M_f v_f^2 + \frac{1}{2} M_\alpha v_\alpha^2 \quad (9)$$

Using Eqn. (7) in Eqn. (9),

$$Q = \frac{1}{2} M_\alpha v_\alpha^2 + \frac{1}{2} M_f \frac{(M_\alpha v_\alpha)^2}{(M_f)^2}$$

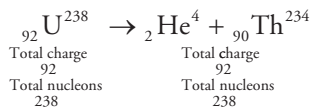
$$Q = \frac{1}{2} M_\alpha v_\alpha^2 + \frac{1}{2} \frac{M_\alpha^2 v_\alpha^2}{M_f}$$

$$Q = \frac{1}{2} M_\alpha v_\alpha^2 \left[1 + \frac{M_\alpha}{M_f} \right] \quad (10)$$

$$Q = E_\alpha \left[1 + \frac{M_\alpha}{M_f} \right] \quad (11)$$

From Eqn. (11), it is clear that the disintegration energy of nuclei is more than energy of alpha particle.

- (iv) The total charge and number of nucleons also remain conserved for α -emission process as demonstrated below:



1. Geiger–Nuttall Law

In 1911, Geiger–Nuttall correlated the empirical facts regarding α -emission as Geiger–Nuttall law. During their studies on α -particles, they found that the most energetic α -particles are emitted by shortest lived nuclides having high value of decay constant. Similarly, least energetic α -particles are emitted by longest lived nuclides. It was found that the α -particle range from 4.06 to 9 MeV.

α -particles have a range which is defined as the critical distance traveled by α -particle before getting absorbed. The relation between range and energy of particle is given by

$$R = 0.318 E^{3/2} \quad (12)$$

The relation between disintegration constant (λ) and number of atoms is given by

$$N = N_0 e^{-\lambda t} \quad (13)$$

$N \rightarrow$ number of atoms in substance after time t

$N_0 \rightarrow$ number of atoms in substance at $t = 0$

λ is defined as the ratio of amount of substance disintegrating/time to the amount of substance present. The relation between disintegration constant λ and range R of α -particles is given by

$$\log \lambda = A + B \log R \quad (14)$$

(range is in cm and standard air) A and B are constants. B is the slope of line and A is the intercept (Figure 7.2). To understand Figure 7.2, we should have an understanding of uranium, thorium, and actinium series. When a radioactive element emits α - or β -particle, it gets transformed to new element (daughter nuclide). If the daughter nuclide is also radioactive, then it will also disintegrate. This process will continue until and unless a stable state is reached this constitute a series which involve the step by step disintegration of parent nuclei to daughter nuclei by emitting radioactive particles. For uranium series (${}_{92}\text{U}^{238}$), the end product is Pb^{206} with a half-life of 4.5×10^9 years. For thorium series, ${}_{90}\text{Th}^{232}$ is the parent nuclei and end product is Pb^{208} with a half-life of 4.5×10^{10} years. For actinium series, ${}_{92}\text{U}^{235}$ is parent nuclei and Pb^{207} is the daughter nuclei with a half-life of 7.1×10^8 years.

From Figure 7.2, it is clear that the slope of all the series is almost same. From Eqn. (12), it can be written as follows:

$$R \propto E^{3/2}$$

$$\log R \propto \log E$$

$$\log \lambda = C_1 + C_2 \log E \quad (15)$$

Equation (15) describes the relation between disintegration constant (λ) and energy (E). It is clear from Eqn. (15) that high energetic particle have high disintegration constant and vice versa.

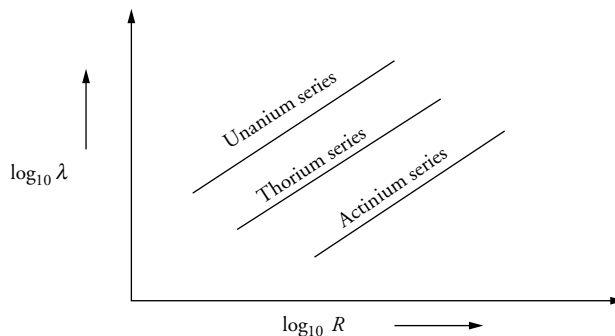


Figure 7.2 Plot of disintegration constant with range of α -particles.

2. Gamow's Theory of α -Decay

Before, we proceed further, there are certain assumptions to be made during the process of α -decay. First, α -particle exists as an entity within heavy nucleus. There is nuclear potential barrier inside which the particle is in constant motion. There is definite probability of tunneling of particle through the potential barrier (height V_0).

From Figure 7.3, we consider a potential barrier of width. The potential distribution is given by

$$\begin{aligned} V &= 0 & \text{for } x < 0 & \quad (\text{Region 1}) \\ V &= V_0 & \text{for } 0 < x < L & \quad (\text{Region 2}) \\ V &= 0 & \text{for } x > 0 & \quad (\text{Region 3}) \end{aligned}$$

The energy E of particle is less than V [$E < V$].

We will use Schrödinger equation to solve this problem:

$$\text{i.e.,} \quad \frac{d^2\varphi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\varphi = 0 \quad [\varphi \text{ is wavefunction describing the position of particle}] \quad (16)$$

For $x < 0$, potential $V = 0$ in region 1

$$\begin{aligned} \frac{d^2\varphi_1}{dx^2} + \frac{2mE}{\hbar^2}\varphi_1 &= 0 \\ \frac{d^2\varphi_1}{dx^2} + k_1^2\varphi_1 &= 0 \end{aligned} \quad (17)$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad (18)$$

The solution of Eqn. (17) is given by

$$\varphi_1 = \underbrace{A_1 e^{ik_1 x}}_{\text{Incident } \alpha\text{-particle}} + \underbrace{A_2 e^{-ik_1 x}}_{\text{Reflected } \alpha\text{-particle}} \quad (19)$$

For $0 < x < L$, potential $V = V_0$ in region 2.

$$\begin{aligned} \frac{d^2\varphi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\varphi_2 &= 0 \\ \frac{d^2\varphi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\varphi_2 &= 0 \end{aligned}$$

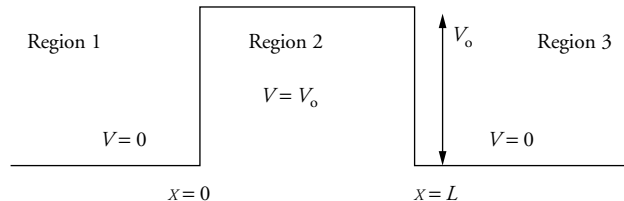


Figure 7.3 One-dimensional potential barrier.

$$\frac{d^2\varphi_2}{dx^2} - k_2^2\varphi_2 = 0 \quad (20)$$

where

$$k_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \quad (21)$$

The solution of Eqn. (20) is given by

$$\varphi_2 = \underbrace{B_1 e^{k_2 x}}_{\text{Refracted wave through potential barrier}} + \underbrace{B_2 e^{-k_2 x}}_{\text{Reflected wave through the potential barrier in region 3}} \quad (22)$$

For $x > 0$, potential $V = 0$ in region 3.

$$\begin{aligned} \frac{d^2\varphi_3}{dx^2} + \frac{2mE}{\hbar^2}\varphi_3 &= 0 \\ \frac{d^2\varphi_3}{dx^2} + k_1^2\varphi_3 &= 0 \end{aligned} \quad (23)$$

The solution of Eqn. (23) is given by

$$\varphi_3 = \underbrace{C_1 e^{+ik_1 x}}_{\text{Transmitted wave}} + \underbrace{C_2 e^{-ik_1 x}}_{\text{Reflected wave}} \quad (24)$$

As there is no further potential barrier after region 3, $C_2 e^{-ik_1 x}$ is zero because there can be no reflection.

$$\varphi_3 = C_1 e^{ik_1 x} \quad (25)$$

To determine the constants, we have to use boundary conditions as follows:

$$\varphi_1 \Big|_{x=0} = \varphi_2 \Big|_{x=0} \quad (26a)$$

$$\varphi_2 \Big|_{x=L} = \varphi_3 \Big|_{x=L} \quad (26b)$$

$$\frac{d\varphi_1}{dx} \Big|_{x=0} = \frac{d\varphi_2}{dx} \Big|_{x=0} \quad (26c)$$

$$\frac{d\varphi_2}{dx} \Big|_{x=L} = \frac{d\varphi_3}{dx} \Big|_{x=L} \quad (26d)$$

Using Eqs (19), (22), and (26a),

$$A_1 + A_2 = B_1 + B_2 \quad (27)$$

Using Eqs (19), (22), and (26c),

$$ik_1(A_1 - A_2) = k_2(B_1 - B_2) \quad (28)$$

Using Eqs (22), (25), and (26b),

$$B_1 e^{k_2 L} + B_2 e^{-k_2 L} = C_1 e^{ik_1 L} \quad (29)$$

Using Eqs (22), (28), and (26d),

$$k_2(B_1 e^{k_2 L} - B_2 e^{-k_2 L}) = ik_1 C_1 e^{ik_1 L} \quad (30)$$

Adding and subtracting Eqs (29) and (30),

$$\text{After adding } \Rightarrow B_1 = \frac{C_1}{2} e^{ik_1 L} \left[1 + \frac{ik_1}{k_2} \right] e^{-k_2 L} \quad (31)$$

$$\text{After subtracting } \Rightarrow B_2 = \frac{C_1}{2} e^{ik_1 L} \left[1 - \frac{ik_1}{k_2} \right] e^{k_2 L} \quad (32)$$

Substituting Eqs (31) and (32) in Eqs (27) and (28), we obtain

$$A_1 + A_2 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) - \frac{ik_1}{2} \sin h(k_2 L) \right] \quad (33)$$

and

$$A_1 - A_2 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) + \frac{ik_2}{k_1} \sin h(k_2 L) \right] \quad (34)$$

Adding and subtracting Eqs (33) and (34),

$$\text{After adding } \Rightarrow A_1 = C_1 e^{ik_1 L} \left[\cos h(k_2 L) + \frac{i}{2} \left[\frac{k_2}{k_1} - \frac{k_1}{k_2} \right] \sin h(k_2 L) \right] \quad (35)$$

and

$$\text{After subtracting } \Rightarrow A_2 = -\frac{iC_1}{2} e^{ik_1 L} \left[\left(\frac{k_1}{k_2} + \frac{k_2}{k_1} \right) \sin h(k_2 L) \right] \quad (36)$$

We can define transmission coefficients as the ratio of transmission probability current density to the incident probability current density.

Probability current density = velocity of particle \times probability

[where v is the velocity of particle]

$$T = \frac{v \varphi_3^* \varphi_3}{v \varphi_1^* \varphi_1} \quad [\text{incident and transmitted particle have same velocity as } k_1 = k_2]$$

$$T = \frac{C_1 e^{ik_1 x} C_1^* e^{-ik_1 x}}{A_1 e^{ik_1 x} A_1^* e^{-ik_1 x}} \quad [\text{from Eqs (25) and (19)}]$$

$$T = \frac{C_1 C_1^*}{A_1 A_1^*} = \frac{C_1 C_1^*}{C_1 e^{ik_1 L} \left[\cos h(k_2 L) + \frac{i}{2} \left[\frac{k_2}{k_1} - \frac{k_1}{k_2} \right] \sin h(k_2 L) \right] C_1^* e^{-ik_1 L} \left[\cos h(k_2 L) - \frac{i}{2} \left[\frac{k_2}{k_1} - \frac{k_1}{k_2} \right] \sin h(k_2 L) \right]}$$

$$T = \frac{1}{\cos h^2(k_2 L) + \frac{1}{4} \left[\frac{k_2}{k_1} - \frac{k_1}{k_2} \right]^2 \sin h^2(k_2 L)}$$

$$T = \frac{1}{1 + \left[\frac{k_2^2 + k_1^2}{2k_1k_2} \right]^2 \sin^2 h^2(k_2L)} \quad (37)$$

Substituting Eqs (18) and (21),

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sin^2 h^2 \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} L}$$

Using binomial expansion $(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \dots$

$$T \approx \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sin^2 k_2L \right]^{-1}$$

$k_2L \gg 1$; hence, $\sin^2 k_2L = \frac{1}{4}e^{2k_2L}$

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \times \frac{1}{4}e^{2k_2L} \right]^{-1}$$

Neglecting 1

$$T = \frac{16E}{V_0} \left[1 - \frac{E}{V_0} \right] e^{-2k_2L} \quad (38)$$

Disintegration constant and transmission coefficient are same, that is,

$$\lambda = \frac{16E}{V_0} \left[1 - \frac{E}{V_0} \right] e^{-2k_2L} \quad (39)$$

Taking log on both sides:

As $E < V_0$, $\frac{E}{V_0}$ can be neglected

$$\log \lambda = \log \left(\frac{16E}{V_0} \left[1 - \frac{E}{V_0} \right] \right) - 2k_2L \quad (40)$$

$$\log \lambda = \log \left(\frac{16E}{V_0} \right) - 2k_2L$$

$$\log \lambda = \log \left(\frac{16E}{V_0} \right) - 2\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} L$$

$$\log \lambda = -\frac{2}{\hbar} \sqrt{2m(V_0 - E)} L + \log \left(\frac{16E}{V_0} \right) \quad (41)$$

Equation (41) can predict finite probability of tunneling of α -particles through nuclear potential. The emission of α -particles can be explained with Gamow's theory.

George Antonovich Gamow was born on March 4, 1904, Odessa, Russian Empire. He was a physicist as well as cosmologist. Gamow went to Leningrad University, where he briefly met A.A. Friedmann who was a mathematician and cosmologist. Friedmann suggested that the universe should be expanding to which Gamow did not agree much. Gamow started working on quantum theory and genetic theory especially on deoxyribonucleic acid (DNA). He developed quantum theory of radioactivity, which provided the first successful explanation of the behavior of radioactive elements. This achievement of Gamow earned him a fellowship at the Copenhagen Institute of Theoretical Physics in 1928. He worked on theoretical nuclear physics. He proposed the famous "liquid drop" model of atomic nuclei. This model is the backbone of many modern theories of nuclear fission and fusion. In collaboration with F. Houtermans and R. Atkinson, he developed a theory, which could describe the rates of thermonuclear reactions inside the core of stars. Gamow emigrated from the Soviet Union in 1934 to Washington. He was appointed as the professor of physics at George Washington University. There he met with Edward Teller and then they collaborated with each other. They developed the theory of β -decay in 1936. Gamow also tried to interpret stellar evolution using theories of nuclear reactions. He found from his work on stellar evolution that the Sun's energy results from thermonuclear processes. He died on August 19, 1968, leaving his genius ideas behind.



**GEORGE GAMOW
AND ACTRESS ANN
BLYTHE**

7.4.2 β -Decay

During β -decay, the atomic number changes by one unit and atomic mass remains unchanged. β -particles get deflected by positive plate. The β -decay can occur through three processes, that is, emission of positron (β^+ decay), emission of electron (β^- decay), or capture of orbital electron (κ -capture). All the three processes are described below.

1. β^- -decay (Negatron Emission)

When electrons are emitted by nucleus in order to achieve stabilization, it is known as electron/negatron emission or β -decay. The main question arises, how can nucleus emit an electron, when electron is revolving in outer shells. This is explained as follows:

- (i) Neutron is converted to proton by the process



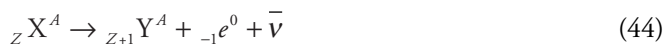
The electron that is formed during Eqn. (42) gets released immediately from the nucleus.

- (ii) According to Eqn. (42), the law of conservation of angular momentum and energy are violated. Hence, Pauli proposed the concept of neutrines, which is a neutral particle of zero rest mass and spin $\frac{1}{2}$. Hence, Eqn. (42) is modified as



$\bar{\nu}$ is called antineutrino.

The generalized equation is given by



For electron emission to take place, the rest mass of initial parent nucleus is greater than the rest mass of final daughter nuclei. When the parent nucleus is at rest, the kinetic energy is zero. According to law of conservation of energy

$$M_i c^2 = M_f c^2 + E_f + m_e c^2 + E_e \quad (45)$$

The disintegration energy Q is given by

= kinetic energy of products - kinetic energy of reactants

$$Q = (E_f + E_e) - 0$$

$$Q = (M_i - M_f - m_e) \quad (46)$$

For β -decay, $Q > 0$, which states

$$M_i > M_f + m_e \quad (47)$$

2. β^+ decay (Positron Emission)

In contrast to β^- decay, the positron is emitted from nuclei to achieve higher stability. This is usually the case when the nuclei is proton rich, then the protons are converted to neutrons by the following mechanism:



where ν (neutrino) is emitted to conserve energy as well as momentum. The generalized equation is given by the following equation:



${}_{+1} e^0$ and ${}_{-1} e^0$ share the same perspectives except the type of charge they carry, that is, positron is a positively charged electron. Similar to negatron emission, the positron emission takes place only when the mass of parent nuclei is more than the mass of daughter nuclei.

3. Electron Capture

The electron capture process is competitive to positron emission. In the case of electron capture, Coulomb barrier tends to prevent emission of positron. Hence, the nucleus captures orbital electron to stabilize itself. Upon the absorption of orbital electron, the proton gets converted to neutron and atomic number gets decreased by one group (to left). Neutrino is emitted during the process. For heavier element, the orbital electrons are closer to the nucleus because of small radii. Hence, the heavier elements exhibit more electron capture than positron emission. After the electron is captured by nucleus, vacancy is created in the orbit. To fill this vacancy, electrons from higher shells jump to the vacant positions to fill empty space. During this transition, the characteristic X-rays are emitted. Therefore, electron capture process is accompanied by the emission of X-rays.

The equation for electron capture is



The generalized equation is same as that of positron emission. Moreover, similar to other β -decay processes, the mass of initial parent nuclei is more than the final daughter nuclei.

4. Fermi Theory of β -Decay

Using Pauli's neutrino hypothesis, Fermi formulated the theory of β -decay in 1934. This theory takes into account the following certain assumptions:

- (i) During the process of β -decay, energy and angular momentum are conserved.
- (ii) Whenever a neutron is converted to proton, antineutrino is emitted. Whereas during the conversion of proton to neutron, neutrino is emitted. The neutrino has zero rest mass.
- (iii) The β -decay is taken analogous with the emission of electromagnetic radiations by an atom. As electromagnetic radiations have a field surrounding them, similarly there is electron neutron field in β -decay process. The nucleons have strong nuclear force field, but the electron–neutron field is weak compared with nucleons.
- (iv) The coupling constants are very small, hence time-dependent perturbation theory is used.
- (v) Nuclear parity does not change during β -decay. The calculations are made in nonrelativistic regime as the nucleons have velocity of $\frac{c}{10}$. The negatrons, positrons, neutrinos, and antineutrinos are produced at the time of emission.

During the process of β -decay, proton can get converted to neutron (positron emission) and neutron can get converted to proton (negatron emission). During these decay processes, neutrino or antineutrino are formed in order to conserve momentum and energy. To find out the probability of transition of nucleon from initial to final state, we will use perturbation theory as follows:

$$P dp = \frac{2\pi}{\hbar} \left| \int \varphi_f^* H \varphi_i dV \right|^2 \frac{dN}{dT} \quad (51)$$

where φ_i and φ_f are the wave functions of initial and final states, respectively. H is the interaction energy operator that represents the interaction between electron neutrino field and nucleon. Basically, H is the backbone of Fermi theory. $\frac{dN}{dT}$ represents energy density of final states (statistical factor). We can write Eqn. (51) as

$$P dp = \frac{2\pi}{\hbar} |H_{if}|^2 \frac{dN}{dT} \quad (52)$$

where

$$H_{if} = \int \varphi_f^* H \varphi_i dV \quad (53)$$

is called interaction matrix element.

Let us explain it with the help of decay scheme

$$p \rightarrow n + {}_{+1}e^0 + \nu$$

$$\text{Wave function of final products} = \varphi_f = \varphi_n \varphi_\beta \varphi_\nu \quad (54)$$

where φ_n wave function of neutron
 φ_β wave function of positron
 φ_ν wave function of neutrino

The wave function is treated as plane wave because due to first approximation, the distortion of wave function of positron or electron due to nuclear charge is neglected. Hence, the wave function can be normalized as follows:

$$\int_0^V \varphi_\beta^* \varphi_\beta dV = 1 \quad \left[V \rightarrow \begin{array}{l} \text{volume occupied by} \\ \text{free particle wave} \end{array} \right]$$

The φ_β is obtained as

$$\varphi_\beta = \frac{1}{\sqrt{V}} \exp\left[\frac{i}{\hbar} p_\beta \cdot r\right] \quad (55)$$

where $\frac{1}{\sqrt{V}}$ is normalization constant and p_β is momentum of β -particle. Similar case is applied for neutrino as it interacts very weakly with matter.

Therefore,

$$\varphi_\nu = \frac{1}{\sqrt{V}} \exp\left[-\frac{i}{\hbar} p_\nu \cdot r\right] \quad (56)$$

where p_ν is momenta of neutrino. The reason behind assumption of plane waveform is to neglect the possible interaction of β -particle and neutrino with nucleus. Another constant “ G ” is used, which is known as “Fermi coupling constant.” This constant determines the strength of coupling because the form of interaction operator H is unknown. G has value of $0.9 \times 10^{-4} \text{ MeV fm}^3$ and is analogous to electron charge. The equations are symmetrical if we replace φ_ν by φ_ν^* because absorption of antineutrino and emission of neutrino is equivalent. Therefore, Eqn. (53) can be written as follows:

$$\begin{aligned} H_{if} &= G \int [\varphi_f^* H \varphi_i] dV \\ H_{if} &= G \int [\varphi_f^* \varphi_\beta^* \varphi_\nu^* H \varphi_i] dV \\ H_{if} &= G \int [\varphi_n^* \varphi_\beta^* \varphi_\nu] M \varphi_i dV \end{aligned} \quad (57)$$

M is dimensionless matrix element.

Now, from Eqs (55) and (56),

$$\begin{aligned} \varphi_\beta^* \varphi_\nu &= \frac{1}{\sqrt{V}} \exp\left[\frac{i}{\hbar} p_\beta \cdot r\right] \frac{1}{\sqrt{V}} \exp\left[-\frac{i}{\hbar} p_\nu \cdot r\right] \\ \varphi_\beta^* \varphi_\nu &= \frac{1}{V} \exp\left[-\frac{i}{\hbar} [p_\beta + p_\nu] \cdot r\right] \end{aligned} \quad (58)$$

$$\varphi_\beta^* \varphi_\nu = \frac{1}{V} \left[1 - \frac{i}{\hbar} [p_\beta + p_\nu] \cdot r - \frac{1}{2\hbar^2} [[p_\beta + p_\nu] \cdot r]^2 + \dots \right] \quad (59)$$

We can approximate

$$p_\nu \approx p_\beta \approx m_0 c$$

$$\frac{p_v r_o}{\hbar} \approx \frac{p_\beta r_o}{\hbar} \approx \frac{m_o c r_o}{\hbar} \approx \frac{1}{100}$$

$$\frac{(p_v + p_\beta) r_o}{\hbar} \approx \frac{1}{50}$$

Hence, we can ignore all the higher order terms and Eqn. (59) can be written as

$$\varphi_\beta^* \varphi_v = \frac{1}{V} \quad (60)$$

Substituting Eqn. (60) in Eqn. (57),

$$H_{if} = G \int \left(\varphi_n^* \frac{1}{V} M \varphi_i \right) dV$$

$$H_{if} = \int \varphi_n^* \frac{G}{V} M \varphi_i dV$$

$$H_{if} = \frac{G}{V} |M_{if}| \quad (61)$$

where

$$|M_{if}| = \int \varphi_n^* M \varphi_i dV \quad (62)$$

M_{if} is the overlap integral between the wave function of final and initial nuclei. $|M_{if}|^2 \approx 1$ is the maximum value.

7.4.3 γ -Decay

γ -rays are electromagnetic radiations with electric and magnetic component perpendicular to each other as well as direction of propagation of wave. γ -rays are produced during nuclear transition as X-rays are produced by atomic transitions. One of the following processes is involved for the nuclear transition, that is, γ -ray emission, internal pair creation, and internal conversion. The energies of transition can be given by the difference between nuclear levels.

γ -rays are produced by electrons in X-ray tubes, synchrotrons, accelerators, and betatrons. The energy spectrum produced is continuous in nature. During nuclear transitions, γ -radiation may be emitted as a prompt radiation along with the formation of α - or β -particle. Geiger–Müller counters (GM counters), scintillation counters, and portioned counters are used for detection of λ -rays. γ -rays also blacken the photographic emulsion. γ -rays discolor the transparent solids. We will discuss the processes in nuclear transition as follows.

1. Multipole Radiations (γ -Emission)

The parent nucleus disintegrates to daughter nuclei by emitting α - or β -particles. Sometimes, the daughter nuclei is still in an excited state and it comes to ground state by emitting γ -radiation (or em radiation). Various factors determine emission of γ -radiations. The γ -rays can be categorized as follows:

- (i) Electric γ -rays, which are due to changes or reorientation of electric charges in the nucleus.
- (ii) Magnetic γ -rays, which are due to reorientation of magnetic poles or changes in current distribution of nuclei.

To obtain emission and absorption of light, the quantum analysis of light is done (by using quantum theory of light). The nucleus radius R is considered to be smaller than the wavelength of radiation, that is,

$$R < \lambda \quad (63a)$$

$$\frac{\lambda}{R} > 1$$

$$\frac{\tilde{\lambda}}{R} > 1 \quad \left[\tilde{\lambda} = \lambda / 2\pi \text{ order remains same} \right]$$

$$\frac{c}{2\pi f R} > 1$$

$$\frac{c}{\omega R} > 1$$

$$\frac{\hbar c}{\hbar \omega R} > 1 \Rightarrow \frac{\hbar c}{ER} > 1$$

$$E < \frac{\hbar c}{R} \Rightarrow E < 20 \text{ MeV} \quad (63b)$$

Hence, during γ -emission, the photons produced are less than energy 20 MeV. For further analysis, we will use Maxwell's equation for uniform isotropic lossless media (source-free region).

i.e., $\rho = 0$

Hence, the Maxwell equations can be written as

$$\nabla \times E = -\frac{\partial B}{\partial t} \quad (\text{faraday's law}) \quad (64a)$$

$$\nabla \times B = \mu_0 \epsilon_0 \frac{\partial E}{\partial t} \quad (\text{Ampere's law}) \quad (64b)$$

$$\nabla \cdot E = 0 \quad (\text{Gauss's law}) \quad (64c)$$

$$\nabla \cdot B = 0 \quad (\text{No monopoles}) \quad (64d)$$

The electric and magnetic field have sinusoidal dependence on position as well as time. The field equations can be written as

$$E(r, t) = E(r) e^{-i\omega t} + E^*(r) e^{i\omega t} \quad (65a)$$

$$B(r, t) = B(r) e^{-i\omega t} + B^*(r) e^{i\omega t} \quad (65b)$$

Equations 64(a)–(b) can be solved using Eqs (65a) and (65b).
[if we consider no reflection, hence $E^* e^{i\omega t} = 0$]

$$\nabla \times B = -i\omega \mu_0 \epsilon_0 E \quad (66)$$

and

$$\nabla \times E = i\omega B \quad (67)$$

Take curl on Eqn. (67),

$$\begin{aligned}\nabla \times \nabla \times E &= iw(\nabla \times B) \\ \nabla \times \nabla \times E &= iw[-iw\mu_0\epsilon_0 E] \\ \nabla \times \nabla \times E &= w^2\mu_0\epsilon_0 E \\ [\nabla \times \nabla \times -k^2]E &= 0\end{aligned}\quad (68)$$

where $k^2 = w^2\mu_0\epsilon_0$ (69)

Similarly, taking curl on both sides of Eqn. (66),

$$[\nabla \times \nabla \times -k^2]B = 0 \quad (70)$$

$[\nabla \times \nabla - k^2]$ is operator whose value is given by the spherical harmonics and Bessel function. We can rewrite Eqn. (66) as

$$E = \frac{\nabla \times B}{-iw\mu_0\epsilon_0}$$

E is changed to E_c and B to B_c because these fields are electric multipole fields and B does not have any radial component.

$$E_c = \frac{\nabla \times B_c}{-iw\mu_0\epsilon_0} \quad (71a)$$

$$E_c = \frac{-1}{iw\mu_0\epsilon_0} \nabla \times [A^e L j_L(kr) Y_{LM}(\theta, \phi)] \quad (71b)$$

where $B_c = \underset{\text{constant}}{A^c} \underset{\text{angular momentum}}{L} \underset{\text{Bessel function}}{j_L(kr)} \underset{\text{spherical harmonic}}{Y_{LM}(\theta, \phi)}$ (71c)

For magnetic multipole fields, no radial component of E exists and we can write Eqn. (67) as

$$\begin{aligned}B_m &= \frac{\nabla \times E_m}{iw} \\ B_m &= \frac{\nabla \times [A^m L j_L(kr) Y_{LM}(\theta, \phi)]}{iw}\end{aligned}\quad (72a)$$

where $E_m = \underset{\text{constant}}{A^m} \underset{\text{angular momentum}}{L} \underset{\text{Bessel function}}{j_L(kr)} \underset{\text{spherical harmonic}}{Y_{LM}(\theta, \phi)}$ (72b)

Normalization condition is applied to find out the constants.

The magnetic field energy density is given by $\frac{1}{2\mu_0} \int |B|^2 dV$ and electric field energy density is given by $\frac{1}{2} \epsilon_0 \int |E|^2 dV$.

$$\frac{1}{\mu_0} \int |B|^2 dV = \frac{\hbar\omega}{2} = \frac{\hbar ck}{2} \quad (72c)$$

[electromagnetic radiation contains half energy due to electric field and half due to magnetic field]

$$\int |B|^2 dV = \frac{\mu_0 \hbar ck}{2} \quad (73)$$

Using Eqn. (71c) in Eqn. (73),

$$\int |B|^2 dV = |A^e|^2 \int_0^{r_0} |j_L(kr)|^2 r^2 dr \int (LY_{LM})^* (LY_{LM}) \underbrace{2\pi \sin\theta d\theta}_{d\Omega} \quad (74)$$

$d\Omega = 2\pi \sin\theta d\theta =$ solid angle, $r_0 \rightarrow$ radius of sphere

$$\int_0^{r_0} |j_L(kr)|^2 r^2 dr = \frac{1}{k^2} \int_0^{r_0} \cos^2 \left[kr - \frac{r(l+1)}{2} \right] dr \quad (75a)$$

[because Bessel function $|j_L(kr)| = \frac{\cos\left(kr - \frac{r(l+1)}{2}\right)}{kr}$]

Equation (75a) is given by

$$\int_0^{r_0} |j_L(kr)|^2 r^2 dr = \frac{r_0}{2k^2} \quad (75b)$$

L is angular momentum and is regarded as Hamiltonian. Hence,

$$\text{Volume} = dV = r^2 \sin\theta d\theta dr d\phi \quad (75c)$$

Hence, the integral yields following results:

$$\int Y_{LM}^* L^2 Y_{LM} d\Omega = L(L+1)\hbar^2 \quad (75d)$$

Substituting Eqs (75b) and (75d) in Eqn. (74),

$$\begin{aligned} |A^e|^2 \frac{r_0}{2k^2} L(L+1)\hbar^2 &= \frac{\mu_0 \hbar ck}{2} \\ |A^e|^2 &= \frac{ck^3 \mu_0}{r_0 L(L+1)\hbar} \end{aligned} \quad (76)$$

Similar to electric multipole field, the magnetic multipole radiation constant is given by

$$|A^m|^2 = \frac{ck^3}{\epsilon_0 r_0 L(L+1)\hbar} \quad (77)$$

Using Eqs (76) and (77) in Eqn. (71b) and (72a),

$$E_c(LM) = i \left[\frac{ck}{\epsilon_0 \hbar r_0 L(L+1)} \right]^{\frac{1}{2}} \nabla \times L j_L(kr) Y_{LM}(\theta, \phi) \quad (78)$$

and

$$B_c(LM) = -i \left[\frac{ck\mu_0}{\hbar r_0 L(L+1)} \right]^{\frac{1}{2}} \nabla \times L j_L(kr) Y_{LM}(\theta, \phi) \quad (79)$$

Similarly, E_m and B_c can be obtained as follows:

$$E_m(LM) = \frac{-1}{iw\mu_0\epsilon_0} \nabla \times [A^m L j_L(kr) Y_{LM}(\theta, \phi)] \quad [\text{from Eqn. (71b)}]$$

The only difference lies in constant, that is, A^m

$$E_m(LM) = k \left[\frac{ck}{\epsilon_0 \hbar r_0 L(L+1)} \right]^{1/2} \nabla \times L j_L(kr) Y_{LM}(\theta, \phi) \quad (80)$$

B_m can be written as

$$B_m(LM) = k \left[\frac{ck\mu_0}{\hbar r_0 L(L+1)} \right] \nabla \times L j_L(kr) Y_{LM}(\theta, \phi) \quad (81)$$

The parity for these fields can be written as

$$\begin{aligned} E_c &\rightarrow (-1)^{L+1} \\ B_c &\rightarrow (-1)^L \\ E_m &\rightarrow (-1)^L \\ B_m &\rightarrow (-1)^{L+1} \end{aligned} \quad \left[\begin{array}{l} \text{for } L = 0, \text{ all} \\ \text{multipole fields vanish} \end{array} \right]$$

Complete set of equations is formed by the multipole expansions. The fields can be expanded in terms of multipoles. The expansion of electric and magnetic field is given by

$$B(r) = \sum_{L=1}^{\infty} \sum_{m=-1}^L [C_c B_c + C_m B_m] \quad (82a)$$

and

$$E(r) = \sum_{L=1}^{\infty} \sum_{m=-1}^L [C_c E_c + C_m E_m] \quad (82b)$$

where C_e and C_m are amplitudes of electric and magnetic 2^L poles, respectively. The amplitudes are usually dependent on boundary conditions and strength of source.

2 Internal Pair Creation

Excited nucleus may produce electron–positron pair if energy of transition is more than 1.022 MeV rather than ejection of K-shell electron. The pair production takes place in Coulomb's field of nucleus. Moreover, momentum is conserved for the generated pair and nucleus.

The process of pair production is independent of atomic number Z . The probability of pair production is greatest at the distance from nucleus of order of $(Z/137)^2$ times radius of K-shell. Visually, it is of importance for low atomic number nucleus.

3 Internal Conversion

Atom exists in the excited state; similarly, nucleus exhibits quantized excited energy states. When the nucleus is excited, it may jump back to lower energy state. This transition of nucleus from excited state to ground state is accompanied by γ -ray emission. In some of the cases, the nucleus may return to ground state by giving its energy to orbital electron revolving around the nucleus (similar to photoelectric effect). Some excited states may remain in that excited state for several hours. These excited states are unstable intermediate states and are known as metastable states. We call a long-lived nucleus to be an "isomer." Isomers differ only in energy content. For example, ${}_{38}\text{Sr}^{87*}$ have a half-life of 2.8 h compared with ground state of ${}_{38}\text{Sr}^{87}$.

The γ -ray is internally converted to an electron and this process is known as internal conversion. While the excited nucleus returns from excited to ground state, it may follow many steps and γ -ray photon is released. Only those nuclear transitions are allowed, which follow conservation of energy and momentum. These rules are known as selection rules. The kinetic energy for the conversion electron is

$$E = (E_i - E_f) - E_B \quad (83)$$

where $E_i \rightarrow$ Energy of initial level

$E_f \rightarrow$ Energy of final level

$E_B \rightarrow$ Binding energy

In 1932, Taylor and Mott gave the total transition probability from nuclear state 1 to nuclear state 2 as follows:

$$P = P_e + P_\gamma \quad (84)$$

where $P_e \rightarrow$ partial decay constant for electron emission

$P_\gamma \rightarrow$ partial decay constant for gamma emission

$$\alpha = \frac{P_e}{P_\gamma} \quad (85)$$

α is the conversion coefficient and is given by the ratio of two partial decay constants. There is other explanation for α , that is,

$$\alpha = \frac{n_e}{n_\gamma} = \frac{\text{number of conversion electrons emitted for time } t}{\text{number of } \gamma\text{-rays emitted for time } t} \quad (86)$$

For each γ -ray energy with definite value, there are many conversion lines that are due to ejection of electrons from different atomic shells. Hence, we can write:

$$\alpha = \frac{n_K + n_L + n_M + \dots}{n_\gamma} = \alpha_K + \alpha_L + \alpha_M + \dots \quad (87)$$

where α_K , α_L , α_M , etc., are partial conversion coefficients. These constants do not give information of nuclear structure but can be used to determine parity change of nuclear transitions.

Otto Hahn was born in 1879 to a rich entrepreneur Heinrich Hahn in Frankfurt, Germany. His father wanted him to pursue his career in architecture but he wanted to study chemistry and mineralogy. He received his doctorate from the University of Marburg in 1901 in organic chemistry. He pioneered the fields of radiochemistry as well as radioactivity and is known as “the father of nuclear chemistry.” Hahn was an influential citizen of the Federal Republic of Germany who was against the use of nuclear weapons after World War II and Jewish persecution by the Nazis. Hahn joined University College of London in 1904 (where he discovered radiothorium) and continued his research in nuclear chemistry at McGill University in Montreal (where he discovered radioactinium, a radioactive isotope of thorium).

He joined as a lecturer in the University of Berlin, Germany, in 1907. The most astonishing discovery of Hahn and Fritz Strassmann, a fellow chemist, was the barium production when uranium atoms were bombarded with neutrons. This was a legendary discovery, which helped indirectly to develop atomic bomb. Hahn was awarded the Nobel Prize in 1944. In 1946, Otto Hahn joined the Kaiser Wilhelm Society and was the last president of the institution. Along with that, he was the founding president of the Max Planck Society (MPG), from 1948 to 1960. Hahn died on July 28, 1968, at the age of 89 years.



OTTO HAHN WITH HIS STUDENT

7.5 Radiation Detectors

We have studied α , β , γ , and other types of radiations. Now we should know how we can detect them for the study of nuclear phenomenon, radioactivity, and radiation research tools. The detectors can detect the particles and their nature. All the detectors are based on the principle of ionization. The uncharged particles or radiations such as X-rays and γ -rays, etc., are also detected by some detectors as these radiations can impart energy to ionized matter. For the working of detectors, the collection and separation of ion pairs is necessary otherwise they will recombine. In solids, the ionization is produced; where as in the case of gas and photographic emulsions, the tracks of particles are visible. Ionization chamber, Geiger-Muller (GM) counter, and proportional counter fall under the category of gas detectors. Scintillation counters are based on fluorescence. Bubble chamber, spark chamber, cloud chamber, and nuclear emulsions are also known as “track chambers.” Crystals are used in semiconductor detectors. Optical energy can be measured using Cerenkov detectors. We will discuss these detectors in the following sections.

7.5.1 Ionization Chamber

1. Principle

Ionization chamber is based on the principle that charged particles suffer from elastic collisions when they pass through gas. When these ions drift in an electric field, the potential induced on electrode can be measured. Ionization varies according to nature and velocity of particle.

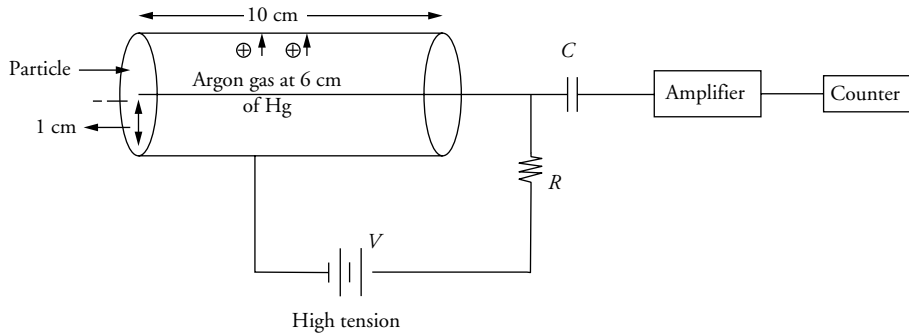


Figure 7.4 Ionization counter.

2. Constructions

A cylindrical tube is filled with argon gas and two electrodes as shown in Figure 7.4. The cylinder is maintained at negative potential w.r.t. positive central wire. The ends have mica windows. When a particle enters through the mica window, it ionizes the gas and separates the ions; some ions recombine on account of small potential difference. At load R , output voltage is obtained. The output voltage depends on the number of ion pairs that are formed per unit length of tube. In addition to specific ionization (number of ion pairs/length), the output voltage depends on tube radius, that is, separation between the electrodes.

That is,

$$\text{Potential}(V) = \frac{\text{charge of } n \text{ pairs of ions}}{\text{chamber capacitance}} \quad (88)$$

The saturation condition is given by

$$I_{\text{sat}} = \frac{dV}{dt} = C \frac{dV}{dt}, \quad [\text{Where } C \text{ is capacitance}] \quad (89)$$

3. Working

The output of ionization chamber is in the form of more or less continuous stream, rather than pulsed output. As the cylinder is at negative potential, the positive ions move toward cylinder and negative ions move toward the central electrode. Under no electric field, the ions may recombine, but when electric field is applied the electrons drift with drift velocity of 10^6 m/s. The ions move slowly as they have higher mass compared with electrons. As the voltage is increased, the ionization current also increases and then becomes almost constant as shown in Figure 7.5.

When applied voltage $< V_1$, the probability of ion recombination is more. Above V_1 , the applied voltage is strong enough to prevent recombination. The ions are collected at their respective electrodes. The constant region of current in Figure 7.5 is called as saturation current (Eqn. 89).

The ionization current can be measured by the charge that is collected at capacitor using Eqn. (89). α -particle produces strong pulses compared with β - or γ -rays, because the ionizing power of α -particles is highest. For ionization counter, almost 35 eV of energy is required to produce ion pair. "RC" is the response time of counter. There is one major drawback of ionization counter, that is, the

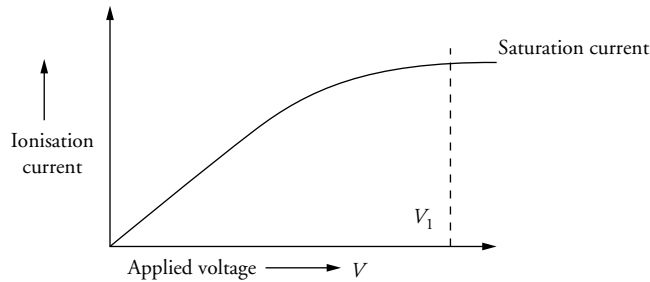


Figure 7.5 Applied voltage and ionization current.

chamber has to wait for milliseconds after the detection of one particle so that it can be ready for other particle. The operating voltage for this counter is 10–200 V.

7.5.2 Proportional Counter

1. Principle

Proportional counter is same as that of ionization counter except the operational voltage. It is based on the principle that when sufficiently large potential difference is applied between the central wire and cylinder, primary ions are produced. These primary ions collide with other atoms of gas and produce secondary ions. The secondary ionization depends on the geometry of apparatus and applied voltage V (generally operating voltage is 200–800V).

2. Construction

About 20 cm long hollow cylinder with 2 cm diameter is used with a fine tungsten wire of 0.1 mm diameter as shown in fig. 7.6. The wire is treated as anode as it is at positive potential. The metallic cylinder serves as a cathode. The anode is connected to load. The cylinder is filled with argon as its atoms prefer to be in metastable states for longer durations. When the excited states return to ground state, the energy is released producing discharges. Usually combination of argon (90 percent) and methane (10 percent) is used in the counter. Methane is used in order to quicken the de-excitation process through collisions. Thin windows of aluminum or mica are used.

3. Working

The gas multiplication factor depends on anode diameter, applied voltage, cathode radius, and nature of filling gas. The anode and cathode are arranged in co-axial arrangement. r_1 is the radius of anode and r_2 is radius of cathode. Hence, the electric field is given by

$$E = \frac{V}{x \log_e \left(\frac{r_2}{r_1} \right)} \quad (90)$$

where x is the distance at which field strength is to be measured. When $x = r_1$, maximum electric field is produced, which causes avalanches. When incident radiation passes through the window, the gas is ionized and the ions get separated due to applied field. The electrons move toward central anode wire and ions drift slowly toward the body of cylinder. The motion of these heavy ions decides the pulse voltage developed at the central wire.

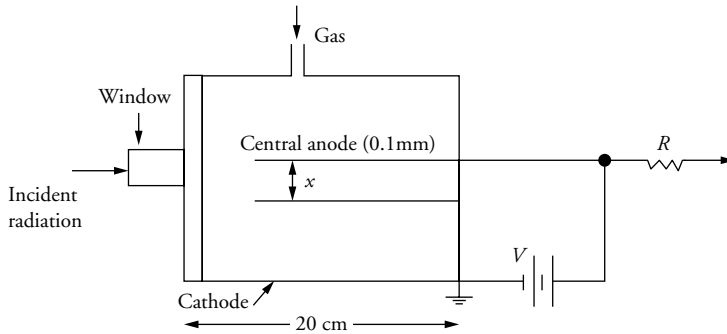


Figure 7.6 Proportional counter.

Initially the pulse is very high as the ions are in strong electric field. Then later on, the positive ions drift in weak field and hence the pulse is also affected. For the proportional counter, the pulse shape is given as in Figure 7.7.

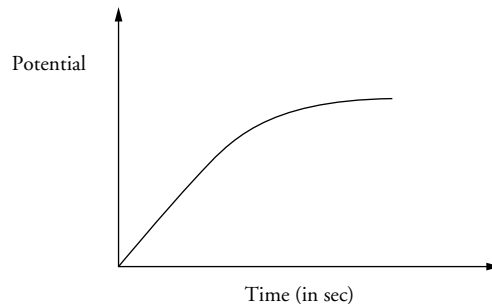


Figure 7.7 Voltage versus time for proportional counter.

The rise time of pulse in proportional counter is shorter compared with ionization chamber which makes it better. Neutrons can also be detected using proportional counter despite the fact that neutral neutrons do not ionize the gas. When an atomic nucleus absorbs the neutron, some charged particle or gamma rays are emitted which can be detected. β -rays, fast protons, and mesons can also be detected using proportional counter.

7.5.3 Geiger-Muller (GM) Counter

For this counter, the collected charge is no longer proportional to the ionization. The gas has complete avalanche or breakdown of gas. The energy of incident particles does not contribute to the electric pulse generated inside the counter.

1. Principle

When a charge particle passes through a gas, the gas ionizes. As the electrons are under high potential, they get accelerated and enhance further ionization. During this process, large number of electrons are produced.

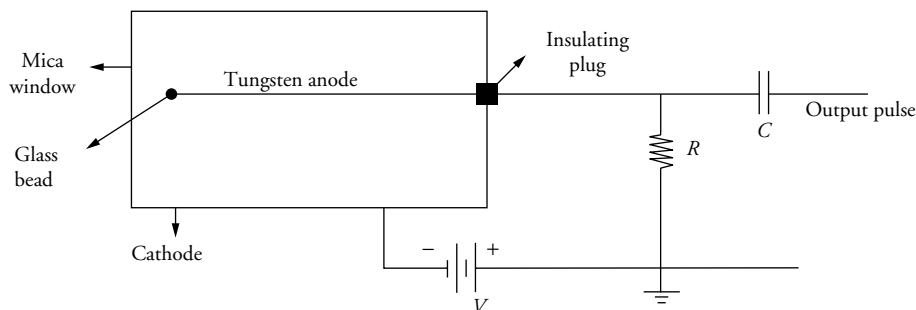


Figure 7.8 GM counter.

2. Construction:

The cylindrical metallic envelope is cathode and tungsten wire is anode (Figure 7.8). Anode at the end is connected to a glass head. The main function of glass bead is to avoid the corona discharge. Usually, the corona discharge is produced at sharp points of conductors. α - and β -particles enter through the thin window of mica. Argon, neon, or helium may be used as the filler gas in the tube. The GM counter operates at high voltage of 900–1300V. GM counter cannot distinguish the source of ions.

3. Working

When a single charge particle enters a GM tube, a bunch of electrons are produced through ionization. The electrons drift toward central anode. During this process, these primary electrons produce further ionization and is known as secondary ionization.

The density of electrons is very high at that stage and current pulse is produced across R . These current pulses are counted by the counting device. Hence, for each pulse recorded, there is one incident particle. After few microseconds, the gas discharge stops due to accumulation of positive charges. The electric field gets reduced to such a level that no more ionization can happen. The pulse height is independent of energy and nature of particle because even a single incident particle can start an avalanche.

4. Quenching:

The positive ions produced have larger masses and hence small accelerations. Virtually, they are stationary. These positive ions tend to move toward the cylindrical cathode. Some positive ions may release electrons upon striking the cathode surface, which may give rise to another avalanche. This avalanche should be stopped because one avalanche will be counted twice otherwise. The positive ions around central wire should be eliminated and the process of elimination of positive charges is known as quenching. The quenching method used is external quenching method and self-quenching. In external quenching method, a very large series resistance is used so that during large current, voltage drop can occur at R . This technique takes large time interval to detect another particle. Hence, the counter is insensitive for some duration, which is called dead time of GM counter (Figure 7.9). Sometimes, an electronic circuit is employed to remove the current so that dead time can be reduced. Recovery time is the time after which the original pulse is restored.

Internal quenching/self-quenching methods are most commonly used methods these days. In this method, some polyatomic gas such as ethyl alcohol is used upto 10 percent in concentration. Ethyl alcohol prevents the release of electrons when positive ion strikes the cathode surface. Hence, the

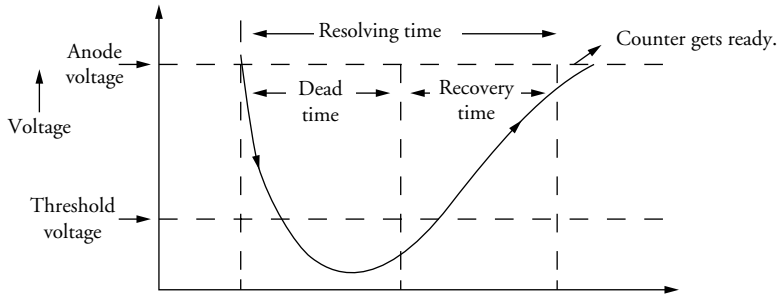


Figure 7.9 Dead time and recovery time of GM counter.

avalanche due to positive ion is stopped and the counter reads only one avalanche. Ethyl alcohol is used at 1 cm of Hg. Halogens such as Br_2 or Cl_2 can also be used as quenching agents at 0.01 cm of Hg. Halogen counters have infinite lifetime as the halogen ions recombine themselves.

When the voltage is increased above 10^3 V (Geiger region), the quenching action is almost incomplete. The count rate is also invalid because the avalanches are not counted correctly. The counter follows continuous discharge, if the voltage is raised further. This may cause damage to the tube. These GM counters have good counting capability with α and β particles, but poor with γ -radiations. GM counters have high pulse, which is independent of nature and energy of incident ions. But uncharged particles cannot be detected using GM counter and amplifier or counter is required.

7.5.5 Ionization Current and Voltage Characteristics (Collective Diagram)

When a radiation enters the chamber produces pulse signal, which depends on voltage between anode and cathode. Different particles (α or β , etc.) have different pulse heights. The variation of pulse height with applied voltage for particle is divided into six different regions as below Figure 7.10

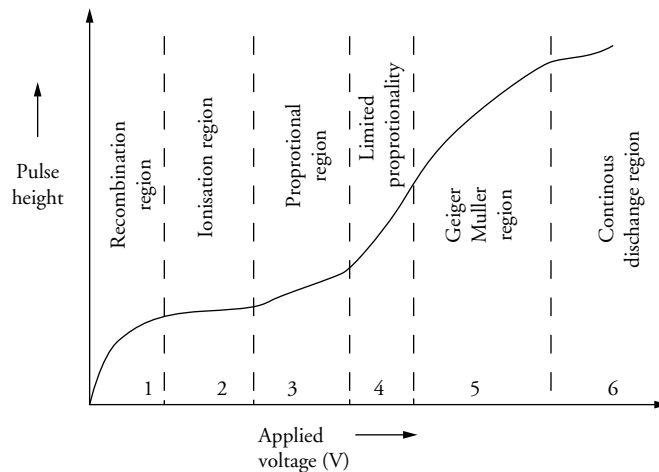


Figure 7.10 The diagram showing the operating regions for all the counters.

Region 1: Recombination Region

In this region, the voltage is not strong enough to keep the ions separated and hence ions and electrons recombine.

Region 2: Ionization Region

As the voltage increases, the recombination of ions is decreased and all the ions are collected at respective electrodes. The pulse height is independent of the applied voltage in this region. Hence, it is known as saturation region. But pulse height depends on the energy of incident particle. Particles with different atomic numbers can be detected in these chambers.

Region 3: Proportional Region

This is the region of gas multiplication. In this region, the voltage is high to accelerate primary electrons, so that they can produce secondary electrons. Hence, a cumulative process sets in producing avalanche of electrons (known as Townsend avalanche) and the charge collected at anode is large. The gas multiplication factor (number of ion pairs formed by collision between electrons while traveling toward anode) depends on particle energy. The pulse height depends on the ionization caused by initial particle.

Region 4: Limited Proportionality

When the applied voltage increases, the pulse height increases but is independent of ionization produced by initial incident particle. This region is not of much use for any applications.

Region 5: Geiger–Müller Region

In this region, very large pulse height is obtained, which is independent of energy and initial ionization of particle. It is a very sensitive region. The counter operated in this region is called Geiger–Müller region and even a single ion pair produces a very large pulse.

Region 6: Continuous Region

In this region, multiple pulses are obtained, and the counter gives continuous discharge.

7.5.6 Scintillation Counter

When α -particles strike some materials such as zinc sulfide, scintillations/light flashes are produced. A low-power microscope is used to measure the individual flashes. Marshall, Coltman, and Kollman introduced photomultiplier tube to count the scintillation produced.

1. Principle

Whenever radiations fall on a fluorescent material, light flashes or scintillations are produced. These scintillations can be detected with photomultiplier tube.

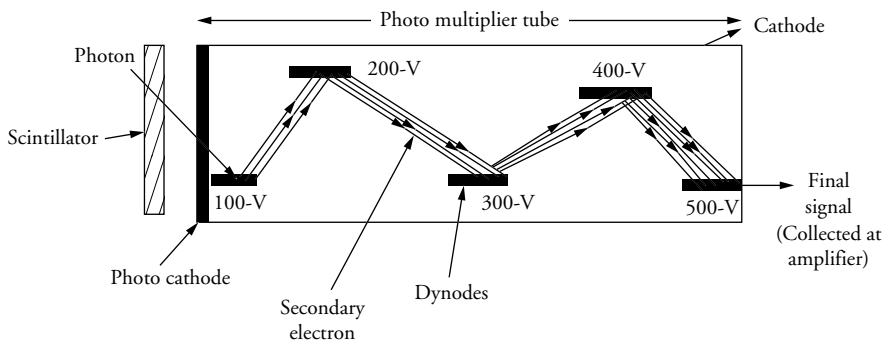


Figure 7.11 Scintillation counter.

2. Construction

The scintillation counter used a scintillating material/phosphor in either solid or liquid form. A photo multiplier tube is used, which detects the light flashes (fig. 7.11). Amplifier circuit is used, which count the electrical impulses. When particle passes through the scintillator atom, the atoms get excited. When the excited scintillator atoms return to ground state, photons are emitted. The intensity of light depends on the energy lost by incident charged particle. Cesium iodide is the common used phosphor for α -particles and protons. To produce maximum effects, thallium is added to the phosphor material. Sodium iodide with thallium is also used as a scintillator. The photomultiplier tube amplifies the output of photoelectrons when they come from a cathode. Then with the help of dynodes the signal is amplified by successive emission of secondary electrons. The process is rapid and dependent on the sensitivity of photo cathode. The height of output pulse is dependent on energy lost in the scintillation by incident particle. The potential at first dynode is small and hence the electrons emitted from first dynode are now very energetic. As the electron reaches second dynode, the electrons get more and more accelerated. This process continues and then the last dynode has highest output, which can be collected. The photomultiplier tube has high vacuum. The electrons have less than 10^{-6} sec between them and can be dedected by scintillation counter.

3. Working

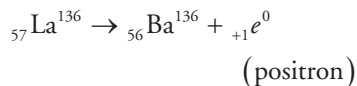
When the ionizing radiation enters the scintillator, short flashes of light are produced. These light photons are absorbed by photocathode and photoelectrons are emitted. Inter dynode voltages accelerate these photoelectrons. The electron multiplication takes place at every dynode, and with increasing voltage the electrons get accelerated. The output at the last dynode is collected by the amplifier. Then, the amplified output is provided to discriminator, which reduces the noise levels. The resolving power of counter is very high and dead time is very small.

SUMMARY

This chapter deals with the phenomena of radioactivity and emission of α -, β -, and γ -radiations from the radioactive nuclei. Soddy and Fajan stated that during radioactive transformation, either α - or β -rays are emitted. Furthermore, it was explained that nuclei with $Z > 82$ disintegrate α -particles in order to stabilize it. Kinetic energy and disintegration energy have a difference that could be explained on the basis of conservation of energy and momentum. The Geiger–Nuttal law demonstrated that the most energetic α -particles are emitted by shortest lived nuclides and vice versa. α -decay was also explained by Gamow's theory and it considered α -particle under the nuclear potential barrier (height V_0). It was explained that β -decay could take place through three processes, that is, negatron emission, positron emission, and electron capture. In negatron and positron emission, the mass of parent nuclei must be greater than the mass of daughter nuclei. Electron capture is competitive to positron emission. Coulomb barrier tends to prevent positron emission. Fermi theory of β -decay assumed β -decay analogous to emission of electromagnetic radiations by an atom. γ -decay was explained using multipole expansions. γ -radiation may be emitted promptly along with the α - and β -radiations. Radioactive detectors are used to detect the radiations. For the working of detectors, collection and separation of ion pairs is necessary to avoid the recombination. Gas detectors such as ionization chamber, Geiger–Müller counter, and proportional counter. Scintillation counters are based on the phenomena of florescence.

SOLVED PROBLEMS

Q.1: Obtain the energy available for β -decay in the following process:



(Given mass of barium = 135.904350 a.m.u.

mass of lanthanum = 135.907380 a.m.u.)

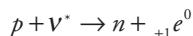
Ans: The mass defect contributes to the kinetic energy of positron particle. Hence,

$$\Delta E = \Delta m \cdot c^2$$

$$\Delta E = [135.907380 - 135.904350] \times 931 \text{ MeV}$$

$$\Delta E \approx 2.865 \text{ MeV}$$

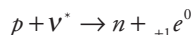
Q.2: Obtain the minimum kinetic energy required to initiate the reaction



Ans: Antineutrino, neutron, and positron have kinetic energy T_{ν^*} , T_n , and T_{β^+} , respectively.

For the antineutrino to initiate the reaction with minimum energy, the kinetic energy for product neutron and positron will be zero.

Hence, from the reaction



We can write energy equation as

$$T_{\nu^*} + m_p c^2 = (T_n + m_n c^2) + (T_{\beta} + m_{\beta} c^2)$$

Here

$$T_n = T_{\beta} = 0$$

$$T_{\nu^*} = (m_n + m_{\beta})c^2 - m_p c^2$$

$$m_p = 1.007825$$

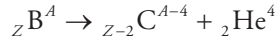
$$m_n = 1.008665 \quad m_{\beta} c^2 = 0.51$$

$$T_{\nu^*} = [1.008665 \times 931 + 0.51 - 1.007825 \times 931] \text{ MeV}$$

$$T_{\nu^*} = [939.067 + 0.51 - 938.285] \text{ MeV}$$

$$T_{\nu^*} = 1.292 \text{ MeV}$$

Q.3: Obtain the value of KE in terms of Q -value of reaction.



Ans: ${}_Z\text{B}^A$ is parent nucleus, whereas ${}_{Z-2}\text{C}^{A-4}$ and ${}_2\text{He}^4$ are daughter nuclei.

If ${}_Z\text{B}^A$ is at rest, then according to momentum conservation principle,
momentum of ${}_{Z-2}\text{C}^{A-4}$ = momentum of ${}_2\text{He}^4$

The kinetic energy is given by $T = \frac{p^2}{2m}$

Hence,
$$T_C = \frac{p_C^2}{2m_C} \quad \text{(a)}$$

and
$$T_{\text{He}} = \frac{p_{\text{He}}^2}{2m_{\text{He}}} \quad \text{(b)}$$

Dividing Eqs (a) and (b)

$$\frac{T_C}{T_{\text{He}}} = \frac{m_{\text{He}}}{m_C} \quad \left[\text{as } p_C = p_{\text{He}} \right]$$

$$\frac{T_C}{T_{\text{He}}} = \frac{4}{A-4} \quad \text{(c)}$$

The Q value of reaction is given by

$$Q = T_C + T_{\text{He}} = \frac{4}{A-4} T_{\text{He}} + T_{\text{He}}$$

$$Q = \left(\frac{AT_{\text{He}}}{A-4} \right) \quad \text{(d)}$$

Q.4: Obtain the energy for and α -particle, which is liberated during the following reaction:



(Given $m_\alpha = 4.00260$ a.m.u .
 $m_{\text{Po}} = 209.98287$ a.m.u .
 $m_{\text{Pb}} = 205.97447$ a.m.u .)

Ans: The energy is given by

$$E = (m_{\text{Po}} - m_{\text{Pb}} - m_{\text{He}})c^2$$

$$E = [209.98287 - 205.97447 - 4.00260] \text{a.m.u.} \times 931 \frac{\text{MeV}}{\text{a.m.u.}}$$

$$E = 0.0058 \text{ a.m.u.} \times 931 \frac{\text{MeV}}{\text{a.m.u.}}$$

$$E = 5.39 \text{ MeV}$$

Q.5: The kinetic energy of α -particles during the decay of ${}_{84}\text{Po}^{210}$ to ${}_{82}\text{Pb}^{206}$ is measured to be 5.39 MeV. Obtain the “ Q ” value for this reaction.

Ans:

$$\text{KE} \approx \left[\frac{A-4}{A} \right] Q$$

$$Q = \left(\frac{A}{A-4} \right) \text{KE}$$

$$Q = \frac{210}{206} \times 5.39 \text{ MeV}$$

$$Q \approx 5.49 \text{ MeV}$$

Q.6: Obtain the energy for α -particle in the following reaction:



(Given $m_{\text{He}} = 4.00260$ a.m.u.
 $m_{\text{Pu}} = 236.046071$ a.m.u.
 $m_{\text{U}} = 232.046071$ a.m.u.)

Ans: The energy is given by

$$E = (m_{\text{Pu}} - m_{\text{U}} - m_{\text{He}})c^2$$

$$E = [236.046071 - 232.0371 - 4.00260] \text{ a.m.u.} \times \frac{931 \text{ MeV}}{\text{a.m.u.}}$$

$$E = 0.00637 \text{ a.m.u.} \times 931 \frac{\text{MeV}}{\text{a.m.u.}}$$

$$E = 5.93 \text{ MeV}$$

Hence, the α -particles have energy of 5.93 MeV after disintegration of plutonium to uranium.

Q.7: Obtain the Q -value of reaction when plutonium ${}_{94}\text{Pu}^{236}$ decays to ${}_{92}\text{U}^{232}$ with the emission of α -particle with energy 5.93 MeV.

Ans: The Q -value equation is

$$\text{KE} = \left[\frac{A-4}{A} \right] \cdot Q$$

$$Q = \left(\frac{A}{A-4} \right) \cdot \text{KE}$$

Here, $A = 236$ and $\text{KE} = 5.93 \text{ MeV}$

$$Q = \frac{236}{232} \times 5.93 \text{ MeV}$$

$$Q = 6.032 \text{ MeV}$$

Q.8: In an ionization chamber, 6×10^6 ion pairs/12 MeV of energy are produced. Obtain the pulse height if capacitance is 30 pF.

Ans:

$$\text{Total charge} = ne$$

Pulse height corresponds to voltage, which is developed after charge/ion pairs are produced.

Hence,

$$\text{Voltage } V = \frac{q}{C} = \frac{ne}{C}$$

$$C = 30 \times 10^{-12} \text{ F}$$

$$V = \frac{6 \times 10^6 \times 1.6 \times 10^{-19}}{30 \times 10^{-12}} = \frac{0.32 \times 10^{-13}}{10^{-12}}$$

$$V = 0.032 \text{ V}$$

Q.9: What would be the kinetic energy of α -particle if 35 eV of energy is spent in producing one pair inside the ionization chamber, provided 1.5×10^5 ion pairs are produced?

Ans:

$$\text{Kinetic energy of particle} = \frac{\text{energy spent}}{\text{ion pair}} \times \text{ion pairs produced}$$

$$\text{KE} = 35 \text{ eV} \times 1.5 \times 10^5$$

$$\text{KE} = 5.25 \text{ MeV}$$

Q.10: What would be the maximum voltage required for a proportional counter if its cylinder size is 1.5 cm and wire size is 0.005 cm?

[Given Maximum radial field = 10^5 V/cm]

Ans:

$$E = \frac{V}{x \log_e \left(\frac{r_2}{r_1} \right)}$$

$r_1 \rightarrow$ radius of anode (wire radius)

$r_2 \rightarrow$ radius of cathode (cylinder radius)

$$\text{Usually } x = r_1$$

$$V = E \times r_1 \log_e \left(\frac{r_2}{r_1} \right)$$

$$V = 10^5 \times (0.005) \times \log_e \left[\frac{1.5}{0.005} \right]$$

$$V = 10^5 \times 0.005 \times 2.477$$

$$V = 10^5 \times 0.01238$$

$$V = 1238 \text{ V}$$

Q.11: Calculate the life-time for proportional counter if it works for 4 h/day at a rate of 2000 counts/min? Given the guaranteed life counts are 10^9 .

Ans: Let total life-time = t years

Hence, the total counts must be equal to the number of counts that are guaranteed.

$$t \times 4 \times 365 \times 60 \times 2000 = 10^9$$

$$t = 5.707 \text{ years}$$

Q.12: Obtain the average current for GM counter if it collects 10^8 electrons/discharge with a counting rate of 700 counts/min.

Ans:

$$\text{Counting rate} = 700 \text{ counts/min}$$

$$\text{Total electrons collected/min} = 700 \times 10^8 = 7 \times 10^{10} / \text{min}$$

$$\text{Change/min in the circuit} = 7 \times 10^{10} \times 1.6 \times 10^{-19} \text{ C/min}$$

$$\text{Average current} = \frac{7 \times 10^{10} \times 1.6 \times 10^{-19}}{60}$$

$$= 0.186 \times 10^{-9}$$

$$I = 1.86 \times 10^{-10} \text{ A}$$

OBJECTIVE QUESTIONS

1. The elements with atomic number greater than are radioactive.

(a) 50

(b) 90

(c) 82

(d) 70

2. X-rays are

(a) “-ve” charged radiations

(b) neutral radiations

(c) neutral radiations

(d) none of the above

3. Radioactivity takes place under

(a) force

(b) pressure

(c) temperature

(d) no force

4. α -rays get deflected toward

- (a) positive plate (b) negative plate
(c) undeflected (d) both positive and negative

5. β -rays are deflected toward

- (a) positive plate (b) negative plate
(c) undeflected (d) both positive and negative

6. Velocity of β -particles can be

- (a) $\approx c$ (b) $\approx c/2$
(c) $0.99c$ (d) $2c$

7. The ionization power of β -particles is

- (a) $\frac{1}{100}$ of α -particle (b) $\frac{1}{10}$ of α -particle
(c) same as α -particle (d) 10 times of α -particle

8. Which of the following can cause fluorescence?

- (a) α -rays (b) β -rays
(c) γ -rays (d) all of them

9. According to Soddy and Fajan

- (a) both α - and β -rays are emitted during radioactive decay
(b) only α -rays are emitted; no β -rays are emitted
(c) only β -rays are emitted; No α -rays are emitted
(d) either α - or β -particle is emitted

10. 1 curie is equal to

- (a) 3.7×10^8 disintegrations/sec (b) 3.7×10^{10} disintegrations/sec
(c) 3.7×10^{12} disintegrations/sec (d) 3.7×10^6 disintegrations/sec

11. 1 Rutherford is equal to

- (a) 10^6 disintegrations/sec (b) 10^8 disintegrations/sec
(c) 10^4 disintegrations/sec (d) 10^{10} disintegrations/sec

12. The relation of KE and disintegration energy (θ) for α -particle is given by

- (a) $KE = \frac{A}{A-4}Q$ (b) $KE = \frac{A}{A-2}Q$
(c) $KE = \frac{A-4}{A}Q$ (d) $KE = \frac{A-2}{A-4}Q$

13. Disintegration energy of nuclei is _____ than the energy of α -particle.
(a) more (b) less
(c) equal (d) none of the above
14. Energy and range are related to each other as
(a) $E = 0.318 R^{3/2}$ (b) $R = 0.5 E^{3/2}$
(c) $R = 0.318 E^{5/2}$ (d) $R = 0.318 E^{3/2}$
15. Disintegration constant λ and range R of α -particles is given as
(a) $\log \lambda = A + B \log R$ (b) $\log R = A + B \log \lambda$
(c) $\log R = B \log \lambda$ (d) $\lambda = A + BR^2$
16. According to Gamow's theory, there is _____ probability of tunneling.
(a) No (b) 100%
(c) finite (d) infinite
17. During β -decay
(a) atomic mass is unchanged
(b) atomic number changes by one unit
(c) the β -decay can happen through three processes
(d) all of the above
18. For electron emission to take place, the rest mass of parent nuclei should _____ than the rest mass of daughter nuclei.
(a) less (b) greater
(c) equal (d) none of the above
19. Coulomb barrier prevents emission of positron in case of
(a) positron emission (b) electron capture
(c) negatron emission (d) all of the above
20. Electron capture is accompanied by the emission of
(a) X-rays (b) γ -rays
(c) UV-rays (d) visible rays
21. For Fermi theory of β -decay, coupling constants are
(a) kept to very small (b) kept to be very large
(c) kept almost equal (d) zero
22. The value of "Fermi-Coupling constant" is
(a) $0.07 \times 10^{-4} \text{ MeV fm}^3$ (b) $0.9 \times 10^{-4} \text{ MeV fm}^3$
(c) $1.9 \times 10^{-5} \text{ MeV fm}^3$ (d) $0.2 \times 10^{-4} \text{ MeV fm}^3$

23. Which process is involved for the nuclear transitions?

- (a) γ -ray emission (b) internal pair creation
(c) internal conversion (d) all of the above

24. During γ -emission, the photons produced have energy less than

- (a) 100 MeV (b) 80 MeV
(c) 20 MeV (d) 50 MeV

25. The probability of pair production is highest at a distance from nucleus of order of

- (a) $\frac{Z}{137}$ times radius (b) $\frac{137}{Z}$ times radius
(c) $\left(\frac{Z}{137}\right)^2$ times radius (d) 10 times radius

26. The conversion coefficient α is given by

- (a) $\frac{P_\gamma}{P_e}$ (b) $\frac{P_\gamma}{P_e^2}$
(c) $P_\gamma \cdot P_e$ (d) $\frac{P_e}{P_\gamma}$

27. For ionization counters, _____ energy is required to produce ion pair.

- (a) 35 eV (b) 10 eV
(c) 25 eV (d) 20 eV

28. For proportional counter, the metallic cylinder serve as

- (a) anode (b) earth
(c) cathode (d) none of the above

29. The electric field for proportional counter is given by

- (a) $E = \frac{V}{x \log_e \left(\frac{r_1}{r_2} \right)}$ (b) $E = \frac{V}{x \log_e \left(\frac{r_2}{r_1} \right)}$
(c) $E = V \log_e \left(\frac{r_1}{r_2} \right)$ (d) $E = V \log_e \left(\frac{r_2}{r_1} \right)$

30. For proportional counter, following gases are used:

- (a) argon and methane (b) neon and methane
(c) methane and oxygen (d) krypton and methane

31. GM Counter operates at

- (a) 800–1000V (b) 600–1000V
(c) 900–1300V (d) 1300–1500V

32. For self-quenching/internal quenching,
(a) ethyl alcohol can be used (b) bromine can be used
(c) chlorine can be used (d) all of the above
33. In continuous region of voltage–pulse characteristics
(a) multiple pulses are obtained (b) no pulse is obtained
(c) two pulses are obtained (d) none of the above
34. Which is most common phosphor for α -particles and protons?
(a) cesium chloride (b) cesium fluoride
(c) cesium iodide (d) cesium bromide
35. With the help of dynodes, the signal is amplified (yes/no).

ANSWERS

- | | | | |
|--------|---------|---------|----------|
| 1. (c) | 10. (b) | 19. (b) | 28. (c) |
| 2. (c) | 11. (a) | 20. (a) | 29. (b) |
| 3. (d) | 12. (c) | 21. (a) | 30. (a) |
| 4. (b) | 13. (b) | 22. (b) | 31. (c) |
| 5. (a) | 14. (d) | 23. (d) | 32. (d) |
| 6. (c) | 15. (a) | 24. (c) | 33. (a) |
| 7. (a) | 16. (c) | 25. (c) | 34. (c) |
| 8. (d) | 17. (d) | 26. (d) | 35. Yes. |
| 9. (d) | 18. (b) | 27. (a) | |

Micro-Assessment Questions

1. What is radioactivity?
2. Which nuclei are considered as radioactive nuclides?
3. What are α -particles?
4. Give the description of radioactive particles.
5. How does penetration power vary for α -, β -, and γ particles?
6. Which radioactive particle exhibits highest ionizing power?
7. γ -rays are not deflected by electric or magnetic field. Explain.
8. Which radioactive particles are deflected toward positive plate?
9. What are β -particles?
10. When is the atomic number of a nuclide increased by one unit?
11. Give the units of radioactivity.
12. Which properties are conserved during α -decay?
13. What is disintegration energy?
14. Write down the relation between range and energy of particle.
15. Define the disintegration constant.
16. Write down the relation between disintegration constant and number of atoms in substance.
17. Give the relation between disintegration constant and range of particle.
18. What do you understand by electron capture?
19. Explain the phenomena of internal conversion.
20. Which condition is necessary for negatron emission?
21. What is positron emission?
22. What are radiation detectors?
23. Why is the detection of particles necessary?
24. What do you understand by scintillators?
25. Explain the dead time and recovery time for a Geiger–Müller counter.
26. Explain the term “avalanche.”

Critical Thinking Questions

1. Give the properties for α -radiations.
2. List the major characteristics for β - and γ -radiations.
3. State and explain the laws of radioactivity.
4. Define 1 curie and Rutherford.
5. Give the relation for the disintegration energy with the masses of nuclides.
6. Why α -emission occurs despite deuterium or tritium emission in certain nuclei?
7. Explain how does momentum conservation happens for α -decay?
8. The mass-energy is conserved during α -decay. Explain.
9. Explain the plot of disintegration constant versus range of α -particle.
10. What is Geiger–Nuttall law?
11. What do you understand by uranium series?
12. Write the differences between actinium and thorium series.
13. Write down the conditions for α -decay.

14. Are the β -particles different from the orbital electrons?
15. What is β -decay?
16. What do you understand by negatron emission?
17. Why neutrino emission is associated with negatron emission?
18. Is electron capture competitive to positron emission? Justify.
19. Explain the importance of Fermi coupling constant.
20. Describe the equations for expansion of electric and magnetic fields.
21. Write down the multipole expansions for γ -emission.
22. Explain internal pair creation. Does it depend on atomic number?
23. Describe the basic principle of working for radiation detectors.
24. Give the principle of ionization chamber.
25. How does proportional counter work?
26. What are the limitations of Geiger–Müller counter?

Graded Questions

1. Correlate the empirical facts for α -decay using Geiger–Nuttall law. Derive the relation between disintegration constant and energy E .
2. Discuss the Gamow's theory for α -decay. Also, obtain the expression for probability of emission of α -particle per second.
3. Derive the transmission coefficient for α -decay. Also, explain the probability of tunneling of α -particle.
4. Write down the three processes through which the β -decay may occur.
5. State and explain the Fermi theory of β -decay. What is the necessity of neutrino emission?
6. What do you understand by γ -decay? Explain the γ -emission process using the concept of multipole radiations.
7. Describe the principle and working of ionization chamber.
8. Write a note on principle, construction, and working of proportional counters.
9. What is a scintillation counter? Explain its principle and working. In addition, list down its advantages and disadvantages.
10. What is the principle of Geiger–Müller counter? How does it work? Which type of particles can be detected using it?
11. Describe the variation of pulse height with applied voltage. Depict the importance of various regions in the graph.

Remember and Understand

1. Radioactivity is disintegration of heavy nuclei into smaller nuclei in the absence of any external force. The elements with atomic number greater than 82 are radioactive in nature.
2. α -, β -, or γ -rays are emitted during the process of radioactivity.
3. When the α - or β -particles are emitted from radioactive nuclei, the atomic number of nuclei changes whereas γ -emission does not change the atomic number or atomic mass of nuclide.
4. During the process of α -decay, energy and momentum are conserved. Hence, the daughter nuclei recoils.

5. According to Geiger–Nuttall law, the least energetic particles are emitted by longest lived nuclides.
6. Negatron emission is emission of electrons to stabilize the nuclei.
7. For negatron emission, the rest mass of parent nuclei should be greater than the daughter nuclei. The antineutrino is emitted along with negatron to conserve the angular momentum.
8. When the positive electron/positron is emitted from the nuclei, it is known as positron emission. Neutrino is also emitted along with it to conserve angular momentum.
9. During electron capture, Coulomb barrier prohibits the positron emission.
10. Fermi theory assumes the β -decay analogous to the emission of electromagnetic radiations by an atom.
11. γ -radiations are produced by nuclear transitions like X-rays are produced by atomic transitions.
12. When the γ -ray is internally converted to an electron, this process is known as internal conversion.
13. For the working of detectors, the separation and collection of ion pairs is necessary, otherwise they will recombine.

Particle Physics

Keywords: Elementary particles, muons, pions, leptons, hadrons, baryons, neutrinos, anti-neutrinos, hyperons, mass determination techniques, intrinsic quantum number, hypercharge, strangeness, quarks, parity, charm quark, color quark, quark model

Learning Objectives

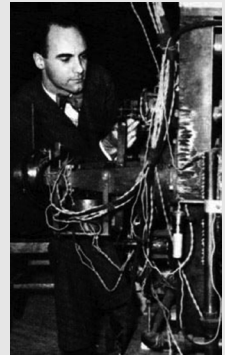
- ◆ To learn about elementary particles and their properties.
- ◆ To understand the classification of elementary particles.
- ◆ To understand the physical significance of symmetric and antisymmetric wave functions.
- ◆ Classification of bosons and fermions.
- ◆ To understand the existence of neutrinos and antineutrinos.
- ◆ To learn about baryons and their classification as nucleons and hyperons.
- ◆ To get insight about the classification of particles on the basis of interactions.
- ◆ To understand the classification of particles on the basis of stability.
- ◆ To understand the parity and its relation to angular momentum.
- ◆ To learn tau-theta puzzle.
- ◆ To learn about mass determination techniques for particles.
- ◆ To learn μ -mesic, kinematic method, and trajectory methods of mass determination.
- ◆ To learn about intrinsic quantum numbers.
- ◆ To understand lepton number (L), baryon number (B), isospin, hypercharge, and strangeness.
- ◆ To get insight of conservation principles that should hold good during the decay process.
- ◆ To understand the quarks and quark model.
- ◆ To learn the properties of quarks such as charm, color, and flavor.

The discovery of electron was a revolutionary step by J.J. Thomson. He determined their charge to mass ratio as well. Rutherford discovered the positive nucleus because atom on whole was neutral, and hence the compensating particle for electron was required. Rutherford model was further improvised by Bohr, when he discovered that the electrons revolve around the nucleus just like the planets revolve around the sun. Moreover, the electrons possess quantized angular moment and energy, which will be lost or gained only when the electrons jump from one orbit to another. As helium atom was found to be four times heavier than hydrogen and lithium was seven times heavier than hydrogen.

Hence, the existence of some third elementary particle was quite probable. This mystery was solved by Chadwick, when he discovered Neutron. The discovery of electron, proton, and neutron was within the classical period, which was from 1897 to 1932. The Planck's photon was also discovered in 1900 while explaining the black-body spectrum for the radiations emitted by wet object. The discovery of "photon" helped Einstein to explain photoelectric effect. The discovery of photon put a revolutionary aspect forward as the Newton's corpuscular theory got the setback. But in 1923, A.H. Compton found the shift of wavelength (Compton shift) when the light is scattered by the atoms of target. Hence, Compton effect treated light as a particle with energy $E = hf$ and zero rest mass.

This particle is photon and is represented by γ . Then came the era from 1934 to 1947 during which the mesons were discovered. The mesons were discovered to define the stability of nucleus and hence nuclear forces. The concept of mesons was proposed by Yukawa in 1934. Meson's mass is $1/6$ times of proton mass. "Meson" means "middle weight." Electron is known as Lepton indicating it is lightweight and protons/neutrons fall under the category of Baryons, which means "heavy." Yukawa meson " π " is produced in upper atmosphere which disintegrates quickly. In 1937, Anderson and Neddermeyer found that cosmic rays have some more lighter particles than the Yukawa " π " mesons. Then, Powell also conducted his independent studies, and he found that cosmic rays have π -meson/pion and μ -meson/muon. With the discovery of these particles, the dualism of Dirac's equation brought new results. According to the dualism of Dirac's equation, for every particle, there must be a corresponding antiparticle having same mass but opposite charge as that of particle. Anderson discovered positron which is a positively charged electron and can be regarded as an antielectron. Neutral particles such as γ -photons are their own antiparticles. Neutrons are also neutral particle, but it is not antiparticle of itself. The other quantum numbers for neutron are different. These quantum numbers are different for neutron and its antiparticle (antineutron).

Carl D. Anderson was born in New York City. His father was Swedish immigrant. He graduated from Caltech in 1930 in physics and engineering. He started his investigations into the world of cosmic rays under the supervision of Robert A. Millikan. He got very interesting results in his cloud chamber photographs, that is, particle tracks could be seen. He explained that these tracks have been created by a particle with an electron-like particle having the same mass as that of electron but opposite electrical charge. Paul Dirac's theoretical prediction of the existence of the positron also got validation due to this discovery. Anderson was the first to detect the particles in cosmic rays. Anderson and Victor Hess shared the Nobel Prize in Physics in 1936 for producing positron-electron pairs by bombarding gamma rays produced by the natural radioactive nuclide thorium into other materials.



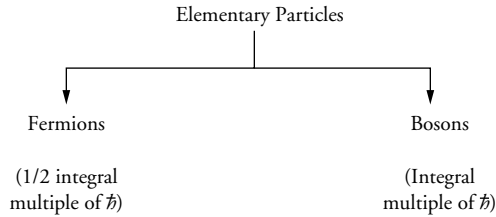
CARL D. ANDERSON

8.1 Introduction to Particle Physics

Before starting with particle physics, the elementary particles should be well understood and discussed. Usually, we understand "elementary" as the entity that cannot be disintegrated into smaller subentities. But at the same time, neutron and proton are regarded as elementary particles despite the fact that they are made up of other small particles. We will define elementary particles as those particles whose lifetime is larger than 10^{-24} sec, i.e., nuclear lifetime. In addition to this, the elementary particles have well-defined spacetime properties and nucleon number ($N = n + p = 0$ or 1). We will classify the elementary particles as follows.

8.1.1 Classification of Elementary Particles

The elementary particles can be classified as follows:



Spin statistics play a vital role in determining the nature of a particle. In 1940, Pauli correlated the spin angular momentum with particle state. The particles that have integral spin $(0, 1\hbar, 2\hbar, 3\hbar, \dots)$ are known as bosons.

In addition to this, the Bose–Einstein statistics is symmetric, that is,

$$\varphi(x, y, z, t) \rightarrow \varphi(-x, -y, -z, t) \quad (1)$$

where $\varphi(x, y, z, t)$ is the wavefunction associated with the particle.

The second category of particles is called fermions. Fermions have half integral spin and their wavefunction is antisymmetric, that is,

$$\varphi(x, y, z, t) \rightarrow -\varphi(-x, -y, -z, t) \quad (2)$$

Electrons, mesons, etc., are fermions, whereas photons and gravitons fall under the category of bosons. The wavefunction can be further divided into spacial and spin part as follows:

$$\varphi = \varphi(1)\varphi(2) \quad (3)$$

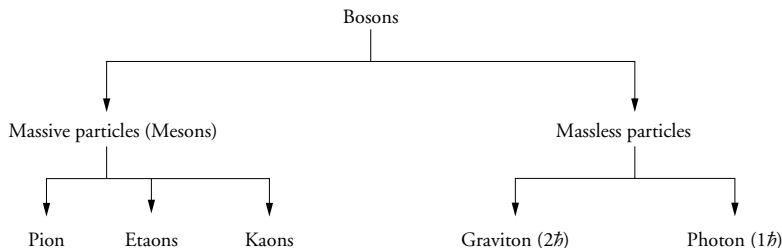
where $\varphi(1)$ is the spacial part and $\varphi(2)$ is the spin-part. When the space coordinates are changed, then the factor $(-1)^l$ is introduced, where l is orbital angular momentum number. When l is odd, then $\varphi(1)$ is antisymmetric and vice versa. In terms of spin part $\varphi(2)$, the wavefunction is symmetric, when the spins of two particles are parallel. When the spins of particles are antiparallel, then the spin wavefunction is negative. Hence, we can say the following:

- (i) For bosons, both the spin and spatial part are either symmetric or antisymmetric.
- (ii) For fermions, either the spin part is antisymmetric or the spatial part is antisymmetric.

For fermions, one particle can be accommodated in one quantum state.

8.2 Classification of Bosons

Bosons can be classified as massive and mass-less particles as follows:



We will discuss these particles one by one below.

8.2.1 Mass-Less Particle

Mass-less particles include gravitons and photons. Gravitons are the quantum of gravitational field and have $2\hbar$ angular momentum. Photons are quantum of light radiations with zero rest mass. The energy of photon is given by hf , and it travels with velocity of light. The angular momentum of photon is $1\hbar$.

8.2.2 Massive Particles (Mesons)

These are strong interacting bosons with zero or integral spins. There are seven types of mesons, and these are discussed below.

1. π -Mesons (π Pions)

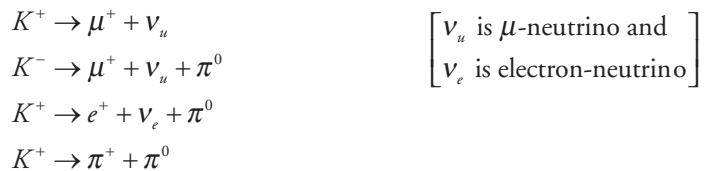
They carry $0\hbar$ angular momentum. They do not have any spin and exist in neutral, positive, and negative states. The decay modes are given by following reaction:



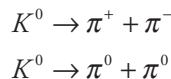
where $\mu^{+/-}$ are mesons and ν_u are neutrinos. The mass of π^0 is $264 m_e$ and mean life is 7×10^{-17} sec. The mass of π^- and π^+ is $273 m_e$ with mean life of 1.82×10^{-8} sec. Neutral pion is its own antiparticle, and it is unstable in nature.

2. Kaons (K)

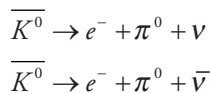
They have $0\hbar$ angular momentum. They are of three types i.e. K^+ , K^- , K^0 . They are heavy mesons as their mass is almost 970 times the mass of electron. It has following decay modes:



The average lifetime of the above reactions is almost 1.2×10^{-8} sec. The neutral pion follows the following decay mode.

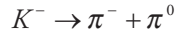


The average lifetime of decay for neutral kaons is almost 10^{-10} sec. Decay mode for $\overline{K^0}$ is given by



The average lifetime of decay is 10^{-10} sec.

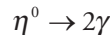
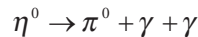
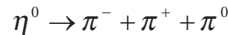
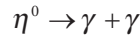
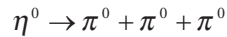
The negative kaon decays as follows:



The average lifetime of negative kaon is 1.2×10^{-8} sec. Neutral pion is heavier than negative and positive kaons. The mass of neutral pion is 975 mass of electron (m_e) and $K^{+/-}$ mass is 967 m_e .

3. Eta-Mesons (η)

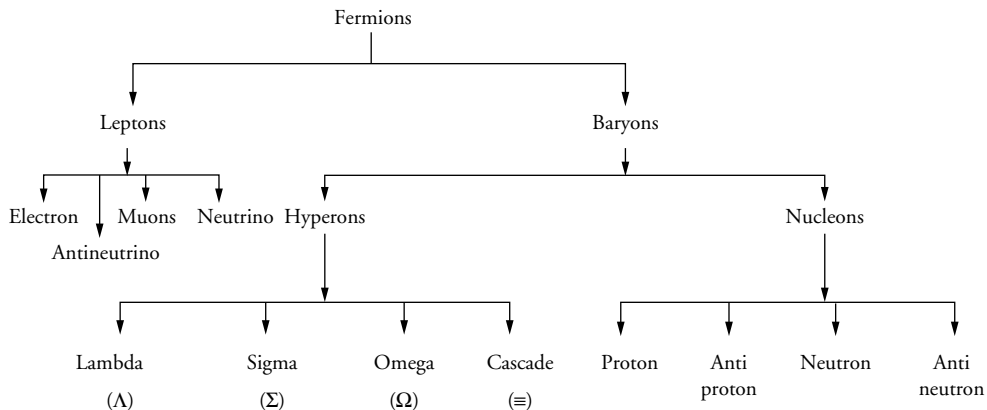
They also possess $0\hbar$ spin. It is neutral particle η^0 , and hence its own antiparticle. It is the heaviest particle among all the bosons, that is, 1074 m_e . Its decay mode is



The average lifetime of decay for eta mesons is almost 10^{-16} sec.

8.3 Classification of Fermions

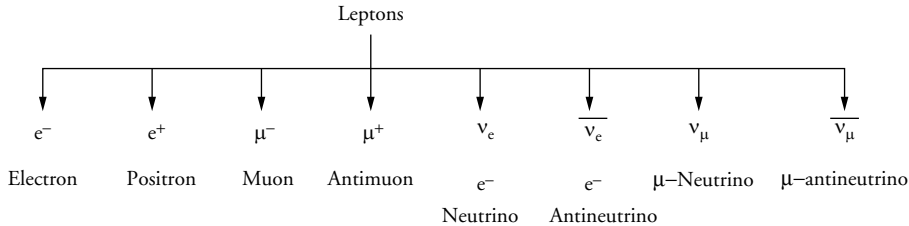
Fermions can be classified as follows:



Fermions can be classified mainly into leptons and baryons as discussed below.

8.3.1 Leptons

They possess $\frac{1}{2}\hbar$ spin angular momentum. Their mass is less than the mass of nucleons and pions. They are subjected to electromagnetic and weak interactions. The general elaborated classification is given as follows:



Members of this group are discussed below.

1. Electrons (e)

The electrons have mass 9.1×10^{-31} kg positron is positive electron. The electrons have charge -1.6×10^{-19} C, whereas the positron has charge $+1.6 \times 10^{-19}$ C. Electrons are stable particles. They have half spin angular momentum of $\frac{\hbar}{2}$.

2. Muons (μ)

There are two types of muons, that is, positive muon and negative muon. The mass of muons is 207 times the mass of electrons. The charge of muon is $\pm 1.6 \times 10^{-19}$ C depending upon whether it is positive muon (μ^+) or negative muon (μ^-). The muons are unstable particles. The half-life for muons is almost 2.2×10^{-6} sec.

The decay modes for muon is given by

$$\mu^+ \rightarrow e^- + \nu_e + \bar{\nu}_\mu$$

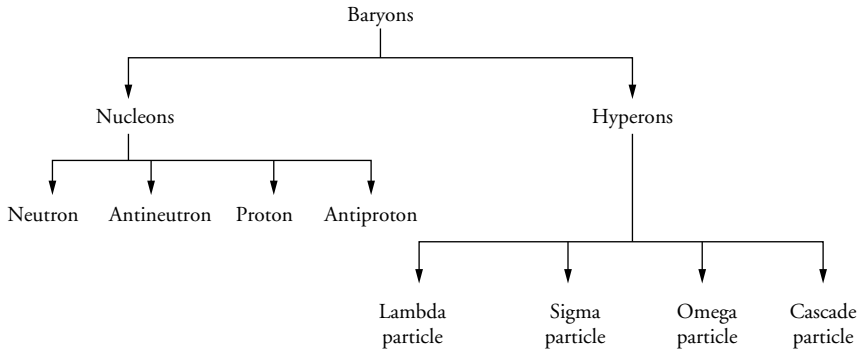
$$\mu^- \rightarrow e^- + \nu_\mu + \bar{\nu}_e$$

3. Neutrinos and Antineutrinos (ν)

In 1930, Pauli proposed the existence of neutrinos to conserve angular momentum, energy, and spin during the process of β^- decay. Neutrinos do not have rest mass and are neutral particles. Neutrinos are stable particle that move with the velocity of light. Neutrinos are of two types, that is, electron neutrino and μ neutrino. The antiparticles of neutrinos are antineutrinos, and they are not very stable particles.

8.3.2 Baryons

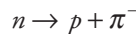
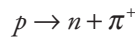
The baryons are fermions and possess half-integral spins. They include the particles with mass equal to or greater than nucleons. The baryons that have mass equal to the mass of proton and neutron are known as nucleons. The baryons with mass greater than nucleons are known as hyperons.



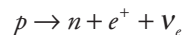
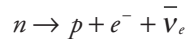
1. Nucleons

Nucleons consist of neutrons and protons. The mass of proton and neutron is the same, that is, 1.67×10^{-27} kg. Neutrons are neutral particles; whereas, protons have a charge equal to antielectron or 1.6×10^{-19} C. The spin of nucleons is $\frac{\hbar}{2}$. The nucleons have same lifetime of 10^{-23} sec within the nucleus. Free neutron and bound proton are unstable. They follow the following decay modes:

Inside the nucleus



Outside the nucleus



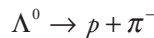
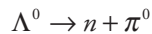
Free neutrons have a lifetime of 933 seconds.

2. Hyperons

The mass of hyperons is more than the nucleons. There are four types of hyperons as explained below:

(a) **Lambda particles (Λ^0)**

The spin of lambda particles is $\frac{\hbar}{2}$ and the mass is $2180 m_e$. The decay modes are given by



The lifetime of lambda particles is 2.1×10^{-10} sec. The antiparticle of lambda particle is $\bar{\Lambda}^0$.

(b) **Cascade particles (Ξ)**

The cascade particle is Ξ^- and Ξ^0 . The mass of negative and neutral cascade particle is $2582 m_e$ and $2570 m_e$, respectively. The decay modes are given by following reactions:



The lifetime of neutral cascade particle is 1.2×10^{-10} sec, whereas the lifetime of negative cascade particle is 1.1×10^{-20} sec. Cascade particles are also known as Xi hyperon. (Their charge is 1.6×10^{-19} C.)

(c) **Sigma particle (Σ)**

Sigma hyperons have $\frac{\hbar}{2}$ angular momentum. There are three sigma particles, that is, positive, negative, and neutral. The mass of positive sigma particle (Σ^+) is $2325 m_e$ and that of negative sigma particle (Σ^-) is $2338 m_e$. Neutral sigma particle (Σ^0) is $2320 m_e$. The decay reactions are given by

$$\Sigma^+ \rightarrow p + \pi^0$$

$$\Sigma^+ \rightarrow n + \pi^+$$

$$\Sigma^- \rightarrow n + \pi^-$$

$$\Sigma^0 \rightarrow n + \gamma$$

The lifetime of Σ^+ is 6×10^{-11} sec and Σ^- is 10^{-10} sec. Neutral sigma particles have a lifetime of 10^{-11} sec. Σ^+ and Σ^- are antiparticle of each other. The charge of $\Sigma^{+/-}$ is $\pm 1.6 \times 10^{-19}$ C

(d) **Omega hyperon (Ω)**

These fermions have charge as that of electron. For Ω^+ , the charge is 1.6×10^{-19} C and for Ω^- the charge is -1.6×10^{-19} C. The omega hyperons have a spin angular momentum of $\frac{3}{2}\hbar$. The mass of Ω^- is $3286 m_e$ and Ω^+ is $3276 m_e$. The decay modes are given by

$$\Omega^- \rightarrow \Xi^0 + \pi^-$$

$$\Omega^- \rightarrow \Lambda^0 + K^-$$

The average lifetime is 1.1×10^{-10} sec.

Seth Neddermeyer was born in Richmond, Michigan, on September 16, 1907. He studied from Stanford University and graduated at the California Institute of Technology in 1935 under the supervision of Carl D. Anderson. In 1936, Neddermeyer and Anderson discovered the negatively charged subatomic particle called "muon." At first, Anderson and Neddermeyer believed that they had seen the pion, which Hideki Yukawa postulated in his meson theory. Later on, they found that it was not the Yukawa pion. J. Robert Oppenheimer from the National Bureau of Standards appointed Neddermeyer to work on the Manhattan Project. Neddermeyer was a group leader in the Ordnance Division for implosion experimentation, although Oppenheimer was full of doubts for the implosion method. However, in January 1944, Neddermeyer was demoted to senior technical advisor, as he could not implement his idea even after struggling with it. Neddermeyer taught at the University of Washington, until his death in 1988. United States Department of Energy awarded him with Enrico Fermi award in 1982.



SETH NEDDERMEYER

8.4 Other General Classifications

The elementary particles can also be classified on the basis of interactions between particles. The interactions between particles depend upon the quanta exchange. Every force has its own quanta through which the forces are transmitted. The second classification is based on the stability of particles, that is, lifetime. First, we will discuss the particles on basis of interaction.

8.4.1 Fundamental Interactions

There are four types of fundamental interactions between particles as discussed below:

1. Gravitational Interaction

Gravitational interaction depends on inertia and hence mass. These interactions are attractive in nature and follow the inverse square law, which means the force between two bodies varies as inverse of square of distance between them. These interactions are very weak in nature. The quanta of gravitational field are gravitons which have spin $2\hbar$ and zero rest mass. Gravitational interaction is central in nature, as it acts along the line joining two bodies. The strength of gravitation is given by a constant G_m (Cavendish gravitational constant).

$$G_m = 6.7 \times 10^{-11} \text{ Nm}^2/\text{kg}^2$$

There is another dimensional interaction constant given by

$$g_m = G_m \left(\frac{M^2}{\hbar c} \right) = 5.82 \times 10^{-39}$$

Where M is the mass of nucleon, c is velocity of light and \hbar is Dirac constant. The gravitons have a characteristic time of 10^{-16} sec.

2. Electromagnetic Interaction

These interactions are based on the nature of charge. These forces can be attractive (between opposite charges) and can be repulsive (between same charges). The quanta of electromagnetic interaction are photon. These are long-range interactions that follow inverse square law. Like gravitational interaction, these are also central in nature. The coupling constant is g_e given by

$$g_e = \frac{e^2}{\hbar c} \approx \frac{1}{137} \quad (\text{C.G.S})$$

These interactions have characteristic time of 10^{-20} sec. The pair production from gamma rays is the process that involves electromagnetic interaction. The interaction between positive charged nucleus and negative charged orbiting electrons is also electromagnetic in nature.

3. Weak Interactions

These interactions are due to W^+ , W^- , and Z^0 bosons. These are short-range interactions which don't obey inverse square law. The weak interactions are involved during decay processes. The characteristic time of decay is 10^{-10} sec. The constant for weak interaction is g_w , which is given by

$$g_w = G_w^2 \left(\frac{1}{\hbar c} \right)^2 \left(\frac{\hbar}{Mc} \right)^{-4} \approx 5 \times 10^{-7}$$

4. Strong Interactions

These are the strongest interactions that exist within the nuclei. These are short-range interactions and charge independent. They do not obey inverse square law. The quanta of these interactions are mesons, which are exchange particles. These interactions overcome the strong repulsions between nucleons of same charge. These interactions are spin dependent. The interaction constant is given by constant g_s , as follows:

$$g_s \approx \frac{(m/2M)^2}{4\pi\hbar^2 c} \approx 8 \times 10^{-2}$$

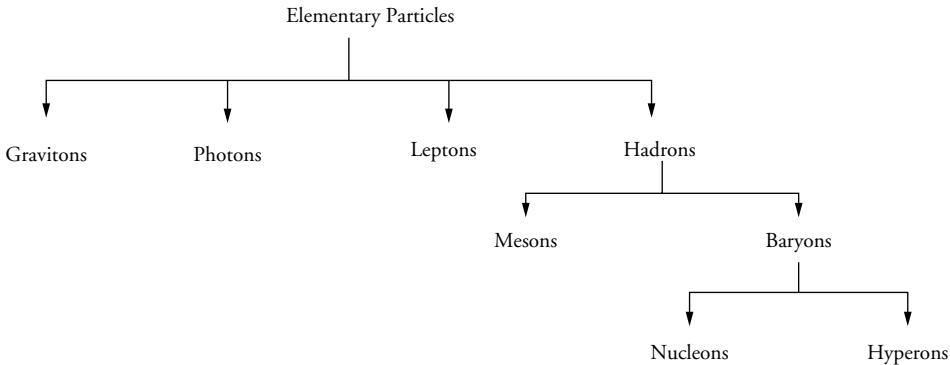
$m \rightarrow$ pion rest mass and M is nucleon rest mass.

$g_s \rightarrow$ is known as pion–nucleon coupling constant. The characteristic time of weak interactions is 10^{-23} sec.

To sum up with, the force and range for the above-mentioned forces is given by

$\left(\begin{array}{l} \text{Range} \\ \text{i.e.,} \end{array} \right.$	$\left(\begin{array}{l} \text{Gravitational} > \text{EM} > \text{Strong} > \text{Weak} \\ \infty : \infty : 10^{-5} \text{ m} : 10^{-17} \text{ m} \end{array} \right)$
$\left(\begin{array}{l} \text{Force} \\ \text{i.e.,} \end{array} \right.$	$\left(\begin{array}{l} \text{Strong} > \text{EM} > \text{Weak} > \text{Gravitational} \\ 1 > 10^{-3} > 10^{-14} > 10^{-39} \end{array} \right)$

8.4.2 Classification on the Basis of Stability



This classification has been familiar to us as we have discussed them in Sections 8.2 and 8.3. Here we have new collective set of particles, which is known as hadrons. Hadrons are collective group of mesons and baryons.

8.5 Parity and Angular Momentum

Parity represents the mirror image or space reflection. If wavefunction changes sign upon inversion of space coordinates, then it is said to odd parity. If the wavefunction does not change sign upon space coordinates, then it is said to have even parity. Parity is also related to angular momentum as $(-1)^l$ is the factor that decides the factor (l is angular momentum). The factor $(-1)^l$ could be obtained for hydrogen atom problem. We know that, the solution to hydrogen value problem (Chapter 4) is given by

$$\varphi(r, \theta, \phi) = R(r)Y_l^{m_l}(\theta, \phi) \tag{4}$$

or

$$\varphi(r, \theta, \phi) = R(r) \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}} P_l^{m_l}(\cos\theta) e^{im_l\phi} \quad [\text{where } m_l \text{ is magnetic quantum number}]$$

When the parity is applied, then the above equation can be written as (after ratio of π) follows:

$$\begin{aligned} \varphi(r, \pi - \theta, \pi + \phi) &= R(r) \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}} P_l^{m_l}(\cos(\pi - \theta)) e^{im_l(\pi + \phi)} \\ &= R(r) \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}} (-1)^{l-m_l} P_l^{m_l}(\cos\theta) (-1)^{m_l} e^{im_l\phi} \\ &= R(r) \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}} (-1)^l P_l^{m_l}(\cos\theta) e^{im_l\phi} \\ &= (-1)^l \sqrt{\frac{(2l+1)(l-m_l)!}{4\pi(l+m_l)!}} P_l^{m_l}(\cos\theta) e^{im_l\phi} \\ \varphi(r, \pi - \theta, \pi + \phi) &= (-1)^l \varphi(r, \theta, \phi) \end{aligned} \quad (5)$$

For a composite system, parity is multiplicative in nature. For example, Let P be the system with P_a, P_b, P_c, \dots parities for the units inside the system, then total parity is given by

$$\text{Parity} = P_a P_b P_c \dots \quad (6)$$

8.6 Parity Conservation

The condition for two operators A and B to be commuting is given by

$$[AB - BA] = 0 \quad \text{or} \quad [A, B] = 0$$

Let us suppose that the Hamiltonian H for a system P -commute with parity operator P , such that

$$\begin{aligned} HP - PH &= 0 \\ HP &= PH \end{aligned} \quad (7)$$

Let the wavefunction $\varphi(r)$ be the eigenfunction of parity operator such that

$$H\varphi(r) = E\varphi(r) \quad (8)$$

Operating with parity P on both sides,

$$\begin{aligned} PH\varphi(r) &= PE\varphi(r) && [\text{using Eqs (7) and (8)}] \\ HP\varphi(r) &= EP\varphi(r) && [\text{where } P\varphi(r) = \varphi'(r)] \\ H\varphi'(r) &= E\varphi'(r) && (9) \end{aligned}$$

If the state is degenerate with energy E , then $\varphi(r)$ and $\varphi'(r)$ can have the same energy. If $\varphi(r)$ and $\varphi'(r)$ are non-degenerate, then they have different energies in their own states.

According to parity conservation, if the following reaction occurs, then

$$x + y \rightarrow x' + y'$$

Then the parity for reactants is given by

$$P | \text{reactants} \rangle = P | x \rangle P | y \rangle | P_{\text{relative motion}} \rangle \quad (10)$$

and for

$$P | \text{products} \rangle = P | x' \rangle P | y' \rangle | P_{\text{relative motion}} \rangle$$

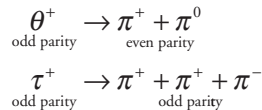
The $| P_{\text{relative motion}} \rangle$ is affected by parity, and hence a factor $(-1)^l$ is introduced for reactants and $(-1)^{l'}$ for products, such that

$$(-1)^l P | x \rangle P | y \rangle = P | x' \rangle P | y' \rangle (-1)^{l'} \quad (11)$$

where l is relative angular momentum between x and y , and l' is relative angular momentum between x' and y' . Parity of neutron, proton, and deuteron is assumed to be positive.

Note: Tau-Theta Puzzle

As per the parity conservation law, for all atomic and nuclear processes, parity should be conserved. But this is not the same for mesons, that is, θ -meson and τ -meson. This can be explained as follows:



Hence, θ^+ and τ^+ are charged mesons with odd parity, which end in states of different parities. This is known as $\tau - \theta$ puzzle.

Tsung-Dao Lee was studied at Kweichow province of China in 1943. Lee moved to Kunming due to Sino-Japanese War. In Kunming, he attended the National Southwest University. During the course of his studies, he met another student Chen-Ning Yang. Both of them received fellowships to study in the United States in 1946. Yang had been with Enrico Fermi from Columbia to the University of Chicago, whereas Lee only had the choice of University of Chicago. Only University of Chicago in the United States then allowed an undergraduate to work toward the PhD without the intermediate degrees. Both of them became very good friends then.

Yang was not very good in experimental physics. He got his doctoral thesis under the supervision of Edward Teller. Lee did his doctoral thesis under Fermi. Fermi gave advice to Yang on his career, which he ignored a bit:

As a young man, work on practical problems; do not worry about things of fundamental importance.

Lee and Yang worked together at the Institute for Advanced Study in Princeton. J. Robert Oppenheimer regarded Lee as "one of the most brilliant theoretical physicists then known." Lee and Yang's work solved the mystery of the *theta-tau puzzle*.

8.7 Mass Determination Techniques for Particles

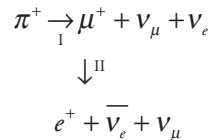
To determine the mass of particles, we will use following three techniques:

1. μ -mesic method
2. Kinematic method
3. Trajectory method

These techniques are discussed as below.

8.7.1 μ -Mesic Method

When nuclei is bombarded with high-energy particles, the π^+ or π^- mesons are emitted from the target nuclei. The π^+ mesons decay to muons as follow:



In the first step, muon is produced along with neutrinos. The muon further decays to electron, μ -neutrinos, and electron antineutrino. The lifetime for π^+ meson is 0.022μ sec and for μ^+ muon is 2.15μ sec. Mesons are heavy electrons ($207 m_e$); and when they travel through matter, then they lose energy by ionization and excitation processes. The μ^- mesons may be captured by Bohr orbits if the thermal energy of μ^- -muons is high.

When the energy of muons is small, then they are scattered rather than being absorbed. The μ^- -muons that are absorbed by Bohr's orbit will fall down to states of lower energy by radiative transitions. Prior to radiative transitions, nonradiative transitions will take place via collisions. During the radiative transitions, mesonic atom would give characteristic X-rays. The radius of mesonic atom is smaller than the atom as follows:

$$\text{Bohr radius } r = \frac{n^2 \hbar^2 \epsilon_0}{\pi m Z e^2} \quad (12)$$

$$\text{Hence, } r \propto \frac{1}{Z} \quad (13)$$

$$Z_{\text{meson}} > Z_{\text{atom}}$$

$$\text{Hence, } r_{\text{meson}} < r_{\text{Bohr atom}} \quad (14)$$

The energy released is given by

$$E = \frac{1}{2} \alpha^2 m Z^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (15)$$

[$\alpha = \frac{1}{137}$, and energy of transition can be obtained]

From Eqs (12) and (15), the mass of mesons can be obtained.

8.7.2 Kinematic Techniques

In kinematic techniques, the principle of conservation of momentum and energy is used, that is,

$$\text{Initial momentum} = \text{Final momentum}$$

$$\text{Initial energy} = \text{final energy}$$

We will explain it using Powell experiment. In 1947, Powell studied the decay of π^+ -meson, that is,

$$\pi^+ \rightarrow \mu^+ + \nu_\mu$$

We can find pion mass using kinematic methods. To start with, let us assume pion at rest, then $m_{\pi^+}c^2$ is rest mass energy of pion. Using conservation of momentum

$$\text{Momentum of } \pi^+ = \text{momentum of } (\mu^+) + \text{momentum of } \nu_\mu$$

$$0 = p_{\mu^+} + p_{\nu_\mu} \quad (16)$$

$$p_{\mu^+} = -p_{\nu_\mu} \quad (17)$$

Using conservation of energy,

$$\text{Energy of } \pi^+ = \text{energy of } \mu^+ + \text{energy of } \nu_\mu$$

$$m_{\pi^+}c^2 = \left(p_{\mu^+}c^2 + m_{\mu^+}^2c^4\right)^{1/2} + \left(p_{\nu_\mu}c^2 + m_{\nu_\mu}^2c^4\right)^{1/2}$$

$$m_{\pi^+}c^2 - \left(p_{\mu^+}c^2 + m_{\mu^+}^2c^4\right)^{1/2} = \left(p_{\nu_\mu}c^2 + m_{\nu_\mu}^2c^4\right)^{1/2}$$

Squaring both sides and using Eqn. (17) $\left[p_{\mu^+}^2 = p_{\nu_\mu}^2\right]$,

$$m_{\pi^+}^2c^4 + m_{\mu^+}^2c^4 - 2m_{\pi^+}c^2\left(p_{\mu^+}^2c^2 + m_{\mu^+}^2c^4\right)^{1/2} = m_{\nu_\mu}^2c^4$$

$$\left(m_{\pi^+}^2 + m_{\mu^+}^2 - m_{\nu_\mu}^2\right)c^2 = 2m_{\pi^+}\left(p_{\mu^+}^2c^2 + m_{\mu^+}^2c^4\right)^{1/2}$$

$$\frac{\left(m_{\pi^+}^2 + m_{\mu^+}^2 - m_{\nu_\mu}^2\right)^2}{4m_{\pi^+}^2} = p_{\mu^+}^2 + m_{\mu^+}^2c^2 \quad (18)$$

$$\text{Using } m_{\mu^+}c^2 = 4.2 \text{ MeV and } m_{\nu_\mu}c^2 = 0 \quad (19)$$

$$\Rightarrow \frac{p_{\mu^+}^2}{2m_{\mu^+}} = 4.2$$

$$\Rightarrow p_{\mu^+} = 29.8 \text{ MeV} \quad (20)$$

Using Eqs (19) and (20) in Eqn. (18),

$$m_{\pi^+}c^2 = 139.3 \text{ MeV} \quad (21)$$

Hence, the mass for elementary particle meson is obtained.

8.7.3 Trajectory Method

From the relation $p = mv$, it is clear that to determine mass, we need to know momentum and velocity. Momentum and velocity are influenced by external conditions; hence, these quantities are extrinsic quantities. Mass do not depend upon the external conditions, and hence mass is an intrinsic quantity. Trajectory method can determine the mass of charged particles provided the extrinsic conditions of temperature, density and pressure are kept constant. In trajectory method, we will determine, mass, velocity, and energy to obtain mass.

1. Determination of Momentum

If the particle is moving with velocity “ v ” under the influence of strong magnetic field B , then the particle experiences force. This force makes the particle to move in circular path (radius r).

The condition for particle of charge e to move in circular orbit of radius r is that the magnetic force should be equal to the centripetal force, that is,

$$\begin{aligned} \frac{mv^2}{r} &= e \left(\vec{B} \times \vec{v} \right) \\ \frac{mv^2}{r} &= Bev \sin\theta \\ \frac{mv^2}{r} &= Bev && \text{[when the velocity is} \\ &&& \text{tangential to charge]} \\ mv &= Ber \\ p &= Ber \end{aligned} \tag{22}$$

Hence, momentum can be obtained from magnetic field, charge, and radius.

2. Determination of Velocity

The time can be determined using time-of-flight technique between two detectors (Figure 8.1).

If particle enters detector D_1 , then the time (t_1) should be noted down. Then, when the particle enters D_2 , then time t_2 is noted down. Let “ L ” be the distance between two detectors. The velocity can be given by

$$\text{Velocity} = \frac{L}{t_2 - t_1} = \frac{L}{t} \tag{23}$$

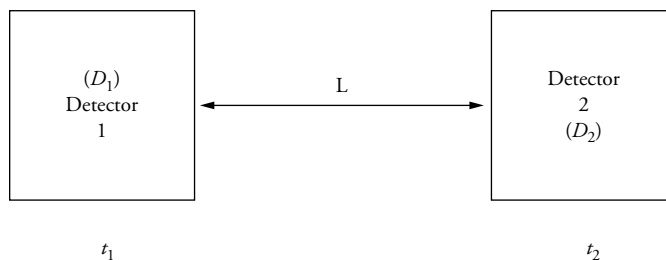


Figure 8.1 Time of flight technique

When environment of detectors change, then the measurements are affected.

3. Determination of Energy

When charged particles pass through matter, then the excitation as well as ionization of medium takes place. During this process, the energy loss occurs, and this is given by $-\frac{dE}{dx}$. The formula for $-\frac{dE}{dx}$ is given by Bethe and Block in 1933 as follow:

$$-\frac{dE}{dx} = \frac{4\pi Z^2 e^4 Z'^2}{m_e v^2} N \ln\left(\frac{2mv^2}{I}\right) \quad (24)$$

where I is the ionization potential, N is the number of particles velocity, Z is the atomic number of charged particle, and Z' is the atomic number of absorbing medium. m_e is mass of electrons and v is the velocity of particle. The range of particle is given by

$$R = \int_E^0 dx \quad (25)$$

Range is the total distance covered by the particle before it comes rest:

$$\begin{aligned} R &= -\int_E^0 \frac{dx}{dE} dE = -\int_0^E -\left[\frac{dE}{dx}\right]^{-1} dE \\ \Rightarrow R &= 0.318 E^{3/2} \\ R &= R_0 E^{3/2} \end{aligned} \quad (26)$$

If we know the range, then energy of particle can be calculated.

8.8 Intrinsic Quantum Numbers

Every particle is associated with certain quantum numbers. These quantum numbers describe the particle completely. Along with s, l, j, m_s, m_l, m_j quantum numbers, there are additional quantum numbers described below, which are used for elementary particles.

8.8.1 Lepton Number (L)

Leptons are “lightweight” particles. Konopinski and Mahmoud introduced lepton number “ L ”. The leptons are electron (e^-), muon (μ^-), electron–neutrino (ν_e), and muon–neutrino (ν_μ). The antileptons include positron (e^+), antimuon (μ^+), antielectron neutrino ($\bar{\nu}_e$), and antimuon neutrino ($\bar{\nu}_\mu$). Following are the rules for lepton number:

- (i) $L = -1$ for antileptons ($e^+, \mu^+, \bar{\nu}_e, \bar{\nu}_\mu$)
- (ii) $L = +1$ for leptons ($e^-, \mu^-, \nu_e, \nu_\mu$)
- (iii) $L = 0$ for all other particles

Until and unless the lepton number conservation is not satisfied, the decay modes are not satisfied. Leptons are created and destroyed during particle–antiparticle pairs.

For example,

$$\begin{array}{l} \gamma \rightarrow e^- + e^+ \\ L \quad 0 \quad -1 \quad 1 \end{array} \left] \sum L_i = \text{constant} \right.$$

$$\begin{array}{l} \gamma \rightarrow p + e^- \\ L \quad 0 \quad 0 \quad 1 \end{array} \left] \sum L_i \neq \text{constant} \right.$$

$$\left. \begin{array}{l} \gamma \rightarrow p + \bar{p} \\ L \quad 0 \quad 0 \quad 0 \end{array} \right\} \sum L_i = \text{constant}$$

8.8.2 Baryon Number (B)

The electric charge Q should be conserved during a decay as follows:

$$\left. \begin{array}{l} p \rightarrow e^+ + \gamma \\ Q \quad 1 \quad 1 \quad 0 \end{array} \right\} \sum Q = \text{conserved}$$

But this decay mode does not exist despite the fact that charge is conserved. Then Stückelberg suggested the concept of baryon number (B). Baryon numbers include nucleons hyperons and their antiparticles. Baryon number has following rules:

- (i) $B = -1$ for antiproton and antineutron and antihyperons

$$\left(\bar{p}, \bar{n}, \bar{\Sigma}^-, \bar{\Xi}^-, \bar{\Omega}^- \right)$$

- (ii) $B = +1$ for protons, neutrons, and hyperons

- (iii) $B = 0$ for leptons, photons, and mesons

For example,

$$\left. \begin{array}{l} \Sigma^+ \rightarrow p + \pi^0 \\ B \quad 1 \quad 1 \quad 0 \end{array} \right\} \sum B_i = \text{constant}$$

$$\left. \begin{array}{l} \Sigma^+ \rightarrow \Lambda^0 + e^+ + \nu \\ B \quad 1 \quad 1 \quad 0 \quad 0 \end{array} \right\} \sum B_i = \text{constant}$$

$$\left. \begin{array}{l} \Sigma^- \rightarrow n + \pi^- \\ B \quad 1 \quad 1 \quad 0 \end{array} \right\} \sum B_i = \text{constant}$$

$$\left. \begin{array}{l} \Lambda^0 \rightarrow n + \pi^0 \\ B \quad 1 \quad 1 \quad 0 \end{array} \right\} \sum B_i = \text{constant}$$

Σ^+ , Σ^- , and Λ^0 are also called strange particles. Nuclei also consist of nucleons, that is, protons and neutrons. Hence, baryon number B is identical to the mass number. When one or more nucleons of a nuclei are replaced by hyperons, then the nuclei is said to be hypernuclei.

8.8.3 Isospin (I)

Before starting for isospin, it should be clear that iso-spin is represented only in iso-spin frame. Heisenberg observed that the mass of protons and neutrons is same, and both particles have same spin of $\hbar/2$. This is the case when there is no electromagnetic interaction. But, in the presence of electromagnetic interactions, the masses are difference due to coulomb forces. In other words, the nucleons can be written as a part of column matrix:

$$p = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \uparrow \quad \text{and} \quad n = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \downarrow$$

up spinor down spinor

Isospin vector I is not in ordinary space and has components $I_1, I_2,$ and I_3 in isospin space. In isospin space, the proton and neutron are not treated as two particles, but two states of the same particle. Hence, proton and neutron are isospin-up and isospin-down states of the nucleon. There are $2I + 1$ orientations corresponding to I . The third component I_3 distinguishes between the nucleons, because $I_3 = \frac{-1}{2}$ for neutron and $I_3 = \frac{1}{2}$ for proton. For the hadron families, many members have almost similar mass but different charges. For pion, $I = 1$, and hence $2I + 1 = 3$ states

- when $I_3 = 1$, it is π^+ -meson
- $I_3 = -1$, it is π^- -meson, and
- $I_3 = 0$, it is neutral meson

Table 8.1 gives the spin and isospin for baryons and mesons.

Table 8.1 Spin and isospin of particles

Elementary Particle	Spin	Isospin	
		I	I_3
p	$\frac{1}{2}$	$\frac{1}{2}$	$+\frac{1}{2}$
n	$\frac{1}{2}$		$-\frac{1}{2}$
Σ^+	$\frac{1}{2}$	1	1
Σ^0			0
Σ^-			-1
Λ^0	$\frac{1}{2}$	$\frac{1}{2}$	0
Ξ^0			$+\frac{1}{2}$
Ξ^-			$-\frac{1}{2}$
Ω^-	$\frac{3}{2}$	0	0
η^0	0	$\frac{1}{2}$	0
K^+			$+\frac{1}{2}$
K^0			$-\frac{1}{2}$
π^+			+1
π^0		1	0

8.8.4 Hypercharge (Y)

Hypercharge is given as twice the average charge (\bar{Q}) of members of the group

$$Y = 2\bar{Q} \quad (27)$$

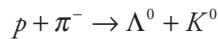
Hypercharge is also given by

$$Y = 2(Q - I_3) \quad \left[\begin{array}{l} Q \text{ is charge and} \\ I_3 \text{ is isospin component} \end{array} \right] \quad (28)$$

For π -mesons, the average charge is zero, which gives zero hypercharge.

8.8.5 Strangeness (S) (Gell-Mann and Nishijima Reaction)

In 1947, Rochester and Butter found V-shaped particles. One of the decay modes was given as follows:



The lifetime for decay is almost 10^{-10} sec. The cross-section is of the order of millibarn for this reaction. Cross-section of order of millibarn represents strong interactions. In contrast to this, the decay lifetime of 10^{-10} sec is characteristic for weak interactions. Conclusively, we can say that the kaons and hyperons are produced by strong interaction and decayed by weak interactions. A. Pais proposed that these V-particles are produced in pairs. Due to their strange behavior, these particles are known as strange particles. According to Pais, the strange particles are always produced in pairs via strong interactions, and then decayed via weak interactions.

Gell-Mann and Nishijima introduced quantum number known as “strange quantum number,” which is additive in nature. The strange quantum number is given by the following equation:

$$S = Y - B \quad (29)$$

[using Eqn. (28)]

$$S = 2(Q - I_3) - B \quad (30)$$

Like hyper charge, strangeness is conserved in strong interactions.

The following points are important:

- (i) $S = 0$ for nucleons and pions
- (ii) $\Sigma S = \text{constant}$ for strong as well as electromagnetic radiations
- (iii) $\Sigma S = \text{not constant}$ for weak interactions.

Hence, “strangeness” represents broken symmetry because it displays different behaviors during strong and weak interactions. Table 8.2 lists the hypercharge and strangeness for particles. It is important to note that for em interactions, isospin is not conserved, whereas for weak interactions, strangeness and parity are not conserved. All the quantum numbers are conserved for strong (hadronic interactions).

Table 8.2 Baryon number, strangeness, hypercharges, and average charge for different particles

Particle	Baryon No.	Strangeness (S)	Hypercharges (Y)	Average Charge
Photon	0	0	0	0
Kaon	0	1	1	$\frac{1}{2}$
Pion	0	0	0	0
Nucleon	1	0	1	$\frac{1}{2}$
Sigma	1	-1	0	0
Lambda	1	-1	0	0
Cascade	1	-2	-1	$-\frac{1}{2}$
Omega	1	-3	-2	-1

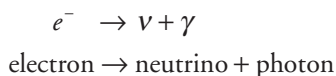
Murray Gell-Mann was born in New York City on September 15, 1929. He did his BSc at Yale University in 1948, and graduated in 1951 at the Massachusetts Institute of Technology. He became a member of the Institute for Advanced Study in 1952. He worked as an instructor at the University of Chicago during 1952–1953. In 1954, he developed the strangeness theory and the eightfold way theory while he was appointed as an associate professor. He became professor in 1956, and his inclination was more toward the theory of weak interactions. In 1959, he received the Dannie Heineman Prize of the American Physical Society. Currently, he is a member of the National Academy of Sciences and fellow of American Physical Society.

**MURRAY GELL-MANN**

8.9 Conservation Principles

Following are the conservation laws that should hold good during the decay process.

1. The total charge Q should remain constant for decay reaction. Many researchers proposed the concept of decay of electron as follows:



The momentum, spin, and energy for this reaction is conserved; hence, the reaction is feasible. If electron comes out of shell, then the electron from higher shell should have jumped to fill the vacancy created by electron. These could have given rise to characteristic X-rays. But no X-rays were observed during the decay process. Hence, the decay is not feasible, which is due to non-conservation of charge. For a reaction or decay to occur,

$$\sum Q = 0$$

Millikan's oil drop experiment proved that charge is quantized, that is, $Q = \pm ne$, where n is the number of charges. n is also said to be charge number. The charge number should also be conserved during a reaction, that is,

For e.g.

$$U + V \rightarrow X + Y$$

$$\text{i.e. } n_u + n_v = n_x + n_y \quad (31)$$

Charge is conserved; it can be proved with the help of symmetry principles. Let us assume that eigenstate φ_e represents state of charge e . Then, the Schrödinger equation is given by the following equation:

$$i\hbar \frac{d\varphi_e}{dt} = H \varphi_e \quad (32)$$

Q is the charge operator and H is the Hamiltonian. Usually, Hamiltonian represents total energy. If charge is conserved, then it should satisfy commuter relation:

$$[H, Q] = 0 \quad (33)$$

Hence, the Hamiltonian and Q should have simultaneous set of eigenfunctions:

$$Q\varphi_e = q\varphi_e \quad (34)$$

q represents eigenvalue of operator Q . We will use Gauge transformation of first kind, that is,

$$\varphi'_e = e^{i\varepsilon Q} \varphi_e \quad (35)$$

where ε is the real parameter and $e^{i\varepsilon Q}$ represents the transformation factor. Gauge invariance states that the φ_e and φ'_e should satisfy the Schrödinger equation, Hence, from Eqn. (32),

$$\begin{aligned} i\hbar \frac{d\varphi'_e}{dt} &= H \varphi'_e \\ i\hbar \frac{d}{dt} (e^{i\varepsilon Q} \varphi_e) &= H (e^{i\varepsilon Q} \varphi_e) \quad [\text{use Eqn. (35)}] \\ i\hbar e^{i\varepsilon Q} \frac{d\varphi_e}{dt} &= H e^{i\varepsilon Q} \varphi_e \end{aligned}$$

Applying $e^{-i\varepsilon Q}$ from both sides,

$$i\hbar \frac{d\varphi_e}{dt} = e^{-i\varepsilon Q} H e^{i\varepsilon Q} \varphi_e \quad (36)$$

From Eqs (32) and (36),

$$H = e^{-i\varepsilon Q} H e^{i\varepsilon Q} \quad (37)$$

Using binomial expansion,

$$\begin{aligned} H &= (1 - i\varepsilon Q) H (1 + i\varepsilon Q) \\ H &= H - i\varepsilon QH + i\varepsilon HQ + \underbrace{\varepsilon^2 QHQ + \dots}_{\text{neglecting higher-order terms}} \\ H &= H + i\varepsilon [HQ - QH] \\ H &= H + i\varepsilon [H, Q] \\ i\varepsilon [H, Q] &= 0 \\ [H, Q] &= 0 \end{aligned} \quad (38)$$

Hence, the charge is conserved, and it is well demonstrated from the gauge invariance. We can sum up the conclusions as follows:

1. The total energy should remain constant
2. The linear and angular momentum should be conserved.
3. The total baryon number and lepton number are conserved.
4. The isospin and hypercharge should be conserved.

Example

$$p + \bar{p} \rightarrow \pi^- + \pi^+ + \pi^0$$

Charge Q	p	\bar{p}	π^-	π^+	π^0	Conserved
	1	-1	-1	1	0	
Spin	1/2	-1/2	0	0	0	Conserved
B	1	-1	0	0	0	Conserved
S	0	0	0	0	0	Conserved
L	0	0	0	0	0	Conserved
Parity		$(-1)^f$	$(-1)^f$			Conserved
Isospin	1/2	-1/2	0	0	0	Conserved

Hence, this decay mode is feasible.

8.10 Quarks and Quark Model

As has been indicated from the evidences that the matter consists of fundamental particles that are known as quarks. Quarks are supposed to carry fractional charges such as $\pm \frac{2}{3}|e|$ and $\pm \frac{1}{3}|e|$. There are six different quarks given below:

- (i) u —(up quark)— $(\frac{2}{3}e)$ (antiquark $-\bar{u}$)
- (ii) d —(down quark)— $(-\frac{1}{3}e)$ (antiquark $-\bar{d}$)
- (iii) s —(strange quark)— $(-\frac{1}{3}e)$ (antiquark \bar{s})
- (iv) c —(charm quark)— $(\frac{2}{3}e)$ (antiquark \bar{c})
- (v) b —(bottom-quark)— $(-\frac{1}{3}e)$ (antiquark \bar{b})
- (vi) t —(top quark)— $(+\frac{2}{3}e)$ (antiquark \bar{t})

Each quark has a baryon number $\frac{1}{3}$; and for antiquark, it is $-\frac{1}{3}$. Three quarks are required to make baryons, and antibaryons have three antiquarks. All the quarks and antiquarks have a spin of $\frac{1}{2}$. In addition to this, the quarks are given colors. The quarks have three basic colors: red, green, and blue; whereas antiquarks have antired (cyan), antigreen (magenta), and antiblue (yellow). For making a baryon, all the quarks are of different colors. Apart from these, the following are the imported properties of quarks:

1. Hadrons prefer to have strong interactions. These interactions are due to quarks. Quarks exchange the particles named “gluons” that move with speed of light and are mass-less particles. Gluon contains color as well as anticolor.

- Quantum chromodynamics is an important aspect of particle physics, which explains the interaction among quarks.
- Mesons are colorless as it consists of quark with color and anticolor. Neutron has one u quark and two d quarks. Proton has two u quarks and one d quark.

$$(u)(d)(d) \rightarrow \text{neutron}$$

$$(\bar{u})(\bar{d})(\bar{d}) \rightarrow \text{antineutron}$$

$$(u)(u)(d) \rightarrow \text{proton}$$

$$(\bar{u})(\bar{u})(\bar{d}) \rightarrow \text{antiproton}$$

- Strange quark has $S = 1$ and antiquark has $S = +1$. All other quarks have $S = 0$.
- Charm quark has charm $C = +1$.
- The composition of some hadrons in terms of quarks is given in Table 8.3 :

Table 8.3 Composition of Hadrons

Hadron	Quark	Charge	Spin	B	S
η^0	udd	$-\frac{1}{3} - \frac{1}{3} + \frac{2}{3} = 0$	$\uparrow\downarrow\downarrow = \frac{1}{2}$	1	0
Ω^-	sss	$-\frac{1}{3} - \frac{1}{3} - \frac{1}{3} = -1$	$\uparrow\uparrow\uparrow = \frac{3}{2}$	1	-3
π^+	$u\bar{d}$	$\frac{2}{3} + \frac{1}{3} = 1$	$\uparrow\downarrow = 0$	0	0
K^+	$u\bar{s}$	$\frac{2}{3} + \frac{1}{3} = 1$	$\uparrow\downarrow = 0$	0	1
p^+	uud	$\frac{2}{3} + \frac{2}{3} - \frac{1}{3} = 1$	$\uparrow\uparrow\downarrow = \frac{1}{2}$	1	0

- The quarks can also be represented by column matrices (as proposed by Gell-Mann)

$$a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, b = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ and } c = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The quark a and b have isospin doublet ($I = \frac{1}{2}$) and c quark is singlet ($I = 0$).

Unitary matrix (U_{ij}) can be used to interchange the matrix.

$$q_i = \sum_{j=1}^3 U_{ij} q_j$$

Three properties of quarks are charm, color, and flavor. In 1964, Dr Glashow proposed the ‘‘charm’’ quark. For all the quarks, Pauli’s exclusion principle should be obeyed; but for nucleons, it is violated. That is why the proposal of different colors came into existence, when W. Greenberg proposed color of quarks. When we say a quark is ‘‘green,’’ it means that it has 1 green color unit and 0 red and blue color unit. Hence, individual quarks have colors, but the elementary particles are neutrals, for example, hadrons are composed of three quarks: red, green, and blue. Either all the colors are in the same amount, or the total amount of colors is zero. The quarks with their quantum properties are given in Table 8.4 :

Table 8.4 Quantum properties of quarks

Quark	Mass	Charge	Spin	Isospin	B	S	C^-	b	T
Up	$330 m_e$	$\frac{2}{3}e$	$\frac{\hbar}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{3}$	0	0	0
down	$330 m_e$	$-\frac{1}{3}e$	$\frac{\hbar}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{3}$	0	0	0
Strange	$500 m_e$	$-\frac{1}{3}e$	$\frac{\hbar}{2}$	0	0	$\frac{1}{3}$	-1	0	0
Charm	$1.6 \text{ GeV}/c^2$	$\frac{2}{3}e$	$\frac{\hbar}{2}$	0	0	$\frac{1}{3}$	0	1	0
Bottom	$4.9 \text{ GeV}/c^2$	$-\frac{1}{3}e$	$\frac{\hbar}{2}$	0	0	$\frac{1}{3}$	0	0	1
top	$20 \text{ GeV}/c^2$	$\frac{2}{3}e$	$\frac{\hbar}{2}$	0	0	$\frac{1}{3}$	0	0	1

SUMMARY

The chapter described the elementary particles as the entities that cannot be disintegrated into smaller subentities. The wavefunction for a particle is given by the spin and spatial part. For bosons, both the spin and spatial part are either symmetric or antisymmetric. For fermions, either the spin part or spatial part is antisymmetric. Bosons can be classified as massive particles and mass-less particles. Fermions are leptons and baryons. Baryons can further be classified as hyperons and nucleons. Leptons possess $\frac{\hbar}{2}$ spin angular momentum. The mass of hyperons is more than the nucleons. Lambda, sigma, omega, and cascade particles fall under the category of hyperons. On the basis of fundamental interactions, the particles can be classified under gravitational interactions: electromagnetic interactions, weak interactions, and strong interactions. On the basis of stability, the elementary particles can be classified as gravitons, photons, leptons, and hardons. It is explained that parity represents the mirror image or space reflection. For a composite system, parity is multiplicative in nature. According to tau-theta puzzle, the θ^+ and τ^+ are charge mesons with odd parity ending in states of different parities. Mass determination techniques for particles include μ -mesic methods: kinematic method and trajectory method. Intrinsic quantum numbers such as s, l, j, m_s, m_l , and m_j describe the particle completely. Other intrinsic quantum numbers include lepton number, baryon number, isospin, hypercharge, and strangeness. According to quark model, the matter consists of quarks. Quarks are supposed to carry fractional charge.

SOLVED PROBLEMS

Q. 1: What would be the energy that is required to annihilate proton and antiproton?

Ans: After annihilation, the reaction becomes

$$p + p^* \rightarrow 2m_p \cdot c^2$$

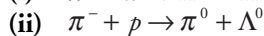
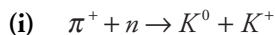
$$\text{Energy required} \approx 2m_p c^2$$

$$\approx 2 \times 931 \text{ MeV}$$

$$\approx 1.862 \text{ MeV}$$

$$\approx 1.862 \text{ BeV}$$

Q. 2: Obtain whether the following reactions are allowed or not:

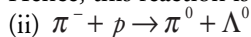


Ans: (i) $\pi^+ + n \rightarrow K^0 + K^+$

$$\pi^+ + n \rightarrow K^0 + K^+$$

Q	1	0	0	1	}	$\Delta Q = 0$
B	0	1	0	0		$\Delta B = 0$
S	0	0	1	1		$\Delta S \neq 1$

Hence, this reaction is forbidden.



$$\pi^- + p \rightarrow \pi^0 + \Lambda^0$$

Q	-1	1	0	0	}	$\Delta Q = 0$
B	0	1	1	0		$\Delta B = 0$
S	0	0	-1	1		$\Delta S = 0$

Hence, this reaction is allowed.

Q. 3: Is $p + p \rightarrow \Sigma^+ + K^+$ forbidden or allowed?

Ans: $p + p \rightarrow \Sigma^+ + K^+$

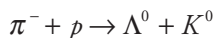
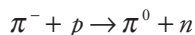
$$p + p \rightarrow \Sigma^+ + K^+$$

Q	1	1	1	1	}	$\Delta Q = 0$
B	1	1	1	0		$\Delta B \neq 0$
S	0	0	-1	1		$\Delta S = 0$

Hence, this reaction is forbidden and will not take place.

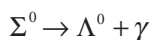
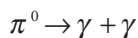
Q. 4: Given examples of two strong and two electromagnetic interactions.

Ans: The examples of strong interactions are the following:



These interactions involve the short-range forces and hadrons.

The examples of electromagnetic interactions are as follows:



These involve emission or absorption of photons.

Q. 5: Is $p \rightarrow e^+ + \gamma$ feasible or not?

Ans:

$$\begin{array}{cccc}
 & p & \rightarrow & e^+ + \gamma \\
 Q & 1 & 1 & 0 \\
 B & 1 & 0 & 0 \\
 L & 0 & -1 & 0
 \end{array}
 \left. \vphantom{\begin{array}{cccc} & p & \rightarrow & e^+ + \gamma \\ Q & 1 & 1 & 0 \\ B & 1 & 0 & 0 \\ L & 0 & -1 & 0 \end{array}} \right] \begin{array}{l} \Delta Q = 0 \\ \Delta B \neq 0 \\ \Delta L \neq 0 \end{array}$$

Hence, it is not feasible.

Q. 6: Is $\pi^- + p \rightarrow \Sigma^0 + \nu$ allowed or forbidden?

Ans:

$$\begin{array}{cccc}
 & \pi^- + p & \rightarrow & \Sigma^0 + \nu \\
 Q & -1 & 1 & 0 & 0 \\
 B & 0 & 1 & 1 & 0 \\
 S & 0 & 0 & -1 & 0 \\
 I_3 & -1/2 & 1/2 & 0 & 0
 \end{array}
 \left. \vphantom{\begin{array}{cccc} & \pi^- + p & \rightarrow & \Sigma^0 + \nu \\ Q & -1 & 1 & 0 & 0 \\ B & 0 & 1 & 1 & 0 \\ S & 0 & 0 & -1 & 0 \\ I_3 & -1/2 & 1/2 & 0 & 0 \end{array}} \right] \begin{array}{l} \Delta Q = 0 \\ \Delta B = 0 \\ \Delta S \neq 0 \\ \Delta I_3 = 0 \end{array}$$

Hence, the reaction is forbidden.

Q. 7: For the electromagnetic decay, $\pi^0 \rightarrow \gamma + \gamma$, how will I and I_3 behave?

Ans:

$$\begin{array}{cccc}
 & \pi^0 & \rightarrow & \gamma + \gamma \\
 I & 1 & 0 & 0 \\
 I_3 & 0 & 0 & 0
 \end{array}
 \left. \vphantom{\begin{array}{cccc} & \pi^0 & \rightarrow & \gamma + \gamma \\ I & 1 & 0 & 0 \\ I_3 & 0 & 0 & 0 \end{array}} \right] \begin{array}{l} \Delta I \neq 0 \\ \Delta I_3 = 0 \end{array}$$

Hence, the component I_3 is conserved but not the isotopic spin I .

Q. 8: Obtain whether strangeness and baryon number of the following decay is conserved or not.

$$p + p \rightarrow p + \Lambda^0 + \Sigma^+$$

Ans:

$$p + p \rightarrow p + \Lambda^0 + \Sigma^+$$

$$\begin{array}{cccc}
 B & 1 & 1 & 1 & 1 & 1 \\
 S & 0 & 0 & 0 & -1 & -1
 \end{array}
 \left. \vphantom{\begin{array}{cccc} B & 1 & 1 & 1 & 1 & 1 \\ S & 0 & 0 & 0 & -1 & -1 \end{array}} \right] \begin{array}{l} \Delta B = 0 \\ \Delta S \neq 0 \end{array}$$

Hence, neither Baryon number nor the strangeness is conserved in the above reaction.

Q. 9: Obtain whether isospin is conserved for the following decays:

(i) $p + p \rightarrow n + p + \pi^+$

(ii) $p + p \rightarrow n + \Lambda^0 + \Sigma^+$

Ans: (i) $p + p \rightarrow n + p + \pi^+$

$$I_3 \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} & 1 \end{bmatrix} \Delta I_3 = 0$$

Hence, the isospin is conserved.

(ii) $p + p \rightarrow p + \Lambda^0 + \Sigma^+$

$$I_3 \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 1 \end{bmatrix} \Delta I_3 \neq 0$$

Hence, isospin is not conserved.

Q. 10: What are weak interactions? Given examples.

Ans: Weak interactions involve leptonic decay of nonstrange and strange particles. Neither parity nor strangeness is conserved in them. Examples are the following:

$$K^0 \rightarrow \pi^+ + \pi^-$$

$$\Xi^- \rightarrow \Lambda^0 + \pi^-$$

$$\Lambda^0 \rightarrow p + \pi^-$$

OBJECTIVE QUESTIONS

1. The lifetime of elementary particles is greater than

(a) 10^{-30} sec

(b) 10^{-24} sec

(c) 10^{-18} sec

(d) 10^{-10} sec

2. Fermions have a spin of

(a) $\frac{1}{2} \hbar$

(b) $\frac{3}{4} \hbar$

(c) \hbar

(d) 0

3. Bosons have a spin of

(a) $\frac{1}{2} \hbar$

(b) $\frac{3}{4} \hbar$

(c) \hbar

(d) 0

4. Wavefunction for fermions is

(a) symmetric

(b) antisymmetric

(c) can be symmetric and antisymmetric

(d) all of the above

5. Wavefunction for bosons is
- (a) antisymmetric
 - (b) can be a symmetric and antisymmetric
 - (c) symmetric
 - (d) All of the above
6. Massive particles or mesons are
- (a) pion
 - (b) etaons
 - (c) kaons
 - (d) All of the above
7. Mass-less bosons are
- (a) graviton
 - (b) photon
 - (c) Both (a) and (b)
 - (d) None of these
8. Mass of neutral pion is
- (a) $264 m_e$
 - (b) $274 m_e$
 - (c) $290 m_e$
 - (d) $300 m_e$
9. The mean life of neutral pion is
- (a) 10^{-16} sec
 - (b) 3×10^{-15} sec
 - (c) 7×10^{-10} sec
 - (d) 7×10^{-17} sec
10. The mass of charged pions (π^- and π^+) is
- (a) $280 m_e$
 - (b) $273 m_e$
 - (c) $260 m_e$
 - (d) $300 m_e$
11. The mass of neutral and charged kaons is _____, respectively
- (a) $975 m_e, 967 m_e$
 - (b) $967 m_e, 975 m_e$
 - (c) $980 m_e, 990 m_e$
 - (d) $1000 m_e, 970 m_e$
12. $K^+ \rightarrow \pi^+ + \pi^0$ has an average lifetime of
- (a) 1.8×10^{-6} sec
 - (b) 2×10^{-7} sec
 - (c) 1.2×10^{-8} sec
 - (d) 1.5×10^{-6} sec
13. $\bar{K}^0 \rightarrow e^- + \pi^0 + \bar{\nu}$ has an average lifetime of
- (a) 10^{-8} sec
 - (b) 10^{-10} sec
 - (c) 10^{-14} sec
 - (d) 10^{-15} sec
14. Eta-mesons (η) have a mass of
- (a) $1000 m_e$
 - (b) $1200 m_e$
 - (c) $800 m_e$
 - (d) $1074 m_e$

15. Electrons and muons fall under
(a) baryons (b) nucleons
(c) hyperons (d) leptons
16. Muons have a mass of
(a) $210m_e$ (b) $207m_e$
(c) $250m_e$ (d) $267m_e$
17. Lambda and sigma particles are
(a) baryons (b) nucleons
(c) hyperons (d) leptons
18. Free neutron and bound proton are unstable. (Yes/No)
19. Free neutrons have a lifetime of
(a) 940 sec (b) 900 sec
(c) 933 sec (d) 1000 sec
20. The mass of lambda particle is
(a) $2180m_e$ (b) $2600m_e$
(c) $1000m_e$ (d) $270m_e$
21. The mass of cascade particles is
(a) $1000m_e$ (b) $1500m_e$
(c) $2083m_e$ (d) $2582m_e$
22. $\Xi^0 \rightarrow \Lambda^0 + \pi^0$ have a lifetime of
(a) 10^{-8} sec (b) 10^{-10} sec
(c) 10^{-15} sec (d) 10^{-18} sec
23. Neutral sigma particles (Σ^0) have a mass of
(a) $2320m_e$ (b) $2500m_e$
(c) $207m_e$ (d) $290m_e$
24. The decay reactions for Σ^+ are
(a) $\Sigma^+ \rightarrow p + \pi^0$ (b) $\Sigma^+ \rightarrow n + \pi^+$
(c) Both (a) and (b) (d) None of the above
25. The decay modes of neutral lambda are
(a) $\Lambda^0 \rightarrow p + \pi^-$ (b) $\Lambda^0 \rightarrow n + \pi^0$
(c) Both (a) and (b) (d) None of the above

26. Σ^+ and Σ^- are antiparticle of each other. (Yes/No)
27. The mass of Ω^+ is
 (a) $3200m_e$ (b) $3276m_e$
 (c) $207m_e$ (d) $100m_e$
28. The magnitude of gravitational interaction force is
 (a) 5.82×10^{-39} (b) 2×10^{-34}
 (c) 9×10^{-18} (d) 6.7×10^{-11}
29. The coupling constant is given by (g_e)
 (a) 137 (b) 150
 (c) $\frac{1}{150}$ (d) $\frac{1}{137}$
30. g_s is the pion–nucleon coupling constant of value
 (a) 10^{-4} (b) 8×10^{-2}
 (c) 10^{-7} (d) 3×10^{-4}
31. Parity is related to angular momentum as follows:
 (a) $(-1)^l$ (b) $(-2)^l$
 (c) $(-1)^{2l+i}$ (d) $(-2)^{2l+i}$
32. Kinematic techniques of mass determination uses
 (a) conservation of energy (b) conservation of momentum
 (c) both (a) and (b) (d) neither (a) nor (b)
33. $m_{\pi^+}c^2$ is obtained to be
 (a) 931 MeV (b) 530 MeV
 (c) 139.3 MeV (d) 253 MeV
34. For e^+ , μ^+ , and $\bar{\nu}_e$, the Lepton number is
 (a) 0 (b) -1
 (c) +1 (d) 2
35. $\gamma \rightarrow p + p^-$ has ΔL_i of
 (a) +1 (b) zero
 (c) -1 (d) 2
36. The proton can be written as
 (a) $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ (b) $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

(c) $\begin{pmatrix} \frac{1}{2} \\ 1 \end{pmatrix}$

(d) $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

37. The neutron can be written as

(a) $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

(b) $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

(c) $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

(d) $\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$

38. Hypercharge (Y) is related to isospin as

(a) $Y = Q - I_3$

(b) $Y = 2Q - I_3$

(c) $Y = 2(Q - I_3)$

(d) $Y = 2I_3$

39. Strange quark has a charge of

(a) $\frac{2}{3}e$

(b) $-\frac{1}{3}e$

(c) $\frac{3}{5}e$

(d) $\frac{1}{2}e$

40. The hadron p^+ has a quark combination of

(a) uud

(b) udd

(c) sss

(d) $u\bar{d}$

ANSWERS

- | | | | |
|---------|---------|---------|---------|
| 1. (b) | 11. (a) | 21. (d) | 31. (a) |
| 2. (a) | 12. (c) | 22. (b) | 32. (c) |
| 3. (c) | 13. (b) | 23. (a) | 33. (c) |
| 4. (b) | 14. (d) | 24. (c) | 34. (b) |
| 5. (c) | 15. (d) | 25. (c) | 35. (b) |
| 6. (d) | 16. (b) | 26. Yes | 36. (d) |
| 7. (c) | 17. (c) | 27. (b) | 37. (a) |
| 8. (a) | 18. Yes | 28. (a) | 38. (c) |
| 9. (d) | 19. (c) | 29. (d) | 39. (b) |
| 10. (b) | 20. (a) | 30. (b) | 40. (a) |

Microassessment Questions

1. What are mesons?
2. Why are mesons known as middle-weight particles?
3. What are elementary particles?
4. Give the basic classification for elementary particles.
5. What are fermions?
6. How do fermions differ from bosons?
7. What do you understand by symmetric and antisymmetric wavefunctions?
8. Explain the spin and spatial part of wavefunction.
9. What are mass-less particles? Give examples.
10. What are kaons?
11. Give the decay mode for neutral kaons.
12. Which is the heaviest particle among all the bosons?
13. What are neutrinos and antineutrinos?
14. Explain (a) leptons (b) baryons.
15. Why are muons unstable particles?
16. What are nucleons?
17. Give the four types of hyperons.
18. Define lambda particles.
19. What is the decay mode followed for neutral lambda particle?
20. Define the quanta for electromagnetic interaction.
21. Give the value of pion–nucleon coupling constant.
22. Write down the relation of weak interaction constant and its value.
23. What are strange particles?
24. What are quarks? Write the quark combination for proton.
25. What are gluons and chromodynamics?

Critical Thinking Questions

1. What are gravitons? How do they differ from photons?
2. Give the classification of mesons/massive particles.
3. What are π -mesons? Give the decay modes given for positive and negative π -mesons.
4. Write down the decay modes for charged kaons.
5. What is the decay lifetime for eta-mesons? Also write down the decay modes.
6. How do sigma and omega particles differ from each other?
7. Write down two main classifications for fermions.
8. Write down the general characteristics of leptons.
9. Write down the decay modes for muons.
10. Give the decay modes for proton inside and outside the nuclei.
11. Write down the decay mode for neutron inside and outside the nuclei.
12. What are cascade particles? How do they decay into neutral lambda and mesons particles?
13. Write down the characteristics for positive and negative sigma particles.
14. What are lifetimes for lambda and cascade particles?

15. Show the decay mode for omega hyperon along with its lifetime.
16. What is the difference between gravitational interaction and electromagnetic interaction?
17. What are weak interactions? Write down their characteristics.
18. Which type of interactions exist within the nucleus? Justify that they are the strongest interactions.
19. How do force and range vary for all forces of nature?
20. Explain the parity and angular momentum for elementary particles.
21. How is the parity conserved for elementary particles?
22. What is tau-theta puzzle?
23. How can kinematic methods be used to measure the mass of particles?
24. What are intrinsic quantum numbers?
25. What is a lepton number? Write down the rules for lepton numbers.
26. What are baryon numbers? Give the rules followed by them.
27. Explain hypercharge and strangeness of particles.
28. Explain the Gell-Mann Nishijima concept of strangeness.
29. Write down three properties of quarks. Are quarks colored?

Graded Questions

1. Explain in detail the classification and subclassification of fermions.
2. Classify the elementary particles on the basis of interactions.
3. Classify the elementary particles on the basis of stability.
4. How can mass be determined for elementary particles? Explain all of the methods in detail.
5. Explain the trajectory method to determine the mass of particles.
6. Why is the concept of isospin necessary? Give the spin and isospin of all the nucleons and kaons.
7. List and explain all the conservation principles that should hold good during decay processes.
8. Explain in detail the quark model and its postulates.

Remember and Understand

1. Most of the particle is unknown before 1930, and cosmic rays were known to be the source of elementary particles.
2. Gravitons and photons are mass-less boson particles with integral spin.
3. Elementary particles are the smallest entities that cannot be further disintegrated into smaller subentities.
4. For bosons, both the spatial and spin particles are symmetric or antisymmetric. For fermions, either of them is symmetric or antisymmetric.
5. Kaons are heavy mesons with mass almost equal to 970 times the mass of electron.
6. Eta-mesons are the heaviest of all the bosons, that is, 1,074 times the mass of electrons.
7. Muons are heavy electrons with mass 207 times than that of electrons.
8. The mass of hyperons is more than the nucleons.
9. Nuclear interactions are the strongest interactions, whereas gravitational interactions possess highest range.
10. Parity gives the mirror image or reflection of wavefunction. For a composite system, parity is multiplicative in nature.

11. Kinematic, trajectory, and mesic methods are used to determine the mass of elementary particles.
12. Isospin vector is not in the ordinary state; it is in isospin space. Proton and neutron can be differentiated on the basis of up and down state of spinor.
13. Hypercharge defines twice the average charge on the members of group.
14. The strange particles are always produced in pair via strong interactions and then decay via weak particles.
15. The total energy, charge, angular/linear momentum, lepton number, baryon number, isospin, and hypercharge are conserved during decay processes.
16. Quarks are supposed to carry fractional charges such as $\pm(2/3) e$ and $\pm(1/3) e$.

Particle Accelerators

Keywords: Van de Graaff generator, cyclotron, betatron, synchrotron, electron synchrotron, synchrocyclotron, LINAC, radio-frequency oscillator, dees, betatron condition

Learning Objectives

- ◆ To learn about the need of particle accelerators
- ◆ To understand the potential and circular orbit of accelerators
- ◆ To know about positive-charge accelerators such that Van de Graaff generator and cyclotron
- ◆ To know about the Cockcroft–Walton machine as voltage multiplier
- ◆ To understand the principle, construction, and working of betatron as an electron accelerator
- ◆ To get an insight of focused magnetic field, Lorentz magnetic field, and Lorentz force while dealing with the accelerators
- ◆ To understand the principle, construction, and working of electron synchrotron
- ◆ To learn the principle, construction, and working of proton synchrotron
- ◆ To understand the construction and working principle of linear accelerators (LINACS)
- ◆ To know about the construction, working, and principle of synchrocyclotron
- ◆ To understand the principle, construction, and working of linear accelerators

In previous chapters, we have studied about the phenomena of radioactivity. In the process of radioactivity, α , β , and γ -rays are emitted. These radioactive particles can be further used to disintegrate other atomic nuclei. For this purpose, the elementary particles need to be accelerated to suitable energies. The particles are accelerated by suitable devices known as particle accelerators. Particle accelerators are specially designed machines that are used to accelerate the elementary particles to desired energy range. Both heavier and lighter nuclei can be used to accelerate the particles. Protons, neutrons, deuterons, electrons, etc., are accelerated using particle accelerators. In addition to these particles carbon, neon, oxygen, and beryllium, etc., are also accelerated. For high-energy particle physics, particle accelerators play an imperative role. This chapter deals with basic particle accelerators and their working principles. There are some requirements that should be satisfied for every particle accelerator. Every accelerator requires a suitable source of particles. The source of particle should have negligible energy spread, high efficiency and exhibit rich output (well collimated). Usually, the particles sources include spark discharge sources, electron oscillation sources, hot and cold cathode sources, and magnetic ion sources.

Once these ions are obtained, then they should be introduced to the defined accelerator using proper accelerating voltage. Once the particle enters the accelerator, then it is under electric/magnetic field and traverses an orbit of radius r and velocity v . The particles are accelerated up to the desired energy. Subsequently, when the desired energy level for the particle is obtained, then the particles are extracted out of the accelerator. The accelerators can work on continuous or pulsed fields. The accelerators should have energy stability and coherence along with good beam intensity. The accelerator should exhibit good particle collimation. In some of the accelerators, the particles are accelerated using constant potential difference. Such accelerators fall under the category of electrostatic accelerators, for example, Van de Graaff generator and Cockcroft–Walton machine. The electrostatic accelerators can give an output of particles with 4–6 MeV energy. When particles form closed-path again and again, then they get accelerated. The accelerators that work on closed-path orbits and yield high energy particles are known as cyclic accelerators, for example, cyclotron, betatron, and synchrotron.

9.1 Van De Graaff Generator

Van de Graaff developed an electrostatic accelerator in 1881, which could accelerate particles up to energy 10 MeV.

1. Principle

- (i) It is based on the principle that sharp pointed surfaces have large charge densities, that is,

$$\sigma = \frac{q}{4\pi r^2}$$

For sharp points, $r \rightarrow 0$, and hence theoretically the charge density $\rightarrow \infty$.

- (ii) If small conducting charged shell of radius r_1 , is located inside a charged and conducting shell of radius r_2 , then the charge q_1 will move from shell A to shell B if both the shells are connected to each other (with key K) (Figure 9.1). Hence, the charge tends to move to outer the surface of spherical shell and does not reside inside the conductor. This leads to increase of the potential of outer surface.

In actual practice the maximum potential on the outer shell does not go infinite because their is electric breakdown of air which surrounds the shell.

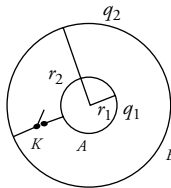


Figure 9.1 Demonstration of charge on hollow conductor.

2. Construction

Two combs C_1 and C_2 are provided with sharp point ends (Figure 9.2). C_1 is maintained at 5–20 kV w.r.t. ground. S is large hollow sphere that is mounted on two pillars D_1 and D_2 . There are two frictionless pulleys P_1 and P_2 over which a well-insulated belt (B) passes over. C_1 is spray comb and C_2 is collector comb. There is discharge tube I which contains positive ions to be accelerated so that they can hit the target (T). The discharge tube is made up of porcelain glass.

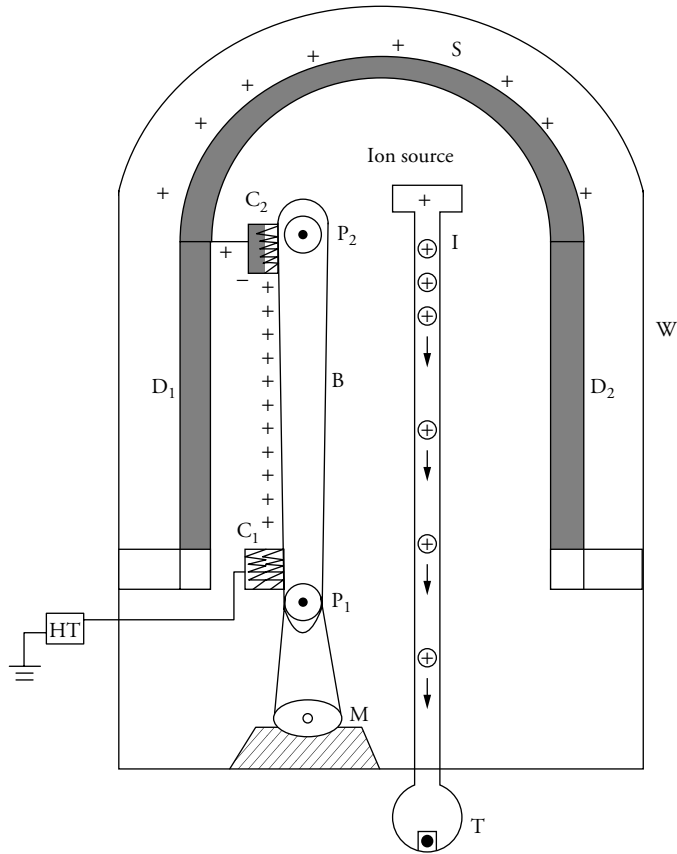


Figure 9.2 Schematic sketch of Van de Graaff generator.

The discharge tube is highly evacuated in order to avoid any discharge inside the tube. The whole apparatus is inside gas tight steel chamber W . Their could be methane, freon (CCl_2F_2), air, or nitrogen inside the chamber.

3. Working

Electric motor M makes a well-insulated belt B rotate over two pulleys P_1 and P_2 . Metallic comb C_1 (Spray comb) is charged to high positive potential. Due to corona discharge action on its sharp points, the spray comb C_1 gives its positive charge to belt. The moving belt carries the charge to collector comb C_2 . Due to induction, “-ve” charge appears on the pointed ends of the comb and in turn “+ve” charge builds up at the base of the C_2 comb. This charge gets transferred to the outer shell S . As the belt moves continuously, hence the charge on outer shell gets accumulated, which is turn raises the potential of outer shell as follows:

If q is charge accumulated over a spherical shell of radius “ r ”, then potential (V) is

$$V = \frac{q}{4\pi\epsilon_0 r}$$

While the charge continues to increase on the spherical shell, the ionization leakage also increases. Hence, the leakage is prevented by steel tank W . The charged particles inside the discharge tube T are at high potential. They get accelerated downward and hit the target after coming out of discharge tube.

Mathematical analysis can be given as follows:

Capacity C for spherical shell = $4\pi\epsilon_0 r$ if r is the radius of spherical shell.

Hence, potential

$$V = \frac{q}{C} \quad (1)$$

Rate at which potential is build up on the shell is given by the following equation:

$$\frac{dV}{dt} = \frac{1}{C} \frac{dq}{dt} = \frac{i}{C} \quad (2)$$

i is charging current that is usually composed of many components as follows:

$$i = i_p + i_1 + i_s + i_c \quad (3)$$

i_p = current due to positive ion source

i_1 = leakage current along the discharge tube

i_s = is the current due to stray/secondary electrons that strike the wall

i_c = current due to breakdown condition as a result of excess potential at surfaces. It is also known as corona current.

If the “S” is made negative, then electrons can also be accelerated. These days, particles up to “20 MeV” energy can be produced using Van de Graaff generator.

Robert Jemison Van de Graaff earned his Bachelor of Science and Master of Science in 1922 and 1923, respectively, from the University of Alabama. Van-de Graaff was awarded PhD in 1928 from Queen's College, Oxford where he was a Rhodes fellow. It was Oxford where he first conceived the idea of high-voltage generator. He was influenced by Rutherford's challenge to produce highly accelerated particles for nuclear disintegrations. He returned to United States in 1929, where he constructed the first working model of the generator while working as a National Research Fellow at Princeton University under the supervision of Karl Taylor Compton. Compton also worked on electrostatic generator as designed by Lord Kelvin. But this electrostatic generator dripped charged water; hence, he thought of exceeding electric field in order to overcome the gravity. He worked as a research associate at the Massachusetts Institute of Technology,



VAN DE GRAAFF (LEFT SIDE)

where he continued his work on accelerating the charged particles. During World War II, he was appointed as the Director of MIT's high-voltage radiographic project. He was the chief of physics of High Voltage Engineering Corporation after the war.

The sphere of Van de Graaff generator holds considerable amount of charge before arc discharge occurs. When we touch the Van de Graaff generator, it releases charge into our body. As the hairs get similar charge, they are repelled from each other.



9.2 The Cyclotron

Cyclotron is a device used to accelerate positively charged particles such as ${}^2\text{He}^4$, protons, and deuterons. These charged particles are further used for the purpose of nuclear disintegrations. Cyclotron was discovered by E.O. Lawrence and M.S. Livingstone in 1934.

1. Principle

It is based on the principle of crossfields, that is, electric and magnetic field should be perpendicular to each other. When a positively charged particle is moved again and again in high-frequency electric field and perpendicular magnetic field, then the particles are accelerated to the desired energy level.

2. Construction

It consists of two hollow metallic chambers D_1 and D_2 which are D-shaped and known as dees as shown in Fig. 9.3. These two dees are separated by small gap between which a positive charge is placed. These dees are connected to high-frequency oscillator that is of magnitude 10^7 Hz. This HF oscillator provides high electric field along the gap of dees. The dees D_1 and D_2 are enclosed inside a box chamber, which is almost at 10^{-3} mm of mercury pressure. These dees are inside the poles of strong electromagnet, which provide perpendicular magnetic field of almost 1.5 T.

3. Working

If dee D_1 is at positive potential and a positive particle is present inside the gap of dees, then the particle will get accelerated toward the “-ve” potential dee D_2 . Inside the hollow dee D_2 , there is no

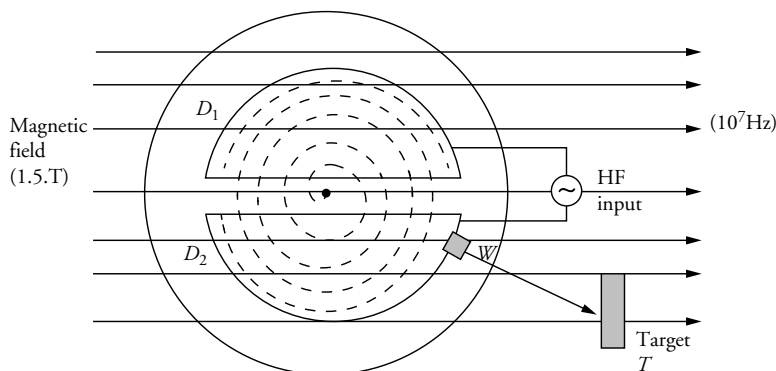


Figure 9.3 Schematic of cyclotron.

electric field. Only magnetic field will act on the particles that are inside dee D_2 . This magnetic field provides necessary centripetal force for a particle to move in circular path, which is given as follows:

Let m be the mass of particle to be accelerated, B is the magnetic field, v is the velocity of particle, q is the charge of particle, and r is the radius of semicircular path traversed by particle.

The Lorentz force acting on particle, when the magnetic field is perpendicular to its motion is given by the following equation:

$$\begin{aligned}\vec{F} &= q(\vec{v} \times \vec{B}) \\ F &= q v B \sin \theta \\ F &= q v B\end{aligned}\quad (4)$$

This force (Eqn. (4)) provides the centripetal force, hence

$$\begin{aligned}q v B &= \frac{mv^2}{r} \\ r &= \frac{mv}{qB}\end{aligned}\quad (5)$$

The particle will traverse a semicircular path of radius r inside dee D_2 and will eventually return to the gap between the dees at the time when polarities of dees are reversed; that is, now the dee D_1 is at negative potential and dee D_2 is at positive potential. The time required by particle to complete one semicircle is given by the following equation:

$$\begin{aligned}t &= \frac{1}{2} \frac{2\pi r}{v} = \frac{\pi r}{v} \\ t &= \frac{\pi r}{v} \\ t &= \frac{\pi}{v} \left(\frac{mv}{qB} \right) = \frac{m\pi}{qB}\end{aligned}\quad (6)$$

Now the particle will enter dee D_1 and again a semicircle is traversed. As can be noted from Eqn. (6), the time taken to reach in between the dees is independent of the radius. Hence, the particle reaches in between the gap after sometime. This process is repeated till the particle reaches the periphery of the dee. Then the particle is deflected by a plate, and it comes out through a window to hit the target. The cyclotron frequency is given by following expression:

Let T be the time period taken by charged particle, hence

$$T = 2t = \frac{2\pi m}{Bq}\quad (7)$$

Hence, the frequency of revolution is given by the following equation:

[also known as magnetic resonance frequency]

$$f = \frac{1}{T} = \frac{Bq}{2\pi m}\quad (8)$$

Equation (8) gives the cyclotron frequency. The angular frequency for cyclotron is given by the following equation:

$$\omega = 2\pi f = \frac{Bq}{m} \quad (9)$$

Similarly, the maximum energy gained by the particles is given by the following equation:

$$\begin{aligned} E &= \frac{1}{2}mv^2 \\ E &= \frac{1}{2}m\left(\frac{qBr}{m}\right)^2 \quad [\text{from Eqn. (5)}] \\ E &= \frac{q^2 B^2 r^2}{2m} \quad (10) \end{aligned}$$

The maximum energy is gained by the particle, when it reaches the periphery of dees, and it is given by the following equation:

$$E_{\max} = \left(\frac{q^2 B^2}{2m}\right) r_{\max}^2 \quad (11)$$

Cyclotron can accelerate the particles through electric field only and not by magnetic field. Magnetic field only deflects the semicircular path for the particles inside the dees. Cyclotron cannot handle/accelerate negative as well as neutral particles. Electrons cannot be accelerated on account of their smaller masses. Due to small mass of electrons, they attain very large energy in small intervals of time, and hence go out of step very quickly. Ions cannot have large velocities comparable to velocity of light inside the cyclotron, because as per following relativistic relation,

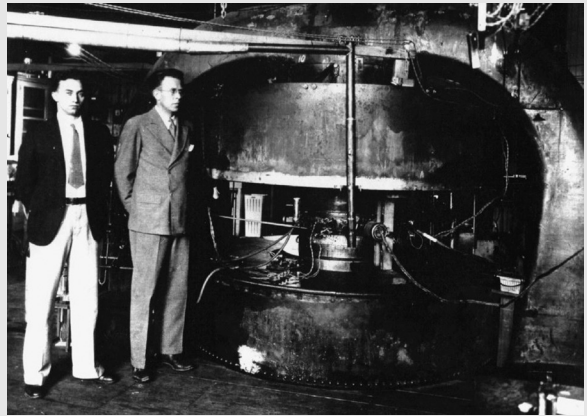
$$m = \frac{m_0}{\sqrt{1 - v^2/c^2}} \quad [m_0 \text{ is rest mass}] \quad (12)$$

Hence, when $v \approx c$, then the particle is of infinite mass. Hence ω becomes

$$\omega = \frac{Bq}{m_0} \left[1 - \frac{v^2}{c^2}\right]^{1/2} \quad (13)$$

Hence, when v increases, then ω decreases and ion will spend more time to traverse the semicircular path inside the dee. This will lead to late arrival of particle inside the gap and hence cannot be accelerated due to time lag. This is also known as “lack of resonance.” Hence, the factor $B\left(1 - \frac{v^2}{c^2}\right)^{1/2}$ should be kept constant. Hence, the magnetic field should be increased such that the product remains unchanged.

The cyclotron is very strong particle accelerator, which was first devised by Ernest Orlando Lawrence. Lawrence was born in South Dakota on August 8, 1901. In 1925, he completed his PhD from Yale. He joined the University of California at Berkeley in 1928, where he served for his whole life. He was awarded the Nobel Prize in 1939 for his invention of cyclotron. He worked with Milton Stanley Livingston at the University of California at Berkeley to build cyclotrons. Milton Stanley Livingston was born in Wisconsin, on May 25, 1905. He chose the PhD topic as suggested by Lawrence when he came to Berkeley in 1930. Livingston's worked on the experimental verification of whether applied voltage could lead to large final energy of moving ions for his thesis. Livingston worked much on the hardware.



**E.O. LAWRENCE (LEFT) &
M.S. LIVINGSTONE (RIGHT)**

At the age of 57, Lawrence died on August 27, 1958, and Livingstone died in 1986. The Radiation Laboratory was officially renamed as the Lawrence Radiation Laboratory in Lawrence's honor.

9.3 The Cockcroft–Walton Machine

The Cockcroft–Walton machine is used as voltage multiplier circuit to get high potential difference.

Principle

According to the principle of Cockcroft–Walton machine, it states that a number of capacitors connected in parallel are charged and then discharged in series when the voltage across them is equal to the sum of voltages on every individual capacitor.

Construction:

Number of capacitors $C_1 \cdots C_n$, having equal capacitance are joined together with rectifiers $R_1 \cdots R_n$. With the help of rectifiers, the current can pass only in one direction (Figure 9.4). A step-up transformer T is used. With the help of step-up transformer, an output voltage of up to 100 keV can be obtained. X is earthed in order to keep the potential at a fixed value. Transformer helps in charging the parallel plate capacitors and then discharged in series. This discharge voltage is further used to accelerate the particles.

Working:

Alternating current is applied across the primary coil of transformer. During the “-ve” half cycle, A becomes negative and w.r.t. point X and the rectifier R , gets forward biased and capacitor C_2 is charged to potential V_{in} . There still exists potential difference between point X and A . The potential difference between X and A is $+V_{in}$ after the capacitor is charged. Before charging of capacitor, the potential difference was $-V_{in}$. During the “+ve” half cycle, A becomes positive and hence R_1 gets reverse biased due to which the rectifier do not conduct. Therefore, during “-ve” half cycle, the potential difference between A and C becomes “0” and during “+ve” half cycle, the potential difference between A and C is $2V_{in}$. When R_2 is conducting then C_1 is charged. These cycles are repeated until the capacitors are charged, and hence the potential difference along the capacitor becomes $2V_{in}$. Hence, potential

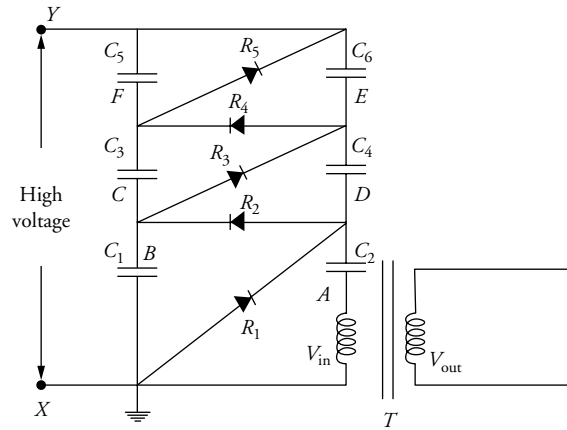


Figure 9.4 Schematic of Cockcroft–Walton machine.

difference between X and F becomes $4V_{in}$. If two rectifiers and two capacitors are joined, then this arrangement is known as voltage doubler. This arrangement is also known as cascade multiplier as “voltage” is multiplied in the arrangement.

If n capacitors are connected via n rectifiers with V_{in} as input voltage, then the output is given as follows:

$$V_{out} = nV_{in} - \frac{1}{12fC} \left[n^3 + \frac{9}{4}n^2 + \frac{n}{2} \right] \tag{14}$$

$f \rightarrow$ frequency of transformer

$C \rightarrow$ capacitance of every capacitor

The ripple voltage is

$$\pm V_{out} = \frac{In(n+2)}{16f \cdot C} \tag{15}$$

$I \rightarrow$ current

C cannot be kept very large. But if we increase the frequency of source, then the ripple voltage increases. High voltage is obtained between X and Y , which is used to accelerate the charged particles. Using this device, particles cannot be accelerated above 5 MeV energy. The capacitors used should be able to withstand high tension. There are many chances of insulation breakdown for this device.

9.4 Betatron

Till now, we have focused on accelerating the “+ve” charged particles. But for producing high energy X-rays and triggering reactions, we require beam of high energy electrons. Betatron is basically used to “accelerate” negative charged particles. The cyclotron had a problem named “out of resonance,” but this has been overcome in betatron. Hence, betatron does not imply any variation in mass with velocity.

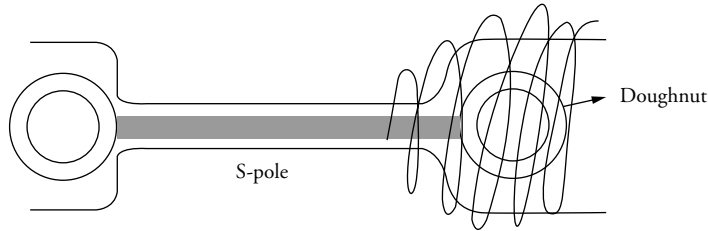


Figure 9.5 (a) Pole pieces for the betatron (doughnut shaped).

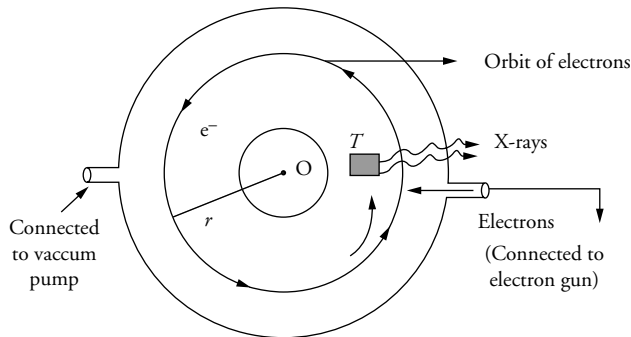


Figure 9.5 (b) Schematic of betatron chamber.

1. Principle

Betatron works on the principle of electromagnetic induction. According to it, an alternating current in the primary coil of a transformer induces a similar current in secondary coil. The primary current produces a magnetic field which induces “potential” in the secondary windings. We can consider the secondary coil of transformer to be moving cloud of electrons in circular orbit due to magnetic field in doughnut-shaped chamber.

2. Construction

A betatron consists of electromagnet pole pieces. This electromagnet works of high voltage A.C. input. The doughnut chambers are arranged in the pole pieces as shown in Figure 9.5(a). The electromagnet produces strong magnetic field at the center of doughnut vacuum chamber (around O in Figure 9.5(b)).

The electron revolves in circular orbit in the doughnut-shaped vacuum chamber. The magnetic flux ϕ associated with orbit changes continuously changes with time. Hence, electrons gain energy by the process of magnetic induction. In cyclotron, the magnetic field always increases the radius of orbiting particle. But in betatron, the transverse magnetic field makes the electrons move in constant orbit. The magnetic field provides the necessary centripetal force, so that electrons move in circular orbit. The magnetic lines of force should be convex outwardly for proper magnetic focusing.

The doughnut chamber is also coated with a silver layer from inside. There should be no accumulation of electrons. Moreover, the generation of eddy currents should be minimized by keeping

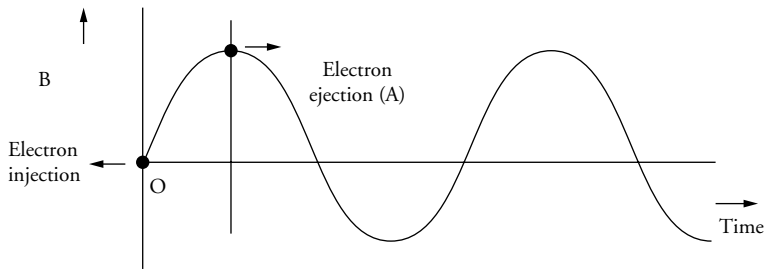


Figure 9.6 The alternating cycle of magnetic field demonstrating the injection and ejection of electrons.

the conductivity of layer to be very small. The eddy currents hinder the operating condition of betatron as they tend to distort the magnetic condition.

3. Working

An electron gun is used to inject the electrons into vacuum chamber. The electron gun consists of a heating filament as electron emitter. The injection of electrons is done when the magnetic field is rising during the first quarter of the alternating cycle as shown in Figure 9.6.

The electrons get accelerated during the rising magnetic field due to increasing potential within the doughnut. Even after increasing kinetic energy of electrons, the electrons orbit in the same orbit of radius r . Then the magnetic field starts decreasing after passing through a maximum. Then the electrons start decelerating as the direction of e.m.f. starts getting reversed. To avoid this effect, the electrons are removed at peak magnitude of magnetic field (point A). These ejected high energy electrons can strike target T to produce X-rays that emerge out of the apparatus. To remove electrons from the orbit, a current of large amplitude is sent through auxiliary coil that abruptly changes the magnetic field. The theory behind the working of betatron can be demonstrated using Faraday's law. According to Faraday's law of electromagnetic induction, the induced e.m.f. due to changing current/magnetic flux linked with a coil is given by the following equation:

$$E = \frac{d\phi_B}{dt} \quad (16)$$

ϕ_B is the magnetic flux which is perpendicular to the plane of circuit

During one revolution, the work done on an electron is given by the following equation:

$$W = q \frac{d\phi_B}{dt} \quad (17)$$

Where q is the charge of electron, the force acting on an electron during one revolution is given by the following equation:

$$F = \frac{\text{Work done}}{\text{Distance travelled during one revolution}}$$

$$F = \frac{q \frac{d\phi_B}{dt}}{2\pi r} \quad (18)$$

We also know that when magnetic field is acting on the charged particle, then it gives rise to Lorentz force:

$$\vec{F} = q(\vec{v} \times \vec{B})$$

$$F = qvB \sin \theta$$

Here, the magnetic field is perpendicular to the velocity of electrons, hence

$$F = qvB \quad (19)$$

This Lorentz force provides the required centripetal force as follows:

$$\begin{aligned} Bqv &= \frac{mv^2}{r} \\ mv &= Bqr \\ p &= Bqr \end{aligned} \quad (20)$$

According to Newton's second law of motion, the rate of change of momentum is given by the following equation:

$$\begin{aligned} F &= \frac{dp}{dt} = \frac{d}{dt}(Bqr) \\ F &= qr \frac{dB}{dt} \end{aligned} \quad (21)$$

From Eqs (18) and (21),

$$\begin{aligned} qr \frac{dB}{dt} &= \frac{q \frac{d\phi_B}{dt}}{2\pi r} \\ \frac{d\phi_B}{dt} &= 2\pi r^2 \frac{dB}{dt} \\ \frac{d\phi_B}{dt} &= 2 \frac{d}{dt}(\pi r^2 B) \end{aligned} \quad (22)$$

Equation (22) is known as flux condition. This condition states that the flux ϕ_B linked with a coil must change at a rate twice the rate if the magnetic field is uniform throughout the orbit in given time interval. This relation holds good in the relativistic and nonrelativistic regime.

From Eqn. (22), we can write

$$2 \cdot \frac{d}{dt}(\pi R^2 \cdot B) = \frac{d}{dt}(\pi R^2 \cdot B_0) \quad (23)$$

Hence,

$$B_0 = 2B \quad (24)$$

Equation (24) is known as betatron condition. Hence, the magnetic field must be shaped such that the average magnetic field (B_0) over the total space enclosed by orbit is equal to twice the magnetic field at orbit. The betatron performance is also limited by some factors. For example, the acceleration of particles becomes very difficult after achieving the relativistic speeds. Secondly, electrons are negatively charged. After their acceleration, the electrons always radiate energy in the form of electromagnetic waves.

The kinetic energy of electrons is also fixed when the energy lost by electrons in the form of electromagnetic radiations becomes equal to energy gained by electrons during their acceleration, then there is no further rise in the kinetic energy of electrons. The betatron usually requires a source of 60 Hz. Betatron has very bulky electromagnet. In the United States, General Electric labs have produced 100 MeV electrons magnet approximately 130 tons and the maximum magnetic field ≈ 0.4 T. This betatron was used during World War II as an intense source of penetrating X-rays.

D.W. Kerst was born on November 1, 1912. Kerst made very important contributions to the field of nuclear physics specially particle accelerators. He worked on betatron, which is the milestone for high energy particle physics. He was a very strong, hard-working and dedicated mentor as he supervised 33 students for their PhD degrees in the betatron group at the University of Illinois. In addition to this, he supervised 42 students for their doctorates in the plasma group at the University of Wisconsin within 17 years. He published the pioneer work based on the first theoretical analysis of betatron oscillations with Robert Serber in 1941. He died on August 19, 1993, at the age of 81 and the community lost one of its most influential physicists.



D.W. KERST

9.5 Electron Synchrotron

Betatron has very bulky electromagnet, which also increases its costs. Hence, source of radio-frequency was used along with ring-shaped magnet. Hence, synchrotron uses the increasing magnetic induction B for an orbit of constant radius. The radio-frequency is synchronized with the electron frequency.

1. Construction

Like betatron, synchrotron also uses doughnut-shaped vacuum chamber in A.C. magnetic field. The weight of the magnet is considerably reduced in synchrotron. Figure 9.7(a) shows the vacuum chamber inside C-shaped magnet. Like other accelerators, the magnetic focusing is required, that is, the pole faces are constructed to provide maximum field at center.

The vacuum chamber is coated with silver from inside to avoid any hindrance in the operation of synchrotron due to eddy current (a gap is kept within the coating) (Figure 9.7(b)). Across, this gap

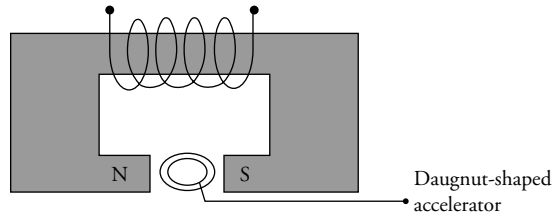


Figure 9.7 (a) The ring magnet.

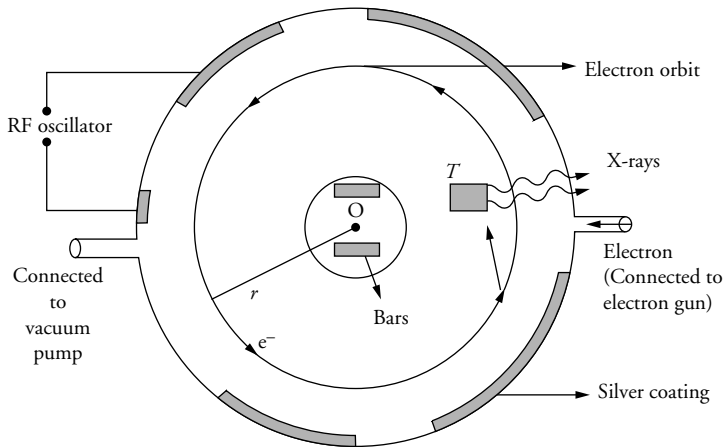


Figure 9.7 (b) The electron synchrotron.

radio-frequency oscillator is used during a proper time. When radio-frequency is applied across the gaps, then the electrons get accelerated every time it crosses the gap (also known as resonance cavity). There are steel bars inside the doughnut, which gets supersaturated easily. These are provided so that the variation of magnetic field takes place only for electron orbit. These bars are of high permeability.

2. Working

With the help of electron gun, electrons are injected into the vacuum chamber with energy range of up to 100 keV. After the electrons are accelerated to high energy, then the electrons may attain velocity comparable to that of light. The bars play a very important role. Once the steel bars get saturated, they no longer obey Faraday's law of electromagnetic induction. Hence, no induced e.m.f. is produced. Hence, it will no longer works as betatron. Now, the chamber works in "synchrotron mechanism." As the electron gains relativistic speed, the mass of electron becomes relativistic and magnetic field also increases. With proper adjustment of frequency at which resonator operates, all the electrons can be kept in phase. The electrons gain energy after every revolution. The magnetic field and orbit radius decide the energy of electrons. After the electrons gain maximum energy, radio-frequency oscillator is turned off and larger current is sent through auxiliary coils so that the electrons change their orbit radius due to unstable magnetic flux. These electrons then strike the target from the inner edge of doughnut chamber. The target releases highly energetic X-rays, when electrons strike the target. The electrons can attain energy up to 330 MeV by synchrotron action and 7–8 MeV by betatron action. The limit of energy can further be increased if the synchrotron is divided into race-type chamber tracks.

The energy of electron with rest mass m_0 is given by the following equation:

$$E = \sqrt{p^2 c^2 + m_0^2 c^4} \quad (25)$$

$$m_0 c^2 \approx 0.51 \text{ MeV}$$

As momentum

$$p = \frac{E}{c}$$

also $p = qBr$ (Eqn. 20),

$$\begin{aligned} qBr &= \frac{E}{c} \\ E &= qBrc \end{aligned} \quad (26)$$

Hence, if we increase the magnetic field, then the energy also increases. We can also obtain the frequency of revolution (when the electron is at relativistic speeds):

$$\begin{aligned} f &= \frac{1}{T} = \frac{1}{2\pi r/c} \\ f &= \frac{c}{2\pi r} \end{aligned} \quad (27)$$

Cyclotron and betatron usually are low energy accelerating machines, whereas synchrotrons are high energy machines. MIT (USA) has a synchrotron with 50 ton magnet, which can accelerate electrons up to 330 MeV. If certain radiation losses occur, then the kinetic energy may drop as per Schwinger's formula (1949):

$$E_{\text{rad}} = \frac{q^2}{3\epsilon_0 r} \left[\frac{m}{m_0} \right]^4 \quad (28)$$

9.6 Proton Synchrotron

With the help of cyclotron, protons can be accelerated up to 10 MeV of energy. But in order to accelerate the particles beyond this value, the proton synchrotron was invented. Proton synchrotron can be used to accelerate deuterons, alpha particles in addition to protons. Using proton-synchrotron, protons can be accelerated up to 10 GeV energy.

1. Construction

The doughnut vacuum chamber for synchrotron is made up of steel (Figure 9.8a). There are four quadrants that produce magnetic field perpendicular to vacuum chamber. The magnetic field increases with time, but the radius of “+ve” charged particle is maintained constant. The doughnut chamber is kept inside the ring as shown in Figure 9.8(b).

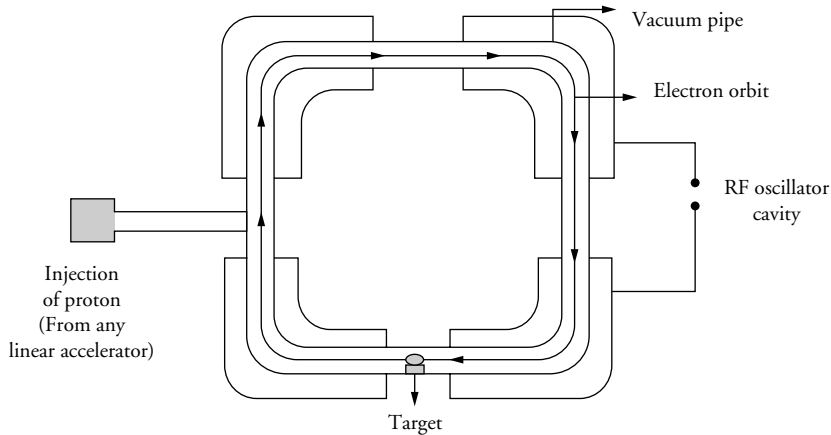


Figure 9.8 (a) Schematic of proton synchrotron.

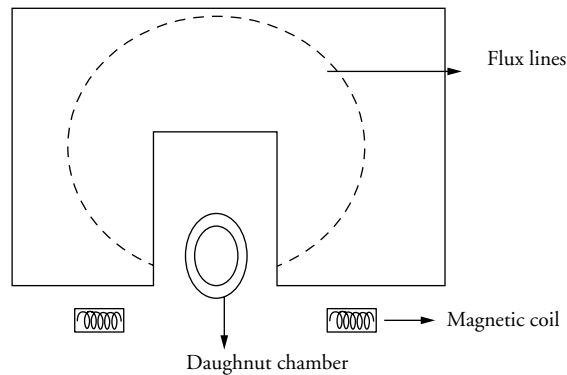


Figure 9.8 (b) Magnet used in proton synchrotron.

2. Working

Using a linear accelerator such as Van de Graaff generator, the protons are accelerated toward the doughnut chamber. Hence, initially the “+ve” particle such as proton can be accelerated up to 10 MeV. These particles are injected when the magnetic field is small. These electrons then come under the influence of radio-frequency oscillator. Moreover, the magnetic field is also increased to keep the electrons in circular orbit of constant radius. In order to avoid any losses due to scattering, the pressure inside the doughnut tube is kept almost 10^{-6} mm of Hg. As proton completes its revolution, it almost gains an impulse of 1 kV/turn, which increases its energy as well as frequency. Hence to maintain the phase stability the frequency of radio-frequency oscillator is also increased in order to synchronize it with the frequency of proton. The range up to which protons can be accelerated is higher than the range of electrons. Hence for proton synchrotron, the radio-frequency adjustments are made quickly. The protons of very high energy (≈ 10 BeV) can be obtained using proton synchrotron. This could be attributed to the fact that the radiation losses for protons are smaller than the losses for electron.

When the protons are accelerated to maximum energy levels, then the radio-frequency is distorted, so that the radius of orbit changes. After the proton gets out of its track, it will strike the target. Theoretically, we could write down the frequency of revolution of positive particle to be

$$f = \frac{(qBc^2)(2\pi r)}{2\pi(K + m_0c^2)(2\pi r_0 + 4l)} \quad (29)$$

$r_0 \rightarrow$ radius of circular section

$l \rightarrow$ section length

$K \rightarrow$ kinetic energy

$B \rightarrow$ Magnetic field

When synchrotron is used to accelerate particles up to 6 BeV, it is also known as betatron. For the proton acceleration of up to 30 GeV, cosmotron are used. Using cosmotrons, nuclear reactions involving energy of cosmic rays are studied. Brookhaven National Laboratory (USA) has such cosmotron, which was built in 1953.

9.7 Synchrocyclotron

As we have studied for cyclotrons that the variation of mass occurs for the ions of accelerator, which further leads to the problem of “loss of resonance.” This problem has been overcome by the use of synchrocyclotrons. They are also known as frequency-modulated cyclotrons because the frequency is varied.

1. Construction

Synchrocyclotron consists of only one dee, which is placed inside the poles of an electromagnet as shown in Figure 9.9. The pole pieces should be shaped to provide magnetic focusing, that is, field decreases outward from the center. The pressure inside the chamber is kept to be 10^{-6} cm of Hg.

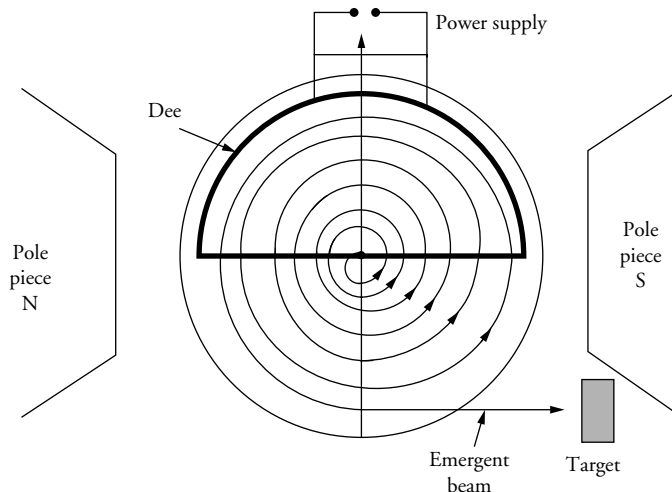


Figure 9.9 Schematic of synchrocyclotron.

High potential is applied across the dee. As compared to cyclotron, the peak value of voltage is quite low ≈ 25 kV. The ions make almost 10^5 revolutions inside the dee. There is only one dee inside the vacuum chamber, so that there can be enough space for the ion source and target. Like cyclotron, the path of the particle is spiral and the ion source is also similar. But still there are some differences; that is for cyclotron, the magnetic field is constant, whereas for synchrocyclotron it decreases. Cyclotron also keeps the frequency to be constant, whereas for synchrocyclotron it varies. The synchrocyclotron may use the magnetic field, which decreases from 1.5 to 1.43 T (Berkley). The Berkley synchrocyclotron is of 400 tons producing the α -particles of almost 380 MeV and deuterons of 190 MeV. The oscillator frequency varies from 11.5 to 9.8 MHz. The frequency is kept at 11.5 MHz during the injection stage; whereas during the ejection stage, it is kept to be 9.8 MHz. The resonance of the ion and the radiofrequency field is usually maintained by decreasing the frequency. In synchrocyclotron, the particle completes 10^5 revolutions before ejection. The frequency of revolution for ions is given by the following equation:

$$v = r\omega$$

$$\omega = \frac{v}{r} \quad [\text{as } mv = Bqr]$$

$$\omega = \frac{Bq}{m}$$

$$\omega = \frac{Bqc^2}{mc^2} = \frac{Bqc^2}{E} \quad (30)$$

$$\omega = \frac{Bqc^2}{\text{K.E.} + m_0c^2}$$

[as total energy $E = \text{K.E.} + \text{rest mass energy}$]

$$f = \frac{Bqc^2}{2\pi(\text{K.E.} + m_0c^2)} \quad (31)$$

Using synchrocyclotron, the electrons cannot be accelerated as well as the output beam current is also very small.

9.8 Linear Accelerators (Linac)

In linear accelerators, the particles are charged in steady steps. Alvarez et al. in 1945 accelerated the protons to 32 MeV using Linacs.

1. Principle

The linear accelerator works on the principle that under an electric field (alternating), the particle is accelerated during (+ve) half cycle and retarded during (\neg ve) half cycle. Moreover, no electric field exists inside hollow conductor moves with uniform velocity.

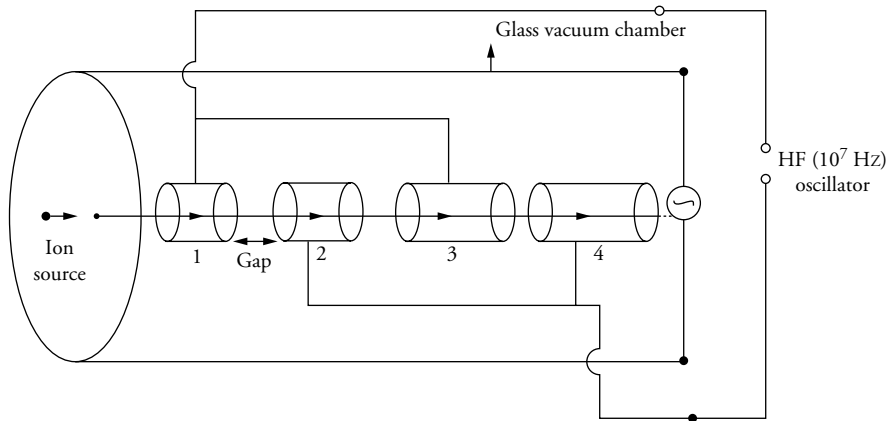


Figure 9.10 Schematic of linear accelerators.

2. Construction

A linear accelerator consists of cylindrical metallic tubes 1 ... n (Figure 9.10). Their axes are along the straight line. The length of cylinders is increasing, that is, the first cylinder is shortest, second is of larger in length than the first, third cylinder is larger in length than the second, and so on. The odd cylinders are connected to one terminal and even cylinders are connected to other terminal. Both terminals are connected to high-frequency oscillator of almost 10^7 Hz frequency. These cylinders are inside evacuated glass chamber. When one set of cylinders get negative, then the second set of cylinders is positive. In next half-cycle, the polarity is reversed and the beam of ions enter the tube along the axis.

3. Working

When the ions enter the tube, then the ions are accelerated only after crossing the gap between the cylinders. Each tube has constant potential; hence, electrons cannot be accelerated within these tubes. If positive charge q enters the accelerator, such that first cylinder is positive, then the second will be negative. The positive ion will get accelerated in between the gap of first and second cylinder. The accelerated ion will now travel through second cylinder with speed faster than it had during travelling through first cylinder. As the length of second cylinder is longer; hence, the ion will reach in the same time to reach in between the gap between second and third cylinder. In the meantime, the polarity gets reversed, that is, the second cylinder will become positive and third will become negative. The ion will again get accelerated in between the gap between second and third cylinder. To keep the ions in phase, the cylinders are made longer in order to compensate for the increasing speed of electrons, that is,

$$t = \frac{\text{cylinder length}}{\text{speed of ion}} = \text{constant} \quad (32)$$

Hence, after passing through every gap, the ion gets accelerated. While passing the tube (which is at constant potential), it moves at constant velocity.

Theoretically, we can conclude as follows:

Let charge q have mass m and V is the potential difference between successive tubes. The velocity of charge; while entering n th cylinder is v_n , then the kinetic energy of ion is $\frac{1}{2}mv_n^2$. The energy picked up by ion after passing through cylinder is qV . For n such gaps, the energy is nqV .

Hence,

$$\begin{aligned} nqV &= \frac{1}{2}mv_n^2 \\ v_n &= \sqrt{\frac{2nqV}{m}} \end{aligned} \quad (33)$$

This equation fails for relativistic velocities, that is, when $v \approx c$. The velocity of ions depends on \sqrt{n} . For example, for the third cylinder, the velocity will become $\sqrt{3}$. During half cycle, the ions travel the distance equal to the length of tube and gap between the cylinders. Hence,

$$L = v_n \frac{T}{2} = \frac{v_n}{2f} \quad [\text{f} - \text{is frequency}] \quad (34)$$

$$L = \frac{1}{2f} \sqrt{\frac{2nqV}{m}}$$

$$L = T \sqrt{\frac{nqV}{2m}} \quad (35)$$

Hence, L varies as \sqrt{n} and velocity v_n also varies as \sqrt{n} , which implies phase stability. Earlier linear accelerators were used to accelerate the protons only, but these days electrons can also be accelerated. Linacs provide a very well-collimated beam of charged particles. Their drawback is their large length, due to which more number of cylinders are required.

SUMMARY

This chapter deals with the particle accelerators. Some accelerators such as Van de Graaff generator and Cockcroft–Walton machines use constant potential difference to accelerate the particles. The output of such oscillators is in the range 4–6 MeV. The accelerators that work on closed-path orbits yielding high energy particles are known as cyclic accelerators, for example, betatrons, synchrotrons, and cyclotrons. Van de Graaff generators and cyclotrons cannot accelerate electrons. The electrons on account of their small size gain velocity very quickly and get out of phase cyclotrons accelerate electrons through electric field only, whereas magnetic fields deflect the semicircular path for electrons.

To avoid any lack of resonance, factor $B \left(1 - \frac{v^2}{c^2}\right)^{1/2}$ should be kept constant. In Cockcroft–Walton

machine, capacitors connected in parallel are charged and discharged in series. Using it, particles cannot be accelerated above 5 MeV, as there are many chances for insulation breakups. To accelerate negative charges such as “electrons,” betatrons and synchrotrons are used. Betatrons produce high

energy X-rays that could trigger further nuclear reactions. No variation of mass with velocity occurs in betatrons; hence, there is no “back of resonance.” Betatrons work on the principle of electromagnetic induction. In betatron, the transverse magnetic field makes the electron to move in constant orbits by providing necessary centripetal force.

Betatron has advantage of very bulky electromagnet. Hence, synchrotrons were introduced which used radiofrequency oscillators and ring-shaped magnet. Cyclotrons and betatrons are low-energy-accelerating machines, whereas synchrotrons are high energy accelerating machines. Particles up to 6 BeV are accelerated using betatron and up to 30 GeV, cosmotrons are used. The synchrocyclotron uses the variation in frequency to avoid and lack of resonance. Unlike cyclotron, the magnetic field in synchrocyclotron decreases. But synchrocyclotron cannot accelerate electrons and output yield is also very small. Linear accelerators use hollow cylinders of increasing lengths. One set of cylinders is positively charged and other set is negatively charged. The particle accelerator in between the gaps of hollow cylinders to keep the ions in phase; the cylinders are made longer to compensate for increasing velocity of ions. LINACS provide very well collimated beam of charge.

SOLVED PROBLEMS

Q. 1: What should be RF frequency for cyclotron, if $B = 1500$ Gauss used for cyclotron.

Ans:

$$f = \frac{Bq}{2\pi m}$$

$$B = 1500 \text{ G} = 1.500 \times 10^{-4} \text{ T}$$

$$q = 1.6 \times 10^{-19} \text{ C}$$

$$m = 1.6 \times 10^{-27} \text{ kg}$$

$$f = \frac{1500 \times 10^{-4} \times 1.6 \times 10^{-19}}{2 \times 3.14 \times 1.6 \times 10^{-27}}$$

$$f = 238.85 \times 10^{-23} \times 10^{27}$$

$$f = 238.85 \times 10^4$$

$$f = 2.39 \text{ MHz}$$

Q.2: What is the period of rotation of deuteron inside a cyclotron? When is it under a magnetic field of 3 Wb/m^2 ?

Ans:

$$T = \frac{2\pi m}{Bq}$$

$$B = 3 \text{ Wb/m}^2 = 3 \text{ T}$$

$$q = 1.6 \times 10^{-19} \text{ C}; \quad m = 3.3 \times 10^{-27} \text{ kg}$$

$$T = \frac{2 \times 3.14 \times 3.3 \times 10^{-27}}{3 \times 1.6 \times 10^{-19}}$$

$$T = 4.3175 \times 10^{-8} \text{ sec}$$

Q.3: A cyclotron with RF frequency 2 MHz is used to accelerate the (i) protons and (ii) deuterons. If the radius of the dees is 50 cm, obtain the magnetic field in tesla for both the particles.

Ans: We know that

$$f = \frac{qB}{2\pi m}$$

(i) For proton,

$$m = 1.67 \times 10^{-27} \text{ kg}$$

$$q = 1.6 \times 10^{-19} \text{ C}$$

$$f = 2 \times 10^6 \text{ Hz}$$

$$f = \frac{1.6 \times 10^{-19} \times B}{2 \times 3.14 \times 1.67 \times 10^{-27}}$$

$$B = \frac{2 \times 3.14 \times 10^{-27} \times 10^6 \times 2}{10^{-19}}$$

$$B = 12.56 \times 10^{-21} \times 10^{+19}$$

$$B = 12.56 \times 10^{-2} = 0.1256 \text{ T}$$

(ii) For deuteron, $m = 3.3 \times 10^{-27} \text{ kg}$

$$B = \frac{2\pi m f}{q}$$

$$B = \frac{2 \times 3.14 \times 3.3 \times 10^{-27} \times 2 \times 10^6}{1.6 \times 10^{-19}}$$

$$B = 25.905 \times 10^{-21} \times 10^{19} \text{ T}$$

$$B = 25.905 \times 10^{-2} \text{ T}$$

$$B = 0.259 \text{ T}$$

Q.4: The radius of the dees is 45 cm and magnetic field is 3000 G. What would be velocity and energy of the protons?

Ans:

$$r = 45 \text{ cm} = 0.45 \text{ m}$$

$$B = 3000 \text{ G} = 3000 \times 10^{-4} \text{ T}$$

$$m = 1.67 \times 10^{-27} \text{ kg}$$

$$q = 1.6 \times 10^{-19} \text{ C}$$

We know that

$$v = \frac{Bqr}{m}$$

$$v = \frac{3000 \times 10^{-4} \times 1.6 \times 10^{-19} \times 0.45}{1.67 \times 10^{-27}}$$

$$v = 1293.41 \times 10^{-23} \times 10^{27}$$

$$v = 1293.41 \times 10^4$$

$$v = 1.29 \times 10^7 \text{ m/sec}$$

Then energy is given by

$$E = \frac{1}{2}mv^2$$

$$E = \frac{1}{2} \times 1.67 \times 10^{-27} \times (1.29 \times 10^7)^2$$

$$E = 1.389 \times 10^{-27} \times 10^{14}$$

$$E = 1.389 \times 10^{-13} \text{ J}$$

$$E = \frac{1.389 \times 10^{-13}}{1.6 \times 10^{-19}} \text{ eV}$$

$$E = 0.86 \text{ MeV}$$

Q. 5: What would be the frequency applied to the dees of cyclotron, which accelerate deuterons when flux density is 2.5 Weber/m².

Ans:

$$f = \frac{Bq}{2\pi m}$$

$$B = 2.5 \text{ Wb/m}^2 = 2.5 \text{ T}$$

$$m = 3.3 \times 10^{-27} \text{ kg}, \quad q = 1.6 \times 10^{-19} \text{ C}$$

$$f = \frac{2.5 \times 1.6 \times 10^{-19}}{2 \times 3.14 \times 3.3 \times 10^{-27}}$$

$$f = 0.193 \times 10^8$$

$$f = 19.3 \times 10^6 \text{ Hz}$$

$$f = 19.3 \text{ MHz}$$

Q. 6: The magnetic field for a cyclotron is 2 T. The extraction radius is 0.8 m. Obtain the frequency and energy for the radiofrequency and accelerated protons, respectively.

Ans:

$$B = 2 \text{ T}$$

$$r = 0.8 \text{ m}, \quad m = 1.67 \times 10^{-27} \text{ kg}$$

The frequency,

$$f = \frac{Bq}{2\pi m}$$

$$f = \frac{2 \times 1.6 \times 10^{-19}}{2 \times 3.14 \times 1.67 \times 10^{-27}}$$

$$f = 0.305 \times 10^8 \text{ Hz}$$

$$f = 30.5 \text{ MHz}$$

Energy

$$E = \frac{B^2 q^2 r^2}{2m}$$

$$E = \frac{4 \times (1.6 \times 10^{-19})^2 \times (0.8)^2}{2 \times 1.67 \times 10^{-27}}$$

$$E = 19.62 \times 10^{-38} \times 10^{27} \text{ J}$$

$$E = 19.62 \times 10^{-11} \text{ J}$$

$$E = \frac{19.62 \times 10^{-11}}{1.6 \times 10^{-19}} \text{ eV}$$

$$E = 12.26 \times 10^8$$

$$E = 0.12 \text{ MeV}$$

OBJECTIVE QUESTIONS

1. Which is the electrostatic accelerator?
 - (a) Van de Graaff generator
 - (b) Cockcroft–Walton machine
 - (c) Both (a) and (b)
 - (d) none of these

2. Which of the following is cyclic accelerator?
 - (a) betatron
 - (b) synchrocyclotron
 - (c) synchrotron
 - (d) all of these

3. Van de Graaff Generator could accelerate particles up to.
 - (a) 10 MeV
 - (b) 5 MeV
 - (c) 20 MeV
 - (d) 50 MeV

4. Following gas can be present inside Van de Graaff generator.
 - (a) methane
 - (b) CO₂
 - (c) H₂
 - (d) fluorine

5. Corona current is due to
 - (a) positive ion source
 - (b) breakdown due to excess potential at surface
 - (c) due to stray/secondary electrons
 - (d) leakage current along discharge tube

6. Cyclotron can accelerate deuterons, protons, and α -particles. (True/False)

7. For the operation of cyclotron,
 - (a) only electric field is required
 - (b) only magnetic field is required
 - (c) electric and magnetic field are parallel
 - (d) electric and magnetic field are perpendicular

8. The high frequency used in cyclotron may use frequency up to:
 - (a) 10^7 Hz
 - (b) 10^5 Hz
 - (c) 10^{10} Hz
 - (d) 10 Hz

9. The electromagnets of cyclotron may have magnetic field up to
 - (a) 2 T
 - (b) 1.5 T
 - (c) 9 T
 - (d) 0.5 T

10. For cyclotron, the radius of the orbit is given by

- (a) $\frac{Bq}{mv}$ (b) $\frac{Bqm}{v}$
 (c) $\frac{mv}{Bq}$ (d) $Bqmv$

11. The time required by particle to complete one revolution in cyclotron is

- (a) $\frac{Bq}{m\pi}$ (b) $\frac{m\pi}{Bq}$
 (c) $\frac{mB\pi}{q}$ (d) $\frac{Bq}{mv}$

12. The maximum energy gained by particles in cyclotron is

- (a) $\frac{2m}{Bqr}$ (b) $\frac{Bqr}{2m}$
 (c) $\frac{B^2 q^2 r^2}{2m}$ (d) $\frac{mv}{Bq}$

13. Cyclotron cannot accelerate

- (a) deuterons (b) alpha particles
 (c) protons (d) electrons

14. Which of the following accelerate the particles in cyclotron?

- (a) Electric field (b) Magnetic field
 (c) Both (a) and (b) (d) None of these

15. Which of the following deflects the particle in cyclotron?

- (a) Electric field (b) Magnetic field
 (c) None of these (d) Both (a) and (b)

16. Which factor should be kept constant to avoid resonance lagging?

- (a) $\frac{B}{\sqrt{1-v^2/c^2}}$ (b) $B(1-v^2/c^2)$
 (c) $B\left(1-\frac{v^2}{c^2}\right)^{+1/2}$ (d) $\frac{B}{(1-v^2/c^2)}$

17. For Cockcroft–Walton machine, the capacitors are charged and discharged in _____

- (a) parallel (b) series
 (c) can be parallel or series (d) cannot be discharged

18. The ripple voltage for Cockcroft–Walton machine in

- (a) $\frac{I(f.C)}{16}$ (b) $\frac{16f.C.}{In(n+2)}$
 (c) $\frac{In(n+2)}{16f.C.}$ (d) $In(16f.C.)$

19. Using Cockcroft–Walton machine, the particles cannot be accelerated above

- (a) 5 MeV (b) 8 MeV
 (c) 10 MeV (d) 1 MeV

20. Betatron works on the principle of

- (a) Superposition (b) Ampere's law
 (c) electromagnetic induction (d) self-induction

21. In betatron, the electron moves in orbit

- (a) of constant radius (b) of variables radius
 (c) of radius as (r^2) (d) of radius as $\frac{1}{r^2}$

22. For magnetic focusing, the magnetic field is

- (a) concave inward (b) convex outward
 (c) radial (d) longitudinal

23. In betatron, the electrons are injected during

- (a) decreasing magnetic field (b) peak magnetic field
 (c) increasing magnetic field (d) O magnetic field

24. The flux condition for betatron is

- (a) $\frac{d\phi_B}{dt} = 4 \frac{d}{dt}(\pi R^2 B)$ (b) $\frac{d\phi_B}{dt} = \frac{d}{dt}(\pi R^2 B)$
 (c) $\frac{d\phi_E}{dt} = \frac{d}{dt}(\pi R^2 B)$ (d) $\frac{d\phi_B}{dt} = 2 \frac{d}{dt}(\pi R^2 B)$

25. General Electric labs have produced electrons up to

- (a) 100 MeV (b) 10 MeV
 (c) 50 MeV (d) 5 MeV

26. Electro synchrotron uses flux bars for

- (a) resonance (b) magnetic field
 (c) supersaturating (d) stability

27. The vacuum chamber are coated with silver to
- (a) avoid any insulation (b) avoid eddy currents
(c) increase the conductivity (d) none of these
28. Synchrotrons are low-energy-accelerating machines. (True/False)
29. The frequency of revolution for synchrotron is
- (a) $\frac{c}{2\pi r}$ (b) $\frac{cr}{2\pi}$
(c) $\frac{2\pi r}{c}$ (d) $\frac{2\pi}{cr}$
30. The energy of particle is synchrotron is
- (a) $\frac{qBr}{c}$ (b) $\frac{c}{qBr}$
(c) $qBrc$ (d) $\frac{qB}{rc}$
31. Using proton synchrotron, the protons can be accelerated up to
- (a) 5 MeV (b) 10 GeV
(c) 10 MeV (d) 1 BeV
32. For proton acceleration up to 30 GeV, which of the following is used?
- (a) Cyclotron (b) Betatron
(c) Betatron (d) Cosmotron
33. In synchrocyclotron, the frequency is
- (a) varied (b) kept constant
(c) varies as q^2 (d) varies as r^2
34. In synchrocyclotron, after completion of one revolution, the electron gains impulse of
- (a) 10 kV/turn (b) 1 kV/turn
(c) 5 kV/turn (d) 10 V/turn
35. For LINAC, the velocity is proportional to
- (a) n (b) n^2
(c) \sqrt{n} (d) $\frac{1}{n}$
36. For LINACs, the distance travelled by ion depends on
- (a) n (b) \sqrt{n}
(c) n^2 (d) $\frac{1}{n^2}$

ANSWERS

- | | | | |
|---------|---------|---------|-----------|
| 1. (c) | 10. (c) | 19. (a) | 28. False |
| 2. (d) | 11. (b) | 20. (c) | 29. (a) |
| 3. (a) | 12. (c) | 21. (a) | 30. (c) |
| 4. (a) | 13. (d) | 22. (b) | 31. (b) |
| 5. (b) | 14. (a) | 23. (c) | 32. (d) |
| 6. True | 15. (b) | 24. (d) | 33. (a) |
| 7. (d) | 16. (c) | 25. (a) | 34. (b) |
| 8. (a) | 17. (b) | 26. (c) | 35. (c) |
| 9. (b) | 18. (c) | 27. (b) | 36. (b) |

Micro-Assessment Questions

1. What are particle accelerators?
2. What is the difference between cyclic and electrostatic accelerator?
3. Write the conditions that the ion source must satisfy for a particle accelerator.
4. Write the conditions for an ideal accelerator.
5. Write down the principle of Van de Graaff generator.
6. What do you understand by corona discharge?
7. Which gases are used inside a Van de Graaff chamber?
8. What do you understand by breakdown current?
9. What is loss of resonance for cyclotron?
10. What is Cockcroft–Walton machine?
11. What is the ripple voltage for Cockcroft–Walton machine?
12. What is betatron?
13. What is synchrotron? How does it differ from synchrocyclotron?
14. What is the disadvantage of cyclotron?
15. What is the advantage of using betatron?
16. What is the difference between Van de Graaff generator and LINAC?
17. What is the principle of betatron?
18. Explain the betatron condition for the betatron.
19. What is the advantage of synchrotron over betatron?
20. List the low-energy and high-energy particle accelerators.
21. Explain the linear accelerators (LINAC).
22. List the disadvantage of synchrocyclotron.

Critical Thinking Questions

1. Give the principle of cyclotron in brief. What is the role of magnetic field in cyclotron?
2. Explain the construction of Van de Graaff generator in detail.
3. What are the various currents that are present in Van de Graaff generator?
4. Derive the energy of particle when it is accelerated under the effect of electric and magnetic field in the cyclotron.
5. Explain the consequences when heavy ions are used in cyclotron.
6. What is the difference between cyclotron and betatron?
7. What is the principle of Cockcroft–Walton machine?
8. With the help of diagram, explain the injection and ejection point for betatron w.r.t. magnetic field.
9. Derive the flux condition linked with the betatron.
10. Which factors limit the performance of betatron?
11. Explain the role of flux bars in synchrotron.
12. Why doughnut chamber is coated with silver from inside?
13. Explain the working of synchrotron.
14. Describe the importance of RF oscillators in accelerators.
15. What is the disadvantage of linear accelerators?

Graded Questions

1. Write in detail the principle, working, and construction for Van de Graaff generator. Which type of particles can be accelerated using Van de Graaff generator?
2. Explain in detail the principle construction and working of cyclotron.
3. Describe the principle, working, and construction of Cockcroft–Walton machine.
4. Write in detail the principle, working, and construction for the betatron. How is the problem of “loss of resonance” resolved?
5. Explain in detail the working of electron synchrotron. How does its working differ from proton synchrotron?
6. Describe the principle, working, and construction for synchrocyclotron. What is the frequency of particle revolution?
7. What are linear accelerators? Give its detailed principle and working.

Remember and Understand

1. The accelerators should have energy stability and coherence along with good beam intensity. The accelerators should also exhibit good particle collimation.
2. Accelerators fall in two categories: electrostatic accelerators in which the particles are accelerated by constant potential difference and cyclic accelerators in which particles form closed path again and again.
3. The Van de Graaff generator is based on the principle of harp pointed surfaces and zero charge inside hollow conductor.
4. Van de Graaff generator can only accelerate positive particles up to 10 MeV. Cyclotron is also used to accelerate positively charged particles that are further used for nuclear disintegration.
5. Cyclotron can accelerate the particles through electric field only. The purpose of magnetic field in cyclotron is to deflect the particles in semicircular path inside the dees.
6. The time period (T) taken by a charged particle in cyclotron is given by the following equation:

$$T = 2t = \frac{2\pi m}{Bq}$$

7. The maximum energy gained by a particle inside the cyclotron is given by the following equation:

$$E_{\max} = \left(\frac{q^2 B^2}{2m} \right) r_{\max}^2$$

8. Electrons can be accelerated by cyclotron due their smaller mass. Electrons gain energy very quickly in small intervals of time and hence go out of step very quickly.
9. Cockcroft–Walton machine uses voltage multiplier circuits to get high potential difference. The capacitors are connected in parallel, which are charged and discharged in series. This accelerator can accelerate particles up to 5 MeV.
10. For producing high energy X-rays and triggering reactions, we require energetic beam of electrons which are negatively charged particles. Betatron is used to accelerate negative-charged particles, and it works on the principle of electromagnetic induction.

11. The particles of energy 100 MeV can be produced by betatron. In betatron, the transverse magnetic field makes the electrons move in constant orbit.
12. The magnetic lines of force should be convex outwardly for proper magnetic focusing.
13. In betatrons the electrons are injected when the magnetic field is rising because the electrons get accelerated due to increase in potential within the doughnut.
14. The flux condition for betatron is given by the following equation:

$$\frac{d\phi_b}{dt} = 2 \frac{d}{dt} (\pi r^2 B)$$

15. In synchrotrons, the bulky electromagnet is replaced with a source of radiofrequency. It can accelerate both positive and negative particles. Although protons can be accelerated using cyclotron, but to accelerate the particles up to 10 GeV energy, proton synchrotrons are used.
16. The problem of loss of resonance has been overcome by the use of sychrocyclotron, which uses variation in frequency. Before ejection, ions revolve for 10^5 revolutions and the frequency is given by the following equation:

$$f = \frac{Bqc^2}{2\pi (\text{K.E.} + m_0c^2)}$$

17. The linear accelerators work on the principle that the particle gets accelerated during positive half cycle and retarded during negative half cycle under an electric field.

Electrostatics

Keywords: Coulomb's law, Gauss's law, electric charge, potential, polarization, law of superposition, electric field, test and source charge, dielectric strength

Learning Objectives

- ◆ To learn about scalar and vector fields
- ◆ To understand the significance of gradient, divergence, and curl
- ◆ To understand the concept of charge and its properties
- ◆ To derive Coulomb's law in terms of position vectors
- ◆ To define the dielectric constant and coulomb
- ◆ To learn how Newton's third law holds good during electrostatic interactions.
- ◆ To get insight into electric field, source, and test charge
- ◆ To understand the importance of electric field lines and their properties
- ◆ To learn the difference between discrete and continuous charge distribution
- ◆ To derive electric field for different charge distributions like line charge, over a circular ring and disc, and due to two infinite charged plane sheet
- ◆ To understand the Gauss theorem as a bridge between electric flux and charge
- ◆ To learn about the electric potential and potential difference
- ◆ To understand the potential for continuous charge distributions
- ◆ To learn about dielectrics, dielectric polarization, and displacement vector
- ◆ To understand different types of polarization, that is, electronic polarizability, ionic polarization, orientation polarization, and space-charge polarization

In day-to-day routine, we deal with many electromagnetic devices. These devices are based on the phenomena exhibited by charges and magnetic field. We have studied about static charges in our previous classes. In this chapter, we will also deal with moving charges. Moving charges give rise to magnetic field and changing magnetic field generates electricity. The branch of physics that deals with electricity and magnetism is known as electromagnetism. It is very important to have thorough knowledge of Maxwell equations to understand electromagnetism. Before we understand these mathematical equations, we should be able to grab the importance and relevance of terms such as “gradient,” “divergence,” and “curl.” In addition, we should understand scalar and vector fields.

10.1 Scalar and Vector Fields

Every physical entity has a region surrounding it, which is of interest. For example, the body of mass m has a gravitational field around it and a body with charge q has electric field around it. Hence, the region that surrounds the entity and is of interest is called field. When the physical quantity is given as a function of position in well-defined space, it is known as point function. When the scalar point function is associated with a field, then the field is said to be scalar field. The scalar function is single-valued continuous function and is given by $\phi(x, y, z)$.

When vector function is associated with the region or field, the field is said to be vector field. The vector function is also single-valued continuous function and is given by $\vec{A}(x, y, z)$.

10.2 Gradient And Its Significance

Let $\phi(x, y, z)$ be scalar point function such that it is continuously differentiable. Mathematically, the gradient is defined by

$$\nabla\phi = \hat{i} \frac{\partial\phi}{\partial x} + \hat{j} \frac{\partial\phi}{\partial y} + \hat{k} \frac{\partial\phi}{\partial z} \quad (1)$$

where “ ∇ ” is “grad” or “nabla” operator. \hat{i} , \hat{j} , and \hat{k} are unit vectors along x -, y -, and z -direction. “ ∇ ” is given by

$$\nabla = \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \quad (2)$$

$\frac{\partial\phi}{\partial x}$, $\frac{\partial\phi}{\partial y}$, and $\frac{\partial\phi}{\partial z}$ are partial derivatives of scalar function w.r.t. x , y , and z . ϕ is a scalar quantity, but $\nabla\phi$ is a vector quantity as indicated from Eqn. (1). Let S_1 and S_2 be level surfaces as shown in Figure 10.1 [by level surface, we mean that the value of temperature or any other physical entity is constant over it].

Let A and B be at a distance dr . For surfaces S_1 and S_2 , the scalar functions have value ϕ and $\phi + d\phi$, respectively. Let $AC = dn$ be the normal to surface S_1 . B and C will have same value of scalar function because the surface is taken to be leveled. Scalar function ϕ changes as $\frac{\partial\phi}{\partial n}$ along AC .

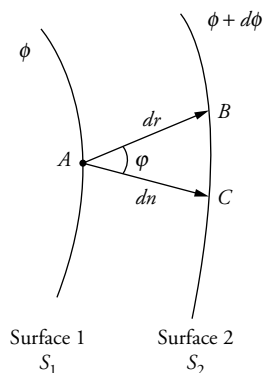


Figure 10.1 Two surfaces with different scalar functions.

In $\triangle ABC$

$$\begin{aligned}\frac{dn}{dr} &= \cos \phi \\ dn &= dr \cos \phi\end{aligned}\quad (3)$$

We can also write Eqn. (3) in terms of unit vector \hat{n}

$$dn = \hat{n} \cdot dr \quad (4)$$

Equation (4) indicates that the rate of increase of ϕ at A is greatest in the direction of unit vector \hat{n} and is given by $\frac{\partial \phi}{\partial n}$. Therefore,

[from Eqn.(4)]

$$d\phi = \frac{\partial \phi}{\partial n} dn = \frac{\partial \phi}{\partial n} \hat{n} \cdot dr \quad [\text{where } \overline{dr} = dx \hat{i} + dy \hat{j} + dz \hat{k}] \quad (5)$$

Now $\nabla \phi \cdot dr$ is given by

$$\begin{aligned}\nabla \phi \cdot dr &= \left(\hat{i} \frac{\partial \phi}{\partial x} + \hat{j} \frac{\partial \phi}{\partial y} + \hat{k} \frac{\partial \phi}{\partial z} \right) \cdot (dx \hat{i} + dy \hat{j} + dz \hat{k}) \\ \nabla \phi \cdot dr &= \frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy + \frac{\partial \phi}{\partial z} dz \\ \nabla \phi \cdot dr &= d\phi\end{aligned}\quad (6)$$

Comparing Eqs (5) and (6),

$$\nabla \phi = \frac{\partial \phi}{\partial n} \hat{n} \quad (7)$$

Equation (7) indicates that gradient of a scalar function ϕ represents the vector with magnitude equal to maximum rate of change of scalar function along the normal to level surface. When a vector field is derived from the gradient of a scalar field, the field is said to be conservative or lamellar field. For example, the electric field E is derived from gradient of potential such that

$$E = -\nabla V = - \left[\hat{i} \frac{\partial V}{\partial x} + \hat{j} \frac{\partial V}{\partial y} + \hat{k} \frac{\partial V}{\partial z} \right] \quad (8)$$

From Eqn. (8), E is the lamellar or conservative field and V is the potential.

10.3 Divergence and its Significance

The divergence can only be performed for a vector point function. Consider \vec{A} to be a vector function with position coordinates $\vec{A} = A_x \hat{i} + A_y \hat{j} + A_z \hat{k}$. Then the divergence of \vec{A} can be given by

$$\begin{aligned}\text{Div. } \vec{A} &= \nabla \cdot \vec{A} = \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \cdot (A_x \hat{i} + A_y \hat{j} + A_z \hat{k}) \\ \nabla \cdot \vec{A} &= \left[\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right]\end{aligned}\quad (9)$$

It should be noted from Eqn. (9) that \vec{A} is a vector quantity, whereas $\nabla \cdot \vec{A}$ gives scalar quantity.

$\nabla \cdot \vec{A}$ can have the following three cases:

- (i) $\nabla \cdot \vec{A}$ can be positive. When divergence of vector field is positive, the vector quantity represents a source.
- (ii) $\nabla \cdot \vec{A}$ can be negative. When divergence of vector field is negative, the vector field represents a sink.
- (iii) $\nabla \cdot \vec{A}$ can be zero. When the divergence of vector field is zero, the vector field is said to be solenoidal. In other words, flux in that region is zero. A solenoidal vector field does not represent either source or sink.

In other terms, divergence of vector \vec{A} can also be given as

$$\nabla \cdot \vec{A} = \frac{\oint \vec{A} \cdot d\vec{s}}{\Delta V} \quad (10)$$

R.H.S. of Eqn. (10) represents the flux density of vector \vec{A} over surface S , which encloses volume V .

10.4 Curl and its Significance

Curl is also performed on a vector field \vec{A} . The curl for vector \vec{A} is given by

$$\begin{aligned} \text{Curl } \vec{A} = \nabla \times \vec{A} &= \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \times (A_x \hat{i} + A_y \hat{j} + A_z \hat{k}) \\ \nabla \times \vec{A} &= \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{bmatrix} \end{aligned} \quad (11)$$

The curl is also given in terms of line integral, that is,

$$\nabla \times \vec{A} = \frac{\oint \vec{A} \cdot d\vec{s} \hat{n}}{\Delta s} \quad (12)$$

Hence, curl can be defined as the line integral of vector field \vec{A} per unit area.

If curl of vector field \vec{A} is zero, then the field is said to be irrotational, that is,

$$\nabla \times \vec{A} = 0 \quad (13)$$

Following are important identities of gradient, divergence and curl:

$$\begin{aligned} \text{(i) } \nabla \cdot (\nabla \phi) &= \nabla^2 \phi \\ &= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \phi \end{aligned} \quad (14)$$

“ ∇^2 ” is known as the “Laplacian operator.”

$$\text{(ii) } \nabla \times (\nabla \phi) = 0 \quad (15a)$$

Hence curl of gradient is zero.

$$(iii) \quad \nabla \times (\nabla \times A) = \nabla(\nabla \cdot A) - \nabla^2 A \quad (15b)$$

$$(iv) \quad \nabla \cdot (\nabla \times A) = 0 \quad (15c)$$

Divergence of curl is zero

$$(v) \quad \iiint_V (\nabla \cdot A) dV = \iint_S A \cdot ds \quad (15d)$$

Equation (15d) is Gauss divergence theorem, which states that the volume integral of divergence of vector \vec{A} over volume V is equal to surface integral of \vec{A} bounded by surface S .

$$(vi) \quad \iint_S (\nabla \times A) \cdot ds = \oint A \cdot dl \quad (15e)$$

Equation (15e) is known as Stoke's theorem, which states that surface integral of vector field \vec{A} over any surface s is equal to line integral of \vec{A} over a closed contour.

10.5 Charge

Charge is the property of body that causes attraction or repulsion. This property is acquired when the bodies rub against each other. The bodies get charged after rubbing against each other and they may attract or repel each other. The charges are of two types, positive and negative. The distance between charges describes whether they are point charges. By point charges, we mean that the distance r between the charges is much larger than the dimensions of charges. The charges can mutually influence or exert forces on each other, which is known as electrostatic interaction. If the charges are moving, the interaction is said to be electromagnetic interaction.

10.6 Coulomb's Law

Let q_1 and q_2 be two point charges with \vec{r}_1 and \vec{r}_2 be the position vectors, respectively (Figure 10.2).

The Coulomb's law states that the force between two charges is

- (i) directly proportional to product of charges

$$F \propto q_1 q_2 \quad (16)$$

- (ii) inversely proportional to the square of distance between the charges

$$F \propto \frac{1}{r^2} \quad (17)$$

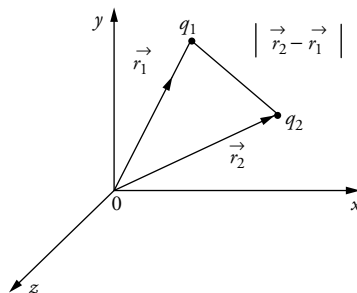


Figure 10.2 Charges showing Coulomb's interaction.

Combining Eqs (16) and (17),

$$F \propto \frac{q_1 q_2}{r^2}$$

$$F = K \frac{q_1 q_2}{r^2} \quad (18)$$

where K is the constant of proportionality. F is known as Coulomb's force which has following properties:

- (i) This force is repulsive for the charges of same polarity and attractive for the charges with opposite polarity.
- (ii) The Coulomb force acts along the line joining the two charges. Hence, Coulomb forces are central in nature.

Let \vec{F}_{21} be the force on charge q_2 due to charge q_1 . Let \vec{F}_{12} be the force on charge q_1 due to charge q_2 . Forces \vec{F}_{12} and \vec{F}_{21} are given by following cases:

- (i) F_{12} for charges with same polarity (Figure 10.3(a))

$$F_{12} = K \frac{q_1 q_2}{|\vec{r}_1 - \vec{r}_2|^2} \quad (19)$$

- (ii) F_{12} for charges with opposite polarity (Figure 10.3(b))

$$F_{12} = \frac{K q_1 q_2}{|\vec{r}_2 - \vec{r}_1|^2} \quad (20)$$

- (iii) F_{21} for charges with same polarity (Figure 10.3(c))

$$F_{21} = K \frac{q_1 q_2}{|\vec{r}_2 - \vec{r}_1|^2} \quad (21)$$

- (iv) F_{21} for charges with opposite polarity (Figure 10.3(d))

$$F_{21} = \frac{K q_1 q_2}{|\vec{r}_1 - \vec{r}_2|^2} \quad (22)$$

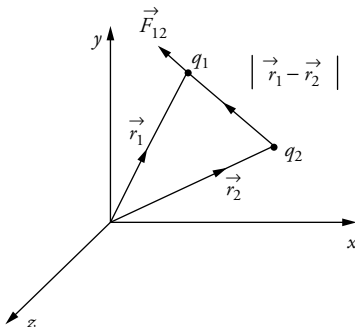


Figure 10.3(a)

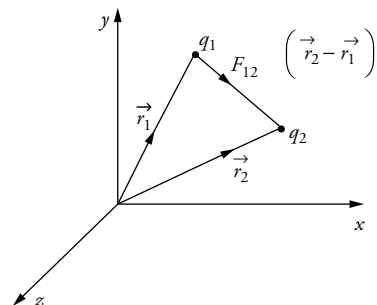


Figure 10.3(b)

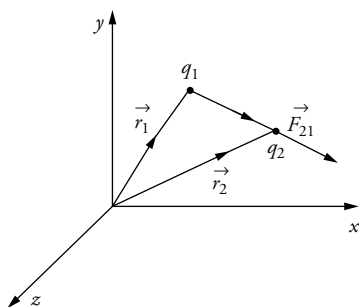


Figure 10.3(c)

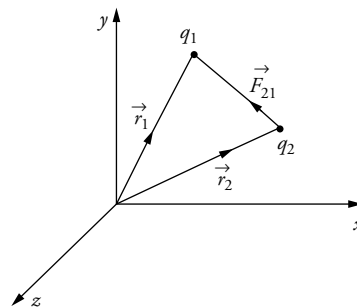


Figure 10.3(d)

Figure 10.3 Coulomb's force for different polarities of charges.

If we have to find out \vec{F}_{21} , then we have to multiply unit vector with F_{21} . The unit vector is given by

$$\hat{n} = \frac{(\vec{r}_1 - \vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} \quad (23)$$

As

$$\vec{F}_{21} = F_{21} \cdot \hat{n}$$

$$\vec{F}_{21} = \frac{K q_1 q_2 (\vec{r}_1 - \vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|^3} \quad (24)$$

We will define charge and constant of proportionality K in the following sections:

Charles-Augustin de Coulomb was an eminent French physicist who formulated the famous Coulomb's law. The law deals with the electrostatic interaction between electrically charged particles and "coulomb," SI unit of electric charge, was named after him. The Coulomb's law was formulated as a consequence of Coulomb's efforts to study the law of electrical repulsions put forward by English scientist Joseph Priestley. He also devised sensitive apparatus in order to evaluate the electrical forces. The device was torsion balance that could measure very small charges and hence experimentally estimate the force of attraction or repulsion between two charged bodies. Then he issued out his theories in 1785–1789.



CHARLES-AUGUSTIN DE COULOMB

Coulomb was born to a wealthy family in Angouleme, France. His father Henri Coulomb was an inspector of the Royal Fields in Montpellier. Later on, the family moved to Paris, where Coulomb studied mathematics at the famous Collège des Quatre-Nations. In 1759, he attended military school of Mézières. He graduated from Ecole du Génie at Mézières in 1761. After his formal studies at the Royal School of Engineering, he embarked on a long career within the Military Engineering Corps. Coulomb worked as a military engineer in the West Indies for almost nine years. His duties were hectic and forced him to make

several necessary moves over time. A particularly long stay in the West Indies left his health in a deteriorated state. Then he came back to France with a bad state of health and never fully recovered. Coulomb lived in Blois during the French Revolution and carried out his scientific research. In 1777, Coulomb was awarded part of the Academy's grand prize for a paper discussing the magnetic compass. In 1781, he received prize for a groundbreaking examination of friction. He also formulated the inverse square law of attraction and repulsion of unlike and like magnetic poles, which further laid out the foundation for the mathematical theory of magnetic forces formulated by French mathematician Siméon-Denis Poisson. He was appointed as an inspector of public instruction in 1802. His health worsened day by day and he died on August 23, 1806, in Paris at the age of 70 years. Posthumously, he was honored by the adoption of an SI unit of electric charge "coulomb" bearing his name.

10.6.1 Coulomb as Unit of Charge

The SI unit of charge is Coulomb. The current is given by

$$\text{Current}(I) = \frac{\text{charge}(q)}{\text{time}(t)}$$

$$1 \text{ ampere} = \frac{1 \text{ Coulomb}}{1 \text{ sec}} \quad (25)$$

One Coulomb is defined as the amount of charge that passes through any section of wire per second carrying current of unit current.

10.6.2 Proportionality Constant (K)

K depends on the medium between charges as well as system of units chosen and is given by

$$K = \frac{1}{4\pi\epsilon_0} \quad (26)$$

where ϵ_0 is the absolute permittivity of free space.

The value of $\epsilon_0 = 8.854 \times 10^{-12} \text{ C}^2/\text{Nm}^2$.

The value of $K = 9 \times 10^9 \text{ Nm}^2/\text{C}^2$ in SI and the value of $K = 1$ in c.g.s.

Let $q_1 = q_2 = q$ and $|\vec{r}_1 - \vec{r}_2| = 1 \text{ m}$.

Let $F = 9 \times 10^9 \text{ N}$, Eqn. (24) can be written as

$$q^2 = 1 \Rightarrow q = \pm 1 \quad (27)$$

Hence, one coulomb is defined as the amount of charge, which will attract/repel similar or opposite charge respectively, when placed at a distance 1 m apart from each other in vacuum with a force of $9 \times 10^9 \text{ N}$.

From Eqs (20) and (22), when we take forces between opposite charges, then

$$\vec{F}_{12} = -\vec{F}_{21} \quad (28)$$

Similar is the case for force between charges with same polarity. Hence, Coulomb's force obeys Newton's third law of motion.

Following are the points about the charge:

1. Charge is a conserved quantity, which will not change with time for an isolated system.
2. Charge can be added and subtracted like ordinary numbers. Hence, charge is a scalar quantity.
3. Charge is quantized as the total charge of body and is given by discrete values. Total charge q is given by

$$q = \pm ne \quad (29)$$

Hence, total charge can be expressed as integral multiple of smallest unit of charge e . n can take integral values only and cannot take any fractional value.

Andre Marie Ampère was the famous French physicist and mathematician who is mainly known for giving fundamental basis of electrodynamics. He was the first person who demonstrated the generation of magnetic field when two parallel wires are charged with electricity. He invented the astatic needle, which is a significant component of the astatic galvanometer.

Andre Marie was born on January 20, 1775, in Lyon, France. He was the son of Jean-Jacques Ampère who was a local government official and an affluent businessman. At a very young age, Ampère spent most of his time reading in the library of his family home. While reading, he developed an interest for philosophy, history, geography, literature, and above all natural sciences. His father was a support and motivation for him. He used to give him Latin lessons and encouraged him to pursue his passion for mathematics.

During 1820, the Danish physicist, H.C. Oersted accidentally discovered that by a voltaic current, magnetic needle shows movement. This phenomenon established was the background of relationship between electricity and magnetism. Ampère was very much influenced by Oersted's discovery. He performed systematic series of experiments in order to elucidate the exact nature of the relationship between electric current-flow and magnetism. He also emphasized on the behavior of electric currents in various types of conductors. Furthermore, he demonstrated from his experiments that two parallel wires carrying electric currents magnetically attract each other if the currents are in the same direction and repel if the currents are in opposite directions. Then, Ampère formulated his famous law of electromagnetism, which is known as Ampère's law. This law gives the mathematical description of the magnetic force between two electrical currents. After a week of Oersted's discovery, his findings were reported in the Académie des Sciences, which laid a solid foundation of electrodynamics. Ampère died on June 10, 1836, at Marseille and was buried in the Cimetière de Montmartre, Paris. Posthumously, The SI unit of measurement of electric current was named as Ampere.



"Either one or the other [analysis or synthesis] may be direct or indirect. The direct procedure is when the point of departure is known-direct synthesis in the elements of geometry. By combining at random simple truths with each other, more complicated ones are deduced from them. This is the method of discovery, the special method of inventions, contrary to popular opinion."

André-Marie Ampère

ANDRE MARIE AMPÈRE

10.7 Electric Field

Electric field is the inherent space property of charge by virtue of which the surroundings of source charge (q) is modified, so that incoming test charge q_0 experiences a force on it. Hence, electric field is the space around the vicinity of charge. The source charge produces electric field and test charge experiences force on it when it comes in the field region of source charge.

Mathematically, electric field (\vec{E}) is given by force experienced by test charge (\vec{F}) per unit test charge (q_0).

$$\vec{E} = \lim_{q_0 \rightarrow 0} \frac{\vec{F}}{q_0} \quad (30)$$

In Figure 10.4, we have fixed source charge q located at position vector \vec{r} . \vec{r}_0 is the position vector of test charge q_0 . The force \vec{F} on test charge is given by

$$\vec{F} = \frac{1}{4\pi\epsilon_0} \frac{q q_0 (\vec{r}_0 - \vec{r})}{|\vec{r}_0 - \vec{r}|^3}$$

$$\vec{E} = \lim_{q_0 \rightarrow 0} \frac{\vec{F}}{q_0} = \frac{q (\vec{r}_0 - \vec{r})}{4\pi\epsilon_0 |\vec{r}_0 - \vec{r}|^3} \quad (31)$$

From Eqn. (31), it is clear that the direction of electric field is always from source to test charge. Moreover, source charge contributes to electric field. When the source charge is at origin, $\vec{r} = 0$

$$\vec{E} = \frac{q \vec{r}_0}{4\pi\epsilon_0 r_0^3} = \frac{q \hat{r}_0}{4\pi\epsilon_0 r_0^2}$$

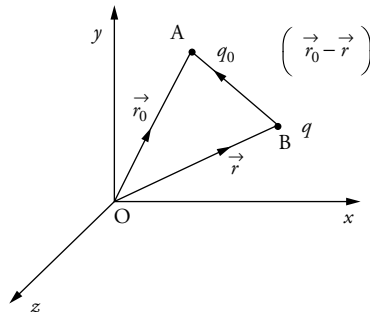


Figure 10.4 Electric field between test and source charge.

$$|\vec{E}| = \frac{q}{4\pi\epsilon_0 r_0^2} \quad (32)$$

From Eqn. (30), it should be noted that test charge q_0 tends to zero, which means the magnitude of test charge should be very small. The small test charge will not displace source charge and hence accurate value of electric field is obtained. If the source charge is fixed, then the magnitude of test is immaterial and Eqn. (30) is given by

$$\vec{E} = \frac{\vec{F}}{q_0} \quad (33)$$

10.8 Principle of Superposition

Let us take n charges q_1, q_2, \dots, q_n with respective position vectors $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n$. Let q be the test charge on which we want to determine the force as well as electric field. Then according to principle of superposition “for a group of charges, the force on any charge is the vector sum of individual forces exerted on it due to all other charges.” Hence, we can write

$$\vec{F} = \vec{F}_1 + \vec{F}_2 + \dots + \vec{F}_n \quad (34)$$

All forces are independent of each other.

Let F_n be the force between charge q_n and q (Fig. 10.5). Then Eqn. (34) can be given as

$$\vec{F} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q (\vec{r} - \vec{r}_1)}{|\vec{r} - \vec{r}_1|^3} + \frac{1}{4\pi\epsilon_0} \frac{q_2 q (\vec{r} - \vec{r}_2)}{|\vec{r} - \vec{r}_2|^3} + \dots + \frac{1}{4\pi\epsilon_0} \frac{q_n q (\vec{r} - \vec{r}_n)}{|\vec{r} - \vec{r}_n|^3} \quad (35)$$

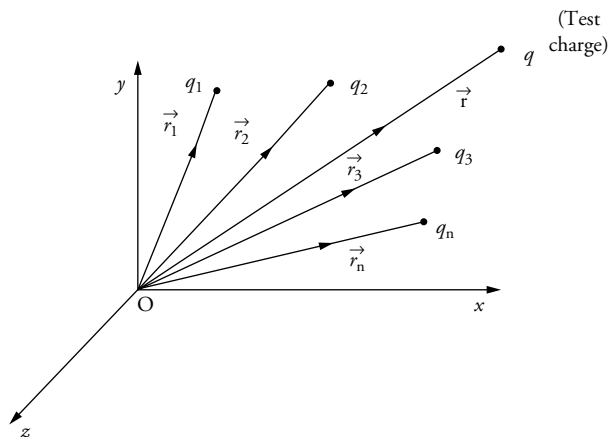


Figure 10.5 Group of n charges and their position vectors.

$$\vec{F} = \frac{q}{4\pi\epsilon_0} \left[\frac{q_1(\vec{r} - \vec{r}_1)}{|\vec{r} - \vec{r}_1|^3} + \frac{q_2(\vec{r} - \vec{r}_2)}{|\vec{r} - \vec{r}_2|^3} + \dots + \frac{q_n(\vec{r} - \vec{r}_n)}{|\vec{r} - \vec{r}_n|^3} \right] \quad (36)$$

$$\vec{F} = \frac{q}{4\pi\epsilon_0} \sum_{i=1}^n \frac{q_i(\vec{r} - \vec{r}_i)}{|\vec{r} - \vec{r}_i|^3} \quad (37)$$

If charge q lies at origin, then Eqn. (37) can be written as

$$\vec{F} = \frac{q}{4\pi\epsilon_0} \sum_{i=1}^n \frac{q_i \vec{r}_i}{r_i^3} \quad (38)$$

The electric field can be given as force per unit test charge q . Equation (37) can be written as

$$\vec{E} = \frac{\vec{F}}{q} = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{q_i(\vec{r} - \vec{r}_i)}{|\vec{r} - \vec{r}_i|^3} \quad (39)$$

For the charge q lying at origin, Eqn. (39) can be written for electric field as

$$\vec{E} = \frac{\vec{F}}{q} = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{q_i \vec{r}_i}{r_i^3} \quad (40)$$

10.9 Electric Lines of Force

An electric line of force is defined as the path along which unit positive charge will tend to move, when it is free (under no force). The intensity of electric field is represented by the density of field lines. Electric field lines have the following properties:

1. Lines of force are normal to surface of body where they originate or terminate (Fig. 10.6).
2. There is no line of force inside the conductor. Hence, electric field lines are not closed curves.

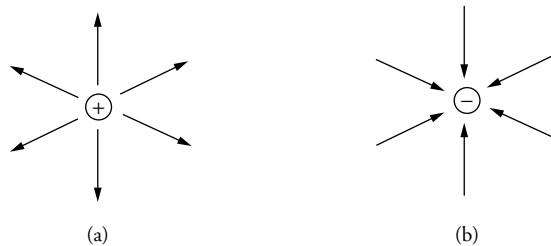


Figure 10.6 Electric field lines for positive and negative charge.

3. Lines of force start from positive charge and terminate at negative charge.
4. The electric lines of force have the same direction as that of electric field.
5. Lines of force never intersect each other. When the lines intersect, at the point of intersection two tangents can be drawn, which gives two directions of electric field at the same point. This is quite contradictory.
6. The lines of force moving in the same direction repel each other and moving in opposite direction attract each other.

10.10 Continuous Charge Distribution

Till now, we have obtained the force and electric field due to discrete charge distribution. When the charges are distributed in an entire surface, within a volume or along a length, we have to use continuous charge distribution. Following are three kind of distributions:

1. Line Charge Distribution

For line charge distribution, the charge is spread all along the length (can be wire). Let q be the total charge distributed along the whole length PQ of wire (Figure 10.7). Then dq is the charge for small length dl of wire PQ . Then line charge density is given by

$$\lambda = \frac{dq}{dl} \quad (41)$$

Then, the electric field becomes

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \int \frac{dq \hat{R}}{R^2}$$

$$\vec{E} = \frac{\lambda}{4\pi\epsilon_0} \int \frac{dl \hat{R}}{R^2} \quad (42)$$

λ is constant only if the charge is distributed uniformly over a length.

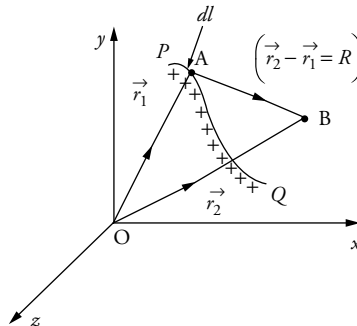


Figure 10.7 Line charge distribution.

2. Surface Charge Distribution

For surface charge distribution, the charge is continuously distributed over an entire surface. Let q be the total charge distributed on surfaces (Figure 10.8). Then dq is small charge for small area ds , such that surface charge density is given by

$$\sigma = \frac{dq}{ds} \quad (43)$$

The electric field can be written as

$$\vec{E} = \frac{\sigma}{4\pi\epsilon_0} \int \frac{ds \hat{R}}{R^2} \quad (44)$$

For uniform charge distribution, σ is constant for entire surface.

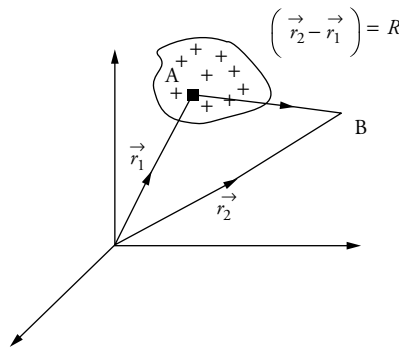


Figure 10.8 Surface charge distribution.

3. Volume Charge Distribution

For volume charge distribution, the charge is distributed inside whole volume. Let q be the total charge distributed inside a volume (Figure 10.9). Then dq be small charges for small volume dV , such that volume charge density is given by

$$\rho = \frac{dq}{dV} \quad (45)$$

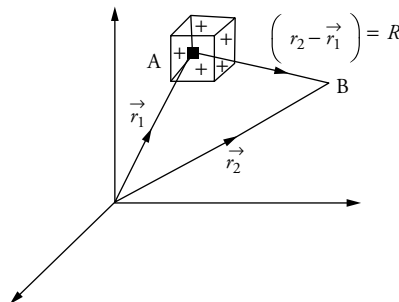


Figure 10.9 Volume charge distribution.

The electric field can be written as

$$\vec{E} = \frac{\rho}{4\pi\epsilon_0} \int \frac{dV \hat{R}}{R^2} \quad (46)$$

Like line and surface charge distributions, volume charge density ρ is constant for homogenous uniform distribution. In the following sections, we will find electric field in different geometries such as line, ring, sheets, etc.

10.10.1 Uniformly Charged Infinite Wire

Let us take an infinite wire along y -axis (Figure 10.10). Take a small part PQ of length dl such that it has charge dq [q is distributed along whole length of infinite wire].

Then,

$$\lambda = \frac{dq}{dl} \quad (47)$$

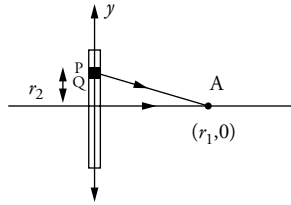


Figure 10.10 Uniformly charged infinite wire.

$$\begin{cases} \vec{r}_1 = x\hat{i} \\ \vec{r}_2 = y\hat{j} \end{cases}$$

and

$$\begin{aligned} d\vec{E} &= \frac{1}{4\pi\epsilon_0} \frac{dq(\vec{r}_1 - \vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|^3} \\ \Rightarrow \vec{E} &= \int_{-\infty}^{\infty} dE = \int_{-\infty}^{\infty} \frac{\lambda dl(x\hat{i} - y\hat{j})}{4\pi\epsilon_0(x^2 + y^2)^{3/2}} \\ \vec{E} &= \frac{\lambda}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{dl(x\hat{i} - y\hat{j})}{(x^2 + y^2)^{3/2}} \\ \vec{E} &= \frac{\lambda x\hat{i}}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{dl}{(x^2 + y^2)^{3/2}} - \frac{\lambda y\hat{j}}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{y dl}{(x^2 + y^2)^{3/2}} \end{aligned}$$

Substitute

$$y = x \tan \theta$$

then

$$dy = x \sec^2 \theta d\theta$$

then

$$y = -\infty \Rightarrow \theta = -\pi/2$$

$$y = \infty \Rightarrow \theta = \pi/2$$

$$\vec{E} = \frac{\lambda x \hat{i}}{4\pi\epsilon_0} \int_{-\pi/2}^{\pi/2} \frac{\cos\theta d\theta}{x^2} - \frac{\lambda \hat{i}}{4\pi\epsilon_0} \int_{-\pi/2}^{\pi/2} \sin\theta d\theta$$

$$\Rightarrow \vec{E} = \frac{\lambda \hat{i}}{4\pi\epsilon_0 x} \quad (48)$$

The electric field due to infinite long wire is along x -axis and inversely proportional to the distance.

10.10.2 Uniformly Charged Ring

Let (r_0) be the radius of charged ring. Let PQ be the small arc over which charge dq is distributed (Figure 10.11). Then,

$$\lambda = \frac{dq}{dr}$$

$$dq = \lambda dr \quad (49)$$

Using the relation $\text{angle} = \frac{\text{arc}}{\text{radius}}$

$$d\theta = \frac{dr}{r_0}$$

$$dr = r_0 d\theta \quad (50)$$

Let A be the observation point with coordinates $(0, 0, z)$, such that the position vector of A is \vec{r} . Hence,

$$\vec{r} = z \hat{k} \quad (51)$$

The electric field is given by

$$d\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{dq(\vec{r} - \vec{r}_0)}{|\vec{r} - \vec{r}_0|^3} \quad (52)$$

$$[\vec{r}_0 = x\hat{i} + y\hat{j}]$$

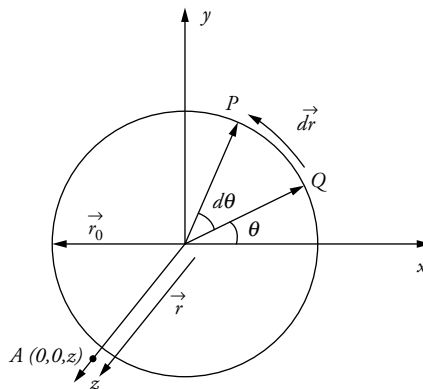


Figure 10.11 Uniformly charged ring.

$$\vec{r} - \vec{r}_0 = z \hat{k} - (r_0 \cos \theta \hat{i} + r_0 \sin \theta \hat{j}) \quad (53)$$

$$|\vec{r} - \vec{r}_0| = (z^2 + r_0^2)^{1/2} \quad (54)$$

Equation (52) can be written as

$$\begin{aligned} \vec{E} &= \int_0^{2\pi} \vec{dE} = \frac{1}{4\pi\epsilon_0} \int_0^{2\pi} \frac{\lambda r_0 d\theta (z \hat{k} - (x \hat{i} + y \hat{j}))}{(z^2 + r_0^2)^{3/2}} \\ E &= \frac{\lambda r_0}{4\pi\epsilon_0 (z^2 + r_0^2)^{3/2}} \int_0^{2\pi} (z \hat{k} d\theta - r_0 \hat{i} \cos \theta d\theta - r_0 \hat{j} \sin \theta d\theta) \\ E &= \frac{\lambda r_0}{4\pi\epsilon_0 (z^2 + r_0^2)^{3/2}} [2\pi z \hat{k}] \\ \vec{E} &= \frac{\lambda r_0 z \hat{k}}{2\epsilon_0 (z^2 + r_0^2)^{3/2}} \quad (55) \end{aligned}$$

λ can also be given as $\lambda = \frac{q}{2\pi r_0}$

$$\vec{E} = \frac{q z \hat{k}}{4\pi r_0 (z^2 + r_0^2)^{3/2}} \quad (56)$$

Hence, if the ring is in x - y plane, then the electric field should be along z -direction.

Special Case: This case can be applied to circular disc also (Fig. 10.12). We consider a disc with radius r_1 and r_2 (outer edge). We consider a small elementary ring of thickness dr_1 . The area of the ring is $2\pi r_1 dr_1$. The surface charge density can be given by

$$\sigma = \frac{dq}{ds}$$

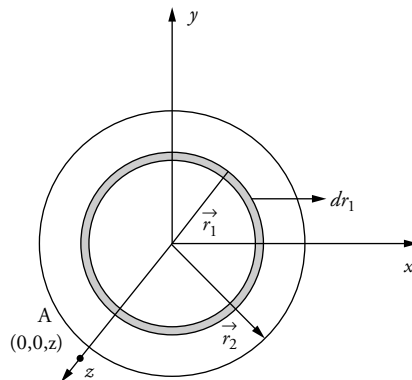


Figure 10.12 Circular disc.

$$dq = \sigma ds = \sigma 2\pi r_1 dr_1 \quad (57)$$

From Eqn. (56),

$$\overline{dE} = \frac{dq z \hat{k}}{4\pi\epsilon_0 (z^2 + r_1^2)^{3/2}} \quad (58)$$

$$\overline{E} = \int_0^{r_2} dE = \frac{1}{4\pi\epsilon_0} \int_0^{r_2} \frac{dq z \hat{k}}{(z^2 + r_1^2)^{3/2}}$$

$$\overline{E} = \frac{1}{4\pi\epsilon_0} \int_0^{r_2} \frac{\sigma 2\pi r_1 dr_1 z \hat{k}}{(z^2 + r_1^2)^{3/2}}$$

Put	$z^2 + r_1^2 = x$	}	limit charge to	$x = z^2$
	$r_1 dr_1 = \frac{dx}{2}$		$x = z^2 + r_2^2$	

$$\overline{E} = \frac{2\pi\sigma z \hat{k}}{4\pi\epsilon_0} \int_{z^2}^{z^2+r_2^2} \frac{dx}{2x^{3/2}}$$

$$\overline{E} = \frac{\sigma z \hat{k}}{2\epsilon_0} \left[\frac{1}{|z|} - \frac{1}{(z^2 + r_2^2)^{1/2}} \right] \quad (59)$$

Hence, again the electric field is in z -direction. If $|z| = z$, then Eqn. (59) is given by

$$\overline{E} = \frac{\sigma \hat{k}}{2\epsilon_0} \left[1 - \frac{z}{\sqrt{z^2 + r_2^2}} \right]$$

$$|E| = \frac{\sigma}{2\epsilon_0} \left[1 - \frac{z}{\sqrt{z^2 + r_2^2}} \right] \quad (60)$$

Equation (60) indicates that when z tends to infinity, electric field decreases.

When $z = 0$,

$$|E| = \frac{\sigma}{2\epsilon_0} \quad (61)$$

When $|z| = -z$, Eqn. (59) becomes

$$|E| = -\frac{\sigma}{2\epsilon_0} \left[1 + \frac{z}{\sqrt{z^2 + r_2^2}} \right] \quad (62)$$

Hence, the center acts as a point of discontinuity and electric field can take sudden jump on either side.

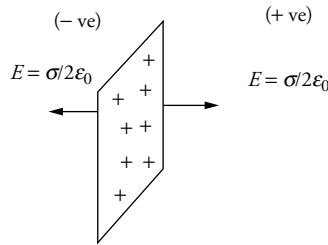


Figure 10.13 Infinite sheet.

When $r_2 \rightarrow \infty$, disc behaves as an infinite sheet of charge (Figure 10.13). Two cases arise when $r_2 \rightarrow \infty$ i.e.

(i) When $|z| = z$

$$\vec{E} = \frac{\sigma}{2\epsilon_0} \hat{k} \tag{63a}$$

(ii) When $|z| = -z$

$$\vec{E} = \frac{-\sigma}{2\epsilon_0} \hat{k} \tag{63b}$$

Hence, the electric field is no longer dependent on the distance between the observation point and source charge. Across the boundary, the electric field jumps from negative to positive.

10.10.3 Field Due to Two Infinite Charge Plane Sheet

Let X and Y be two plane sheets (Fig. 10.14) separated by “ d .” X has surface charge density “ σ ” and Y has surface charge density of “ $-\sigma$.”

We will find electric field at three points as follows:

(i) For point A

We have
$$\vec{E}_x = \frac{-\sigma}{2\epsilon_0} \hat{k}$$

Similarly,
$$\vec{E}_y = -\left(\frac{-\sigma}{2\epsilon_0}\right) \hat{k}$$

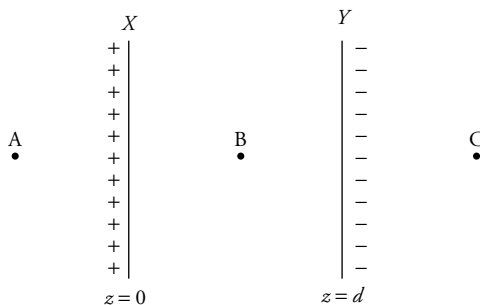


Figure 10.14 Two infinite plane sheets separated by distance d .

Hence,
$$\vec{E} = \frac{-\sigma \hat{k}}{2\epsilon_0} + \frac{\sigma}{2\epsilon_0} \hat{k} = 0 \quad (64a)$$

(ii) For point B , we have

$$\vec{E}_x = \frac{\sigma \hat{k}}{2\epsilon_0}$$

and

$$\vec{E}_y = -\left(\frac{-\sigma \hat{k}}{2\epsilon_0}\right)$$

$$\vec{E} = \frac{\sigma}{2\epsilon_0} \hat{k} + \frac{\sigma}{2\epsilon_0} \hat{k} = \frac{\sigma}{\epsilon_0} \hat{k} \quad (64b)$$

(iii) For point C , we have

$$\vec{E}_x = +\frac{\sigma}{2\epsilon_0} \hat{k}$$

Similarly,

$$\vec{E}_y = -\frac{\sigma}{2\epsilon_0} \hat{k}$$

$$\vec{E} = E_x + E_y = 0 \quad (64c)$$

Hence, the electric field exists only between the parallel plates and is independent of the distance.

10.11 Gauss Theorem

The density of field lines around the charge describes the intensity of field. We will define electric flux density (D). The electric field E at a distance r is given by

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2} \hat{r} \quad (65)$$

$$\epsilon_0 \vec{E} = \frac{q \hat{r}}{4\pi r^2} \quad (66)$$

$$\vec{D} = \frac{q \hat{r}}{4\pi r^2} \quad (67)$$

Here $\Rightarrow \vec{D} = \epsilon_0 \vec{E}$ is known as displacement density.

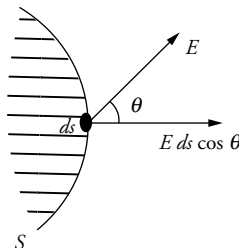


Figure 10.15 Flux over a surface.

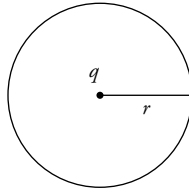


Figure 10.16 Spherical surface enclosing charge q .

Let ds be the small area over a sphere (Figure 10.15). Then the number of lines passing through small area ds is

$$d\phi = \vec{E} \cdot \vec{ds}$$

Hence, the total flux is given by (for a closed surface)

$$\phi = \int d\phi = \oiint_s \vec{E} \cdot \vec{ds} \quad (68)$$

If for a spherical surface with radius r and enclosing charge q as shown in Figure 10.16, then electric field is given by (magnitude only)

$$E = \frac{q}{4\pi\epsilon_0 r^2}$$

From Eqn. (68)

$$\phi = \oiint E ds \cos\theta$$

When electric field and area vector are in same direction then $\theta = 0$

$$\phi = \oint \frac{q(4\pi r^2)}{4\pi\epsilon_0 r^2}$$

$$\phi = \frac{q}{\epsilon_0} \quad (69a)$$

Hence,

$$\oiint \vec{E} \cdot \vec{ds} = \frac{q}{\epsilon_0} \quad (69b)$$

According to Gauss theorem, “The total electric flux emanating out of a closed surface is $\frac{1}{\epsilon_0}$ times the total charge (q) enclosed inside the surface.” Other alternative definition is “The surface integral of electric field over a closed surface is $\frac{1}{\epsilon_0}$ times the total charge (q) enclosed inside the surface.”

The flux is outward for positive charge and inward for negative charge. The flux is only due to the charges that are enclosed inside a surface. The charges outside the closed surface do not contribute to the electric flux.

10.11.1 Deduction of Coulomb's Law

Let us take a Gaussian surface enclosing charge q and r is the radius as shown in Figure 10.17. As E and ds (area vector) are radial, hence Gauss's law is given by

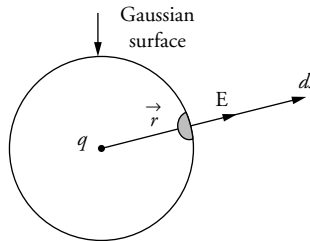


Figure 10.17 Surface enclosing charge q .

$$\oint E \cdot ds = \frac{q}{\epsilon_0}$$

$$\oint E ds = \frac{q}{\epsilon_0} \quad \left[\begin{array}{l} \text{for radial electric field,} \\ \theta = 0 \end{array} \right]$$

$$E \oint ds = \frac{q}{\epsilon_0}$$

$$E = \frac{q}{4\pi r^2 \epsilon_0}$$

$$\vec{E} = \frac{q \hat{r}}{4\pi \epsilon_0 r^3} \quad (70)$$

Hence, Coulomb's law can be obtained from Gauss's law.

10.11.2 Differential Form of Coulomb's Law

Consider a surface S enclosing charge q (Figure 10.18). Let \vec{ds} be a small part on entire surface S . The area vector \vec{ds} is normal to the surface, such that it makes an angle θ with the electric field. For a volume charge distribution,

$$\rho = \frac{dq}{dV} \quad \left[\begin{array}{l} \text{where } dV \text{ is the small volume} \\ \text{enclosing charge } dq \end{array} \right] \quad (71a)$$

From Eqn. (69b)

$$\oint \vec{E} \cdot \vec{ds} = \frac{q}{\epsilon_0} \quad (71b)$$

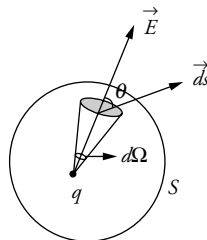


Figure 10.18 Small surface showing area vector and electric field.

From Eqn. (10)

$$\bar{\nabla} \cdot \bar{A} = \frac{\oint \bar{A} \cdot \bar{d}s}{\Delta V}$$

$$(\bar{\nabla} \cdot \bar{A}) \Delta V = \oint \bar{A} \cdot \bar{d}s$$

For total volume, the flux emanating can be written as

$$\iiint_v (\bar{\nabla} \cdot \bar{A}) dV = \oint \bar{A} \cdot \bar{d}s \quad (71c)$$

Using Eqn. (71c) in Eqn. (71b), we can write

$$\iiint_v (\nabla \cdot E) dV = \frac{q}{\epsilon_0} \quad (72)$$

From Eqn. (71a), we write

$$q = \iiint_v \rho dV \quad (73)$$

Using Eqn. (73) in Eqn. (72)

$$\iiint_v (\bar{\nabla} \cdot \bar{E}) dV = \iiint_v \frac{\rho}{\epsilon_0} dV$$

$$\iiint_v \left(\bar{\nabla} \cdot \bar{E} - \frac{\rho}{\epsilon_0} \right) dV = 0$$

As the volume cannot be zero, the term in bracket is zero:

$$\bar{\nabla} \cdot \bar{E} = \frac{\rho}{\epsilon_0} \quad (74)$$

Equation (74) is known as the differential form of Gauss's Law.

Carl Friedrich Gauss was born on April 30, 1777, in Brunswick, Germany, to a very poor family. His father was a gardener and brick layer. His mother put lot of efforts to educate him. The Duke of Brunswick observed the computing and mathematical skills when Gauss was only 14 years old. After meeting Gauss, the Duke was so impressed that he financially supported him to continue his studies at Caroline College. He further financed Coulomb's stay at the Brunswick Collegium Carolinum, Hanover. Gauss attended the University of Göttingen from 1795 to 1798; afterwards he got his doctorate in 1799 at the University of Helmstedt. At the end of his college years, Gauss made a magnificent discovery of finding a regular polygon with 17 sides, which could be drawn using just a compass and straight edge. Gauss was immensely happy and proud of his discovery. He decided to give up his intention to study languages and turned to mathematics.



CARL FRIEDRICH GAUSS

In 1807, Gauss was appointed as the director of the Göttingen Observatory. He worked hard to establish the laboratory; furthermore, his hard work of six years with Wilhelm Weber led to the invention of primitive telegraph device, which could send messages over a distance of 1,500 m. Carl Friedrich Gauss wrote more than 300 papers, mostly in Latin and made calculations of the orbits of the asteroids Ceres and Pallas. He won the Copley Medal in 1838. He died on February 23, 1855, in Göttingen, Germany, at the age of 77 years.



STATUE OF WEBER AND GAUSS

10.12 Electrostatic Potential

Electrostatic potential is defined as the amount of work done in bringing a unit positive charge from infinity to an observation point. Electric field is zero at infinity. Mathematically, the potential is written by following expression:

$$V = -\int_{\infty}^A \vec{E} \cdot d\vec{l} \quad (75)$$

Hence, potential can be defined as the line integral of electric field. Similarly, we can find out the potential difference between two points. Let a charge q is moved through distance dl , from point A to B . Suppose F is the force on the charge that is equal to electrostatic force qE , the work done is given by

$$dW = -\vec{F} \cdot d\vec{l}$$

$$dW = -q\vec{E} \cdot d\vec{l}$$

[the charge is to be moved against the electrostatic force]

$$W_{AB} = -\int_A^B q\vec{E} \cdot d\vec{l}$$

$$\frac{W_{AB}}{q} = -\int_A^B \vec{E} \cdot d\vec{l}$$

$$\frac{W_{AB}}{q} = V_B - V_A = -\int_A^B \vec{E} \cdot d\vec{l} \quad (76)$$

Equation (76) represents the work done in moving a charge from point A to B . The potential difference is defined as the amount of work done in moving unit charge from one point to another point.

We will define 1V now. From Eqn. (76)

$$\frac{1 \text{ Joule}}{1 \text{ Coulomb}} = 1 \text{ Volt} \quad (77)$$

The potential difference is said to be 1 Volt when 1 Joule of work is done in moving 1 Coulomb charge from one point to another. We can express electric field in terms of potential V .

$$\text{Let} \quad V(a) = -\int_0^a \vec{E} \cdot d\vec{l} \quad (78a)$$

$$\text{and} \quad V(b) = -\int_0^b \vec{E} \cdot d\vec{l} \quad (78b)$$

Potential difference becomes [subtract Eqs (78b) and (78a)]

$$V(b) - V(a) = -\int_a^b \vec{E} \cdot d\vec{l} \quad (79)$$

From Eqn. (6) [fundamental gradient equation]

$$dV = \nabla V \cdot dl \quad (80a)$$

Substituting Eqn. (80a) in Eqn. (79),

$$\int_a^b \nabla V \cdot dl = -\int_a^b \vec{E} \cdot d\vec{l}$$

$$\text{Hence,} \quad \vec{E} = -\nabla V \quad (80b)$$

Hence, electric field can be expressed as the gradient of the potential. Hence, when potential is known then the electric field can be calculated. Potential also obeys superposition principle, that is,

$$V = V_1 + V_2 + \dots + V_n \quad (81)$$

as potential is scalar in nature; hence, Eqn. (81) gives the ordinary sum, it is not the vector sum.

10.13 Potential for Continuous Charge Distribution

Potential can be given by

$$V(r) = -\int_{\infty}^r \vec{E} \cdot d\vec{r}$$

Hence, for $E = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}$, the above equation can be evaluated as r

$$V(r) = -\frac{1}{4\pi\epsilon_0} \int_{\infty}^r \frac{q}{r^2} dr$$

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{q}{r} \quad (82)$$

Equation (82) represents the potential at a point due to point charge q . For a group of n charges, Eqn. (82) is written as

$$V(r) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{q_i}{r_i} \quad (83)$$

For continuous charge distribution, the potential can be given by

(i) Line charge distribution

As electric field
$$E = \frac{1}{4\pi\epsilon_0} \int \frac{\lambda dl}{r^2} \quad \text{[from Eqn. (82)]}$$

Similarly,
$$V(r) = \frac{1}{4\pi\epsilon_0} \int \frac{\lambda dl}{r} \quad (84a)$$

(ii) Surface charge distribution

$$V(r) = \frac{1}{4\pi\epsilon_0} \int \frac{\sigma ds}{r} \quad (84b)$$

(iii) Volume charge distribution

$$V(r) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho dV}{r} \quad (84c)$$

10.14 Dielectrics

Dielectric materials are nonconducting materials that exhibit polarization under the effect of electric field. When the dielectric materials are kept under the influence of electric field, the charge inside their body gets separated and material exhibits dipole moment. Hence, dielectrics store charge inside them. A good dielectric material is a good insulator also. An insulator material has low conductivity and dielectric materials have high dielectric constant. Greater dielectric constant helps in storing large amount of energy. The dielectric constant is defined as

$$\text{Dielectric constant} = \frac{\text{Capacitance of capacitor with dielectric material}}{\text{Capacitance of same capacitor when dielectric is replaced by vacuum}} \quad (85)$$

$$K = \frac{C}{C_0} \quad (86)$$

Dielectric constant is defined as the ratio of capacitance of capacitor with dielectric material to the capacitance of same capacitor when the dielectric medium is replaced by vacuum. Capacitance is the ability of a capacitor to store charge.

10.14.1 Dielectric Polarization

The molecules are said to be nonpolar when the center of gravity of positive and negative charges coincide with each other. For example, H_2 , N_2 , and O_2 are nonpolar molecules as shown in Figure 10.19(a).

When the nonpolar molecule is kept inside the electric field, the charge separation occurs, that is, positive and negative charges are separated by some distance d as shown in Figure 10.19(b). Hence, the molecule is induced with electric dipole moment. We can treat nonpolar molecule as an electric dipole in the presence of electric field. When electric field is removed, the polar molecule returns to its original re-orientation. Conclusively, when the center of gravity of positive and negative charges is separated by some distance, it is said to be polar molecule.

If the molecule is inherently polar, that is, polar even in the absence of electric field, then there is no net dipole moment on the dielectric. Under the influence of electric field, the dipoles orient along the direction of electric field and is yielded net dipole moment.

The electric polarization \vec{P} of a material is defined as the electric dipole moment of material per unit volume, such that

$$\vec{P} = N \vec{p} \quad (87)$$

where N is number of atoms/molecules per unit volume and \vec{p} is induced dipole moment, which is proportional to electric field. Hence,

$$\begin{aligned} \vec{p} &\propto \vec{E} \\ \vec{p} &= \alpha \vec{E} \end{aligned} \quad (88)$$

α is defined as the molecular polarizability for the dielectric. Figure 10.20 represents the polarization of dielectric.

When electric field is applied to the dielectric, the stretching of molecule occurs. This stretching of the atoms of dielectric material under the influence of electric field is called dielectric polarization. The charges that are displaced are known as polarization charges. We will find out the relation between polarization and surface charge density as follows:

$$P = \frac{\text{dipole moment}}{\text{volume of dielectrics}}$$

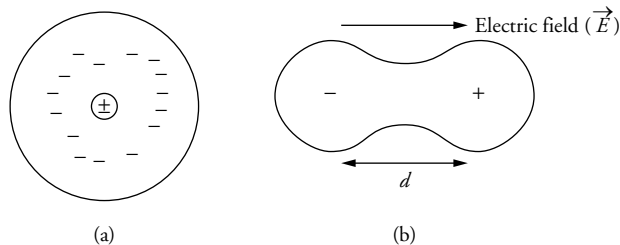


Figure 10.19 (a) Nonpolar molecule (b) Polar molecule

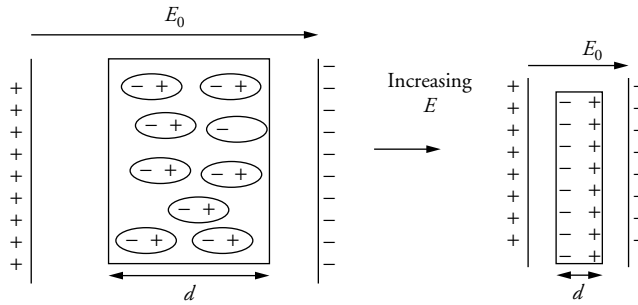


Figure 10.20 Dielectric polarization.

$$\bar{P} = \frac{\text{charge} \times \text{thickness}}{\text{area} \times \text{thickness}}$$

$$\bar{P} = \frac{qd}{Ad} = \sigma_i \quad [\sigma_i = \text{induced charge density}] \quad (89)$$

Hence, the polarization P is equal to surface density of induced charge for a homogenous isotropic dielectric.

10.14.2 Displacement Vector

Displacement vector is given by \bar{D} . There are two types of electric field in the dielectric, that is, external applied field E_0 and induced field due to induced charges E_i as shown in Figure 10.21.

Then the net electric field in the dielectric is given by

$$\bar{E} = \bar{E}_0 - \bar{E}_i$$

$$\bar{E} = \frac{\sigma}{\epsilon_0} - \frac{\sigma_i}{\epsilon_0}$$

$$\epsilon_0 \bar{E} = \sigma - \sigma_i$$

$$\epsilon_0 \bar{E} = \sigma - \bar{P} \quad [\text{from Eqn. (89)}] \quad (90)$$

Furthermore

$$\epsilon_0 \bar{E} = \bar{D} - \bar{P}$$

$$\bar{D} = \epsilon_0 \bar{E} + \bar{P} \quad (91)$$

where \bar{D} is an auxiliary vector with magnitude equal to surface charge density of free charges. Hence, we can say that \bar{E} consists of free and bound charges where \bar{D} is only dependent on free charge density. From Eqn. (90), we can write

$$\bar{P} = \sigma - \epsilon_0 \bar{E} \quad [\sigma = D] \quad (92a)$$

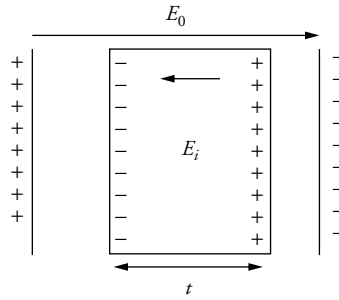


Figure 10.21 Two types of electric field in dielectric (t is the thickness of dielectric).

We know that dielectric constant $K(\epsilon_r)$ is defined as

$$\epsilon_r = K = \frac{E_0}{E}$$

$$E = \frac{E_0}{\epsilon_r} = \frac{\sigma}{\epsilon_0 \epsilon_r} \quad \left[E_0 = \frac{\sigma}{\epsilon_0} \right] \text{ (between the plates of capacitor) } \quad (92b)$$

Using Eqn. (92b) in Eqn. (92a),

$$\vec{P} = \epsilon_0 \epsilon_r \vec{E} - \epsilon_0 \vec{E}$$

$$\vec{P} = (\epsilon_r - 1) \epsilon_0 \vec{E}$$

$$\frac{\vec{P}}{\epsilon_0 \vec{E}} = \epsilon_r - 1 = \chi_e = \text{electric susceptibility}$$

$$\text{Hence, } \epsilon_r = 1 + \chi_e \quad (92c)$$

10.15 Types of Polarization

Under the effect of electric field, the charge distribution can get distorted and hence give rise to induced polarization. If the molecule is already polar in nature, then the field aligns the randomly oriented dipoles. There are four main types of polarization.

10.15.1 Electronic Polarization

When the center of gravity of positive and negative charges gets separated, the atom starts behaving like a dipole. Hence, shifting of electron cloud from the positively charged nucleus results in net dipole moment. The dipole moment is given by

$$p_e = qd \quad (93a)$$

For Eqs (87) and (88), we write electronic polarization as (\vec{P}_e)

$$\vec{P}_e = N \alpha_e \vec{E} \quad (93b)$$

α_e is the electronic polarizability, which is independent of temperature. Furthermore, the dielectric constant can be written as (Eqn. (92c))

$$\begin{aligned}\epsilon_r &= 1 + \chi_e \\ \epsilon_r &= 1 + \frac{\bar{P}_e}{\epsilon_0 \bar{E}} \\ \epsilon_r &= 1 + \frac{N\alpha_e}{\epsilon_0}\end{aligned}\quad (94)$$

Usually, monoatomic gases exhibit electronic polarizability. Hence, the dielectric constant for a monoatomic gas is a function of molecular density (number of molecules/volume) and electronic polarizability.

10.15.2 Ionic Polarization

When electric field is applied to materials, such that anions and cations get separated by a distance giving rise to net dipole moment, then it is known as ionic polarization. p_i is the ionic dipole moment. if \bar{P}_i is the ionic polarization, then

$$\bar{P}_i = N\alpha_i \bar{E} \quad (95)$$

where α_i is ionic polarization. Usually ionic polarizability is 10 times less than the electronic polarizability. The ionic polarizability is given by

$$\alpha_i = \frac{q^2}{w^2} \left[\frac{1}{m_1} + \frac{1}{m_2} \right] \quad (96)$$

where w is optical phonon frequency, q is charge of ion, m_1 and m_2 are masses of ions in even number and odd number planes, respectively.

10.15.3 Orientation Polarization

Some materials such as CH_3Cl , H_2O , etc., possess permanent dipole moment. When these materials are kept under the electric field, the randomly oriented dipoles orient themselves along the direction of electric field (Figure 10.22). This is known as orientation polarization. Orientation polarizations have an inverse relation with temperature. With increasing temperature, the orientation gets distorted and hence the orientation polarization decreases. The orientation polarizability is given by

$$\alpha_0 = \frac{p^2}{3k_B} \quad (97)$$

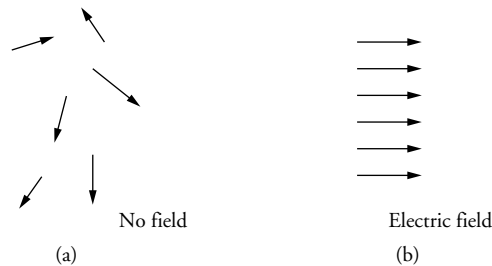


Figure 10.22 Orientation polarization.

where k_B is the Boltzmann's constant. The orientation polarization is given by

$$P_o = \frac{Np^2 E}{3k_B T} \quad (98)$$

Hence, orientation polarization has inverse relationship with temperature.

10.15.4 Space-Charge Polarization

Space-charge polarization is most common for multiphase materials. When multiphase materials are under the influence of electric field, the accumulation of charges takes place at the electrodes or inter phases. When field is applied, the ions get diffused over some appreciable distance. This gives rise to redistribution of charges (Figure 10.23).

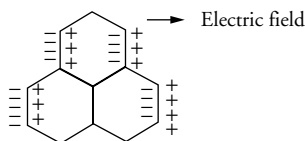


Figure 10.23 Space-charge polarization (P_s)

For single-phase dielectric, there is no space-charge polarization and total polarization is given by

$$P = P_e + P_i + P_o \quad (99a)$$

For multiphase dielectrics, there is space-charge polarization and hence total polarization is given by

$$P = P_e + P_i + P_o + P_s \quad (99b)$$

Michael Faraday was born on September 22, 1791, in Newington Butts, London. Faraday was born in a poor family and his father James was a blacksmith. He could not enjoy the luxuries and had to self-educate himself. He became friends with a local bookbinder and book-seller George Riebau, where he found himself in love with books. He studied inventions and discoveries of eminent scientists and authors where he developed an interest in science, especially in electricity. Furthermore, he began to attend lectures of different famous chemists to gain and learn. He also applied for a job under his chemistry lecturer Humphry Davy, who later appointed him as Chemical Assistant at the Royal Institution in 1813. While working under Davy, Faraday discovered two new carbon chlorides and produced several new kinds of optical glasses. In 1821, Faraday married Sarah Barnard whom he met at the Sandemanian church. After Davy's retirement in 1827, Faraday replaced him as lecturer of chemistry at the Royal Institution.



MICHAEL FARADAY

Faraday is best known for his contributions to electricity and magnetism. In 1821, he was inspired by the work of Hans Christian who was a Danish physicist and chemist. He started his experimentations regarding the conversion of electrical energy into motive force and finally succeeded in devising the electric motor. In 1831, Faraday constructed the first electric dynamo and discovered the induction of electric currents. In 1839, he established that electrostatic force consists of a field of curved lines. He made other discoveries such as the Faraday effect, the process of diamagnetism, and Faraday cage. His famous books are the *Experimental Researches in Electricity* and the *Chemical History of the Candle*. He also received a Doctor of Civil Law degree in 1832 by the University of Oxford. The British government granted him a pension and a house in Hampton Court for his great contribution to science, where he spent the rest of his life after his retirement in 1858. The great British scientist's soul departed from this world on August 25, 1867, leaving the scientific community in shock.

SUMMARY

This chapter introduced scalar and vector fields. Scalar function was used to evaluate the gradient and vector function is used to find curl and divergence. When divergence is zero, the field is solenoidal, whereas when curl of vector is zero, it is known as irrotational. Charge is also understood as a property of body causing attraction or repulsion. Using the charges and distance between them, Coulomb provided concept of electrostatic force of attraction or repulsion. Coulomb force is regarded as conservative force as it follows inverse square law. It also follows Newton's third law of motion and superposition force. Electric field is regarded as the modification of surroundings of source charge, such that test charge feels the force. Electric lines of force determine the direction of force. The electric field for uniformly charged infinite wire varies inversely as the distance between point of observation and source charge. Fields due to infinite charged sheets is independent of the distance. Gauss theorem demonstrated that the surface integral of electric field over a closed surface is $\frac{1}{\epsilon_0}$ times, the charge enclosed within the surface. Electric potential is also given by negative gradient of potential. Dielectric materials are regarded as nonconducting materials exhibiting polarization under the effect of electric-field. The polarization of dielectric depends directly on the electric field. Polarization can be divided in four categories: electronic polarization, ionic polarization, orientation polarization, and space-charge polarization.

SOLVED EXAMPLES

Q.1: If $\phi = 2y^2z + 5x^3y$, obtain the value of $\text{grad } \phi$ at $(1, 1, 2)$.

Ans:
$$\nabla\phi = \hat{i} \frac{\partial\phi}{\partial x} + \hat{j} \frac{\partial\phi}{\partial y} + \hat{k} \frac{\partial\phi}{\partial z}$$

Here, $\phi = 2y^2z + 5x^3y$

$$\frac{\partial\phi}{\partial x} = 15x^2y$$

$$\frac{\partial \phi}{\partial y} = 4yz + 5x^3$$

$$\frac{\partial \phi}{\partial z} = 2y^2$$

$$\nabla \phi = \hat{i}(15x^2y) + \hat{j}(4yz + 5x^3) + \hat{k}(2y^2)$$

Substitute $x = 1, y = 1, z = 2$

$$\nabla \phi = 15\hat{i} + 13\hat{j} + 2\hat{k}$$

Q.2: If $\phi = 6xy - y^2z^2 + 8xz$, obtain $\text{grad } \phi$ at $(-2, 1, 2)$.

Ans:
$$\phi = 6xy - y^2z^2 + 8xz$$

$$\frac{\partial \phi}{\partial x} = 6y + 8z \quad \frac{\partial \phi}{\partial y} = 6x - 2yz^2$$

$$\frac{\partial \phi}{\partial z} = -2y^2z + 8x$$

$$\nabla \phi = \hat{i} \frac{\partial \phi}{\partial x} + \hat{j} \frac{\partial \phi}{\partial y} + \hat{k} \frac{\partial \phi}{\partial z}$$

$$\nabla \phi = \hat{i}(6y + 8z) + \hat{j}(6x - 2yz^2) + \hat{k}(-2y^2z + 8x)$$

For points $(-2, 1, 2)$

$$\nabla \phi = 22\hat{i} - 20\hat{j} - 20\hat{k}$$

Q.3: If $\vec{A} = 2x^2\hat{i} - 3xy\hat{j} + 5y^2z^2\hat{k}$, obtain the divergence of \vec{A} at $(1, -2, 1)$.

Ans:
$$\vec{\nabla} \cdot \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$

Le
$$\vec{A} = 2x^2\hat{i} - 3xy\hat{j} + 5y^2z^2\hat{k}$$

$$\vec{\nabla} \cdot \vec{A} = \frac{\partial}{\partial x}(2x^2) + \frac{\partial}{\partial y}(-3xy) + \frac{\partial}{\partial z}(5y^2z^2)$$

$$A_x = 2x^2, A_y = -3xy, A_z = 5y^2z^2$$

$$\vec{\nabla} \cdot \vec{A} = 4x - 3x + 10y^2z$$

At $x=1$, $y=-2$, and $z=1$

$$\vec{\nabla} \cdot \vec{A} = 4(1) - 3(1) + 10(-2)^2(1)$$

$$\vec{\nabla} \cdot \vec{A} = 4 - 3 + 40$$

$$\vec{\nabla} \cdot \vec{A} = 41$$

Q.4: Given $\vec{A} = 2e^{-x}\hat{i} + 6y^2e^{-x}\hat{j} + 2x^2z\hat{k}$, obtain its divergence.

Ans: $\vec{A} = 2e^{-x}\hat{i} + 6y^2e^{-x}\hat{j} + 2x^2z\hat{k}$

$$A_x = 2e^{-x}, A_y = 6y^2e^{-x}, A_z = 2x^2z$$

$$\frac{\partial A_x}{\partial x} = -2e^{-x}, \frac{\partial A_y}{\partial y} = 12ye^{-x}, A_z = 2x^2$$

$$\vec{\nabla} \cdot \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$

$$\vec{\nabla} \cdot \vec{A} = -2e^{-x} + 12ye^{-x} + 2x^2$$

Q.5: Obtain the curl for position vector \vec{r} .

Ans: $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

$$\vec{\nabla} \times \vec{r} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ x & y & z \end{vmatrix}$$

$$= \hat{i} \left[\frac{\partial z}{\partial y} - \frac{\partial y}{\partial z} \right] - \hat{j} \left[\frac{\partial z}{\partial x} - \frac{\partial x}{\partial z} \right] + \hat{k} \left[\frac{\partial y}{\partial x} - \frac{\partial x}{\partial y} \right]$$

$$= \hat{i}[0-0] - \hat{j}[0-0] + \hat{k}[0-0]$$

$$= 0$$

Q.6: Obtain the curl for $r^n \vec{r}$ and $\left(\frac{\vec{r}}{r^3}\right)$, where \vec{r} is position vector.

Ans: $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$r^n = (x^2 + y^2 + z^2)^{n/2}$$

Hence,

$$\begin{aligned}
 \text{(i)} \quad r^n \vec{r} &= (x^2 + y^2 + z^2)^{n/2} [x\hat{i} + y\hat{j} + z\hat{k}] \\
 &= (x^2 + y^2 + z^2)^{n/2} x\hat{i} + (x^2 + y^2 + z^2)^{n/2} y\hat{j} + (x^2 + y^2 + z^2)^{n/2} z\hat{k} \\
 \vec{\nabla} \times (r^n \vec{r}) &= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ (x^2 + y^2 + z^2)^{n/2} x & (x^2 + y^2 + z^2)^{n/2} y & (x^2 + y^2 + z^2)^{n/2} z \end{vmatrix} \\
 &= \hat{i} \left[\frac{\partial}{\partial y} [z(x^2 + y^2 + z^2)^{n/2}] - \frac{\partial}{\partial z} [y(x^2 + y^2 + z^2)^{n/2}] \right] \\
 &\quad - \hat{j} \left[\frac{\partial}{\partial x} [z(x^2 + y^2 + z^2)^{n/2}] - \frac{\partial}{\partial z} [x(x^2 + y^2 + z^2)^{n/2}] \right] \\
 &\quad + \hat{k} \left[\frac{\partial}{\partial x} [y(x^2 + y^2 + z^2)^{n/2}] - \frac{\partial}{\partial y} [x(x^2 + y^2 + z^2)^{n/2}] \right] \\
 &= \hat{i} \left[zyn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} - yzn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} \right] \\
 &\quad - \hat{j} \left[xzn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} - xzn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} \right] \\
 &\quad + \hat{k} \left[xyn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} - xyn(x^2 + y^2 + z^2)^{\frac{n-2}{2}} \right] \\
 \vec{\nabla} \times (r^n \vec{r}) &= 0
 \end{aligned}$$

$$\text{(ii) For } \frac{\vec{r}}{r^3} = \frac{x\hat{i} + y\hat{j} + z\hat{k}}{(x^2 + y^2 + z^2)^{3/2}},$$

$$\vec{\nabla} \times \left(\frac{\vec{r}}{r^3} \right) = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ x(x^2 + y^2 + z^2)^{-3/2} & y(x^2 + y^2 + z^2)^{-3/2} & z(x^2 + y^2 + z^2)^{-3/2} \end{vmatrix}$$

$$\begin{aligned}
\vec{\nabla} \times \left(\frac{\vec{r}}{r^3} \right) &= \hat{i} \left[\frac{\partial}{\partial y} \left(z(x^2 + y^2 + z^2)^{-3/2} \right) - \frac{\partial}{\partial z} \left(y(x^2 + y^2 + z^2)^{-3/2} \right) \right] \\
&\quad - \hat{j} \left[\frac{\partial}{\partial x} \left(z(x^2 + y^2 + z^2)^{-3/2} \right) - \frac{\partial}{\partial z} \left(x(x^2 + y^2 + z^2)^{-3/2} \right) \right] \\
&\quad + \hat{k} \left[\frac{\partial}{\partial x} \left(y(x^2 + y^2 + z^2)^{-3/2} \right) - \frac{\partial}{\partial y} \left(x(x^2 + y^2 + z^2)^{-3/2} \right) \right] \\
\vec{\nabla} \times \left(\frac{\vec{r}}{r^3} \right) &= \hat{i} \left[-3yz(x^2 + y^2 + z^2)^{-5/2} + 3yz(x^2 + y^2 + z^2)^{-5/2} \right] \\
&\quad - \hat{j} \left[-3xz(x^2 + y^2 + z^2)^{-5/2} + 3xz(x^2 + y^2 + z^2)^{-5/2} \right] \\
&\quad + \hat{k} \left[-3xy(x^2 + y^2 + z^2)^{-5/2} + 3xy(x^2 + y^2 + z^2)^{-5/2} \right] \\
\vec{\nabla} \times \left(\frac{\vec{r}}{r^3} \right) &= 0
\end{aligned}$$

Q.7: Obtain the values a , b , and c if the field is irrotational.

$$\vec{A} = (2y + x + az)\hat{i} + (bx + 6y - z)\hat{j} + (2x - 2z + cy)\hat{k}$$

Ans: For irrotational fields,

$$\begin{aligned}
\vec{\nabla} \times \vec{A} &= 0 \\
\vec{\nabla} \times \vec{A} = 0 &= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ (2y + x + az) & (bx + 6y - z) & (2x - 2z + cy) \end{vmatrix} \\
0 &= \hat{i} \left[\frac{\partial}{\partial y} (2x - 2z + cy) - \frac{\partial}{\partial z} (bx + 6y - z) \right] \\
&\quad - \hat{j} \left[\frac{\partial}{\partial x} (2x - 2z + cy) - \frac{\partial}{\partial z} (2y + x + az) \right] \\
&\quad + \hat{k} \left[\frac{\partial}{\partial x} (bx + 6y - z) - \frac{\partial}{\partial y} (2y + x + az) \right] \\
0 &= \hat{i} [c + 1] - \hat{j} [2 - a] + \hat{k} [b - 2]
\end{aligned}$$

$$c + 1 = 0 \quad \Rightarrow \quad c = -1$$

$$2 - a = 0 \quad \Rightarrow \quad a = 2$$

$$b - a = 0 \quad \Rightarrow \quad b = 2$$

Q.8: Obtain the force between charges $q_1 = 2 \times 10^{-8} \text{ C}$ and $q_2 = 6 \mu\text{C}$ separated 20 cm apart in vacuum.

Ans:
$$F = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r^2}$$

$q_1 = 2 \times 10^{-8} \text{ C}$, $q_2 = 6 \times 10^{-6} \text{ C}$, and $r = 20 \text{ cm} = 0.2 \text{ m}$

$$F = \frac{9 \times 10^9 \times 2 \times 10^{-8} \times 6 \times 10^{-6}}{(0.2)^2}$$

$$F = \frac{108 \times 10^{-5}}{0.04}$$

$$F = \frac{108 \times 10^{-3}}{4} = 27 \times 10^{-3} \text{ N}$$

Q.9: What will be the magnitude of force between two charges of equal magnitude $2 \mu\text{C}$ separated by a distance of 10 cm in kerosene oil (K for kerosene = 2).

Ans:
$$q_1 = q_2 = 2 \times 10^{-6} \text{ C}$$

$$r = 0.1 \text{ m}$$

$$\frac{F_{\text{vac}}}{F_{\text{med}}} = K$$

$$F_{\text{med}} = \frac{F_{\text{vac}}}{K}$$

We will calculate F_{vac} first as follows:

$$F_{\text{vac}} = \frac{9 \times 10^9 \times 4 \times 10^{-12}}{0.01}$$

$$F_{\text{vac}} = 36 \times 10^{-3} \times 100$$

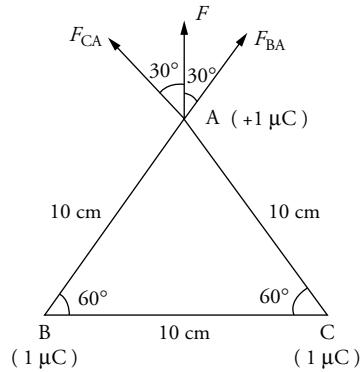
$$F_{\text{vac}} = 3.6 \text{ N}$$

In kerosene, the force changes to

$$F_{\text{med}} = \frac{F_{\text{vac}}}{K} = \frac{3.6}{2} = 1.8 \text{ N}$$

Hence, $F_{\text{med}} = 1.8 \text{ N}$

Q.10: The charges for $+1 \mu\text{C}$ are placed on the vertices of equilateral triangle of side 10 cm. Obtain the magnitude and direction of resultant force on one charge due to other charges.



Ans: The resultant force is F which is obtained from F_{BA} and F_{CA} .

$$F_{BA} = \frac{Kq_Bq_A}{r^2} \quad \text{and} \quad F_{CA} = \frac{Kq_Cq_A}{r^2}$$

$$F_{BA} = \frac{9 \times 10^9 \times (10^{-6})^2}{(0.1)^2}$$

$$F_{BA} = \frac{9 \times 10^9 \times 10^{-12} \times 100}{1}$$

$$F_{BA} = 0.9 \text{ N}$$

Similarly, $F_{CA} = 0.9 \text{ N}$

The resultant force F is given by

$$F = \sqrt{F_1^2 + F_2^2 + 2F_1F_2 \cos \theta}$$

The present case

$$F_1 = F_2 = F_{BA}$$

[θ is angle between \vec{F}_{BA} and \vec{F}_{CA}]

$$F = \sqrt{F_{BA}^2 + F_{BA}^2 + 2F_{BA}^2 \cos \theta}$$

$$F = 2 \times F_{BA} \times \cos \theta / 2$$

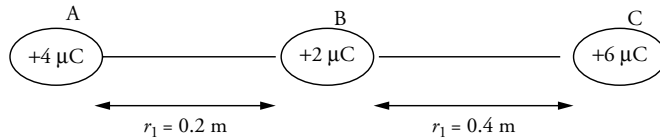
$$F = 2 \times 0.9 \times \cos 30^\circ$$

$$F = 1.8 \times \frac{\sqrt{3}}{2} = 0.9\sqrt{3}$$

$$F = 0.9 \times 1.73$$

$$F = 1.557 \text{ N}$$

Q.11: A charge of magnitude $+2 \mu\text{C}$ is placed in between two charges of magnitude $+4 \mu\text{C}$ and $+6 \mu\text{C}$. If $r_1 = 0.2 \text{ m}$ and $r_2 = 0.4 \text{ m}$, obtain the force on charge of magnitude $+2 \mu\text{C}$.



Ans:

$$F_{BA} = \frac{Kq_1q_2}{r_1^2} = \frac{9 \times 10^9 \times 4 \times 2 \times 10^{-12}}{(0.2)^2}$$

$$F_{BA} = \frac{72 \times 10^{-3} \times 100}{4}$$

$$F_{BA} = 1.8 \text{ N} \quad (\text{a})$$

$$F_{CB} = \frac{Kq_2q_3}{r_2^2}$$

$$F_{CB} = \frac{9 \times 10^9 \times 2 \times 6 \times 10^{-12}}{(0.4)^2}$$

$$= \frac{108 \times 10^{-3} \times 100}{16}$$

$$= 6.75 \times 10^{-1}$$

$$F_{CB} = 0.675 \text{ N} \quad (\text{b})$$

As F_{BA} and F_{CB} will be directed opposite to each other, the net magnitude is given by

$$F = F_{BA} - F_{CB}$$

$$F = 1.8 - 0.675 = 1.125 \text{ N}$$

Q.12: What is the magnitude of electric field between two charges of magnitude $-4 \mu\text{C}$ and $12 \mu\text{C}$ separated by a distance of 0.3 m ?

Ans:
$$E = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}$$

Here, $q = 12 \mu\text{C}$ as source charge is higher in magnitude than the test charge.

Therefore,
$$E = \frac{12 \times 10^{-9} \times 9 \times 10^9}{(0.3)^2}$$

$$E = 12 \times 100 = 1200 \text{ N/m}$$

Q.13: Calculate the magnitude and direction of electric field at point $P(2, -6, 3)$ due to charge of magnitude $4 \mu\text{C}$ at point $Q(0, 0, 0)$ when placed in vacuum.

Ans: The vector \vec{r} is given by

$$\vec{r} = 2\hat{i} - 6\hat{j} + 3\hat{k} \quad (\text{a})$$

$$|\vec{r}| = \sqrt{4 + 36 + 9} = 7$$

$$\hat{n} = \frac{\vec{r}}{|\vec{r}|} = \frac{2\hat{i} - 6\hat{j} + 3\hat{k}}{7} \quad (\text{b})$$

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{q}{|\vec{r}|^2} \hat{n}$$

$$\vec{E} = \frac{9 \times 10^9 \times 4 \times 10^{-6}}{49} \times \left(\frac{2\hat{i} - 6\hat{j} + 3\hat{k}}{7} \right)$$

$$\vec{E} = 0.104 \times 10^3 \times (2\hat{i} - 6\hat{j} + 3\hat{k})$$

$$\vec{E} = 104(2\hat{i} - 6\hat{j} + 3\hat{k})$$

$$\vec{E} = 208\hat{i} - 624\hat{j} + 312\hat{k} \text{ V/m}$$

Q.14: The electric potential V at any point is given by

$$V = 3y(x^2 + y^2)^{1/2} + 2x^2$$

Obtain the Cartesian coordinates of the electric field intensity at that point.

Ans:
$$\vec{E} = -\nabla V$$

$$\left(E_x \hat{i} + E_y \hat{j} + E_z \hat{k} \right) = - \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) V$$

$$\begin{aligned} E_x &= -\frac{\partial V}{\partial x} \\ &= -\frac{\partial}{\partial x} \left(3y(x^2 + y^2)^{1/2} + 2x^2 \right) \\ &= - \left[\frac{3}{2} y (x^2 + y^2)^{-1/2} (2x) + 4x \right] \end{aligned}$$

Hence,
$$E_x = -4x - 3xy(x^2 + y^2)^{-1/2} \quad (\text{a})$$

$$E_y = -\frac{\partial V}{\partial y}$$

$$\begin{aligned}
 E_y &= -\frac{\partial}{\partial y} \left[3y(x^2 + y^2)^{1/2} + 2x^2 \right] \\
 &= -3(x^2 + y^2)^{1/2} - \frac{3}{2}y(x^2 + y^2)^{-1/2} (2y) \\
 E_y &= -3(x^2 + y^2)^{1/2} - 3y^2(x^2 + y^2)^{-1/2} \quad (b)
 \end{aligned}$$

Similarly,

$$\begin{aligned}
 E_z &= -\frac{\partial V}{\partial z} \quad (c) \\
 E_z &= -\frac{\partial}{\partial z} \left[3y(x^2 + y^2)^{1/2} + 2x^2 \right] \\
 E_z &= 0
 \end{aligned}$$

Q.15: Obtain the electric potential for a point (2, 3, 1) where potential is specified by

$$V = 3x^2 - 9yz^2 + 4x^2y^2$$

Ans:

$$\begin{aligned}
 \vec{E} &= -\nabla V = -\left(\frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k} \right) V \\
 \vec{E} &= -\left(\frac{\partial V}{\partial x} \hat{i} + \frac{\partial V}{\partial y} \hat{j} + \frac{\partial V}{\partial z} \hat{k} \right) \\
 \vec{E} &= -\left[(6x + 8xy^2) \hat{i} + (-9z^2 + 8x^2y) \hat{j} + \hat{k}(-18yz) \right]
 \end{aligned}$$

Hence, \vec{E} at $x=2$, $y=3$, and $z=1$

$$\begin{aligned}
 \vec{E} &= -\left[(12 + 144) \hat{i} + (-9 + 96) \hat{j} + (-54) \hat{k} \right] \\
 \vec{E} &= -156 \hat{i} + 87 \hat{j} - 54 \hat{k}
 \end{aligned}$$

Q.16: A crystal is kept under an electric field of 2000V/m and the polarization is $2.8 \times 10^{-8} \text{ C/m}^2$. Obtain the permittivity for the crystal.

Ans:

$$\begin{aligned}
 \frac{\vec{P}}{\epsilon_0 E} &= \epsilon_r - 1 \\
 \epsilon_r &= 1 + \frac{\vec{P}}{\epsilon_0 E} \\
 \epsilon_r &= 1 + \frac{2.8 \times 10^{-8}}{8.85 \times 10^{-12} \times 2000} \\
 &= 1 + 1.58 = 2.58
 \end{aligned}$$

Q.17: Obtain the atomic polarizability of argon when its susceptibility is 4.35×10^{-4} at S.T.P. and n is 2.7×10^{25} atom/m³.

Ans:
$$\vec{P} = N\vec{p} \text{ and } \vec{p} = \alpha\vec{E}$$

$$\vec{P} = N\alpha\vec{E} \quad \text{(a)}$$

Also,
$$\vec{P} = (\epsilon_r - 1)\epsilon_0\vec{E} \quad \text{(b)}$$

Comparing Eqs (a) and (b),

$$N\alpha = (\epsilon_r - 1)\epsilon_0$$

$$\alpha = \frac{\epsilon_0(\epsilon_r - 1)}{N}$$

$$\alpha = \frac{8.85 \times 10^{-12} (4.35 \times 10^{-4} - 1)}{2.7 \times 10^{25}}$$

$$\alpha \approx 1.428 \times 10^{-40} \text{ Fm}^2$$

Q.18: Obtain the polarizability of argon atom ($\epsilon_r = 1.0024$ and $n = 2.7 \times 10^{25}$ atoms/m³).

Ans:
$$\vec{P} = \epsilon_0(\epsilon_r - 1)\vec{E}$$

Also,
$$\vec{P} = N\alpha\vec{E}$$

Hence,
$$N\alpha = \epsilon_0(\epsilon_r - 1)$$

$$\alpha = \frac{\epsilon_0(\epsilon_r - 1)}{N}$$

$$\alpha = \frac{8.85 \times 10^{-12} (1.0024 - 1)}{2.7 \times 10^{25}}$$

$$\alpha = 7.86 \times 10^{-40} \text{ Fm}^2$$

Q.19: For a parallel plate capacitor of area $5.2 \times 10^{-3} \text{ m}^2$ whose plate is separated by distance 10^{-3} m under the application of 20V potential. If material inside capacitor has relative dielectric constant 4, then obtain the displacement vector \vec{D} and polarization \vec{P} .

Ans:
$$\vec{D} = \epsilon\vec{E}$$

Here, we have to obtain ϵ and \vec{E} .

$$\epsilon = \epsilon_0\epsilon_r = 4 \times 8.85 \times 10^{-12} = 3.54 \times 10^{-11} \text{ F/m}$$

$$\vec{E} = \frac{\text{Potential applied}}{\text{Distance between the plates}}$$

$$\vec{E} = \frac{20}{10^{-3}} = 2 \times 10^4 \frac{\text{V}}{\text{m}}$$

Here,

$$\begin{aligned}\vec{D} &= \epsilon \vec{E} \\ &= 3.54 \times 10^{-11} \times 2 \times 10^4 \\ \vec{D} &= 7.08 \times 10^{-7} \text{ C/m}^2\end{aligned}$$

Similarly, the polarization can be obtained on

$$\begin{aligned}\vec{D} &= \epsilon_0 \vec{E} + \vec{P} \\ \vec{P} &= \vec{D} - \epsilon_0 \vec{E} \\ &= 7.08 \times 10^{-7} - (8.85 \times 10^{-12})(2 \times 10^4) \\ \vec{P} &= 7.08 \times 10^{-7} - 17.7 \times 10^{-8} \\ \vec{P} &= (7.08 - 1.78) \times 10^{-7} = 5.30 \times 10^{-7} \text{ C/m}^2\end{aligned}$$

Q.20: The susceptibility for a material is given by 0.97. Obtain the relative dielectric constant and ϵ for the material.

Ans:

$$\begin{aligned}\epsilon_r &= 1 + \chi_e = 1 + 0.97 \\ \epsilon_r &= 1.97 \\ \epsilon_r &= \frac{\epsilon}{\epsilon_0} \Rightarrow \epsilon = \epsilon_0 \epsilon_r \\ \epsilon &= 8.85 \times 10^{-12} \times 1.97 \\ \epsilon &= 1.74 \times 10^{-11} \text{ F/m}\end{aligned}$$

OBJECTIVE QUESTIONS

1. Nabla can be represented as

- (a) ∇ (b) Δ
(c) δ (d) θ

2. In terms of Cartesian coordinates, ∇ can be shown as

- (a) $\frac{\partial^2}{\partial x^2} \hat{i} + \frac{\partial^2}{\partial z^2} \hat{k}$ (b) $\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$
(c) $\frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$ (d) $\frac{\partial^2 x}{\partial x \partial y \partial z}$

3. $\nabla \phi$ is a _____ quantity.

- (a) scalar (b) vector
(c) tensor (d) complex

4. The rate of increase of ϕ is given by
- (a) $\frac{\partial^2 \phi}{\partial n^2}$ (b) $\partial \phi \partial n$
(c) $\frac{\partial n}{\partial \phi}$ (d) $\frac{\partial \phi}{\partial n}$
5. Divergence of a vector is _____ quantity.
- (a) scalar (b) vector
(c) tensor (d) complex
6. Positive divergence represents
- (a) sink (b) source
(c) solenoidal (d) irrotational
7. Negative divergence represents
- (a) solenoidal (b) irrotational
(c) sink (d) source
8. Solenoidal field represents
- (a) $\vec{\nabla} \times \vec{A} = 0$ (b) $\vec{\nabla} \cdot \vec{A} = 0$
(c) $\vec{\nabla} \cdot \vec{A} = -1$ (d) $\vec{\nabla} \cdot \vec{A} = 1$
9. Irrotational field is represented by
- (a) $\vec{\nabla} \times \vec{A} = 0$ (b) $\vec{\nabla} \cdot \vec{A} = 0$
(c) $\vec{\nabla} \cdot \vec{A} = -1$ (d) $\vec{\nabla} \cdot \vec{A} = 1$
10. $\vec{\nabla} \times (\vec{\nabla} \phi)$ yields value of
- (a) 1 (b) 0
(c) $-x^2$ (d) -1
11. $\vec{\nabla} \cdot (\vec{\nabla} \times A)$ yields value of
- (a) 1 (b) -1
(c) 0 (d) 2
12. Coulomb's law is dependent on distance "r" as
- (a) $\frac{1}{r}$ (b) r
(c) r^2 (d) $\frac{1}{r^2}$

13. Coulomb force varies as

- (a) $q_1 q_2$ (b) $\frac{q_1}{q_2}$
(c) $\frac{q_2}{q_1}$ (d) $\frac{1}{q_1 q_2}$

14. Coulomb forces are

- (a) conservative (b) central
(c) both (a) and (b) (d) neither (a) nor (b)

15. 1 Coulomb is given by

- (a) $1 \text{ amp} \times 1 \text{ sec}$ (b) $1 \text{ amp}/1 \text{ sec}$
(c) $1 \text{ amp}^2 \text{ sec}$ (d) 1 amp sec^2

16. The value of ϵ_0 is given by

- (a) $9 \times 10^9 \text{ Nm}^2/\text{C}^2$ (b) $8.85 \times 10^{-12} \text{ C}^2/\text{Nm}^2$
(c) 1 (d) 0.5

17. Value of proportionality constant κ is given by

- (a) 1 (b) $8.85 \times 10^{-12} \text{ Nm}^2/\text{c}^2$
(c) $12 \times 10^{-12} \text{ C}^2/\text{m}^2$ (d) $9 \times 10^9 \text{ Nm}^2/\text{c}^2$

18. According to the quantization of charge,

- (a) $q = \pm \frac{n}{e}$ (b) $q = \pm \frac{e}{n}$
(c) $q = \pm ne$ (d) $q = \pm \frac{n}{2} e$

19. The test charge should be small in magnitude than the source charge. (yes/no)

20. The electric field is given by

- (a) $\frac{\vec{F}}{q_0}$ (b) $\vec{F} q_0$
(c) $\frac{2\vec{F}}{q_0}$ (d) $\frac{\vec{F}}{V}$

21. Which of the following is true for electric field lines?

- (a) No force line exists within the conductor
(b) They start from positive charge
(c) They do not intersect each other
(d) All of the above

22. For a uniformly charged wire, the electric field varies w.r.t. distance (r) as

- (a) $\frac{1}{r}$ (b) $\frac{1}{r^2}$
 (c) r (d) r^2

23. For a uniformly charged ring, the electric field is given by

- (a) $\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{qz \hat{k}}{(z^2 + r_0^2)^{3/2}}$ (b) $\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{qz \hat{k}}{(z^2 + r_0^2)^{3/2}}$
 (c) $\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r^2}$ (d) $\vec{E} = \frac{\lambda \hat{i}}{4\pi\epsilon_0 x}$

24. When $r_2 \rightarrow \infty$, and the disc behaves as an infinite sheet of charge, $|\vec{E}|$ field is given by

- (a) 0 (b) $\frac{\sigma}{\epsilon_0}$
 (c) $\frac{\sigma}{2\epsilon_0}$ (d) 1

25. According to Gauss theorem.

- (a) $\oint E \cdot ds = q\epsilon_0$ (b) $\oint E \cdot ds = \frac{\epsilon_0}{q}$
 (c) $\oint E \cdot dl = \frac{q}{\epsilon_0}$ (d) $\oint E \cdot ds = q / \epsilon_0$

26. The differential form of Gauss's law is

- (a) $\vec{\nabla} \cdot \vec{E} = \frac{q}{\epsilon_0}$ (b) $\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$
 (c) $\nabla^2 E = \frac{q}{\epsilon_0}$ (d) $\nabla^2 E = \frac{\rho}{\epsilon_0}$

27. Electric field can be expressed as

- (a) $-\nabla V$ (b) ∇V
 (c) $\frac{1}{\nabla V}$ (d) $\nabla^2 V$

28. The potential for a charge “ q ” is given by

- (a) $V = \frac{1}{4\pi\epsilon_0} \frac{q^2}{r^2}$ (b) $V = \frac{1}{4\pi\epsilon_0} \frac{q^2}{r}$
 (c) $V = \frac{1}{4\pi\epsilon_0} \frac{q}{r}$ (d) $V = \frac{1}{4\pi\epsilon_0} \frac{q}{r^2}$

29. The electric polarization \vec{P} of material is proportional to
 (a) \vec{p} (b) \vec{E}
 (c) both (d) none of these
30. For a homogenous isotropic dielectric, the polarization is
 (a) greater than surface density of induced charge
 (b) less than surface density of induced charge
 (c) equal to surface density of induced charge
 (d) neither equal nor greater/less
31. Displacement vector is related to polarization as
 (a) $\vec{D} = \frac{\epsilon_0 \vec{E}}{\vec{P}}$ (b) $\vec{D} = \epsilon_0 E + \vec{P}$
 (c) $\vec{D} = \epsilon_0 \vec{E} - \vec{P}$ (d) $\vec{D} = \frac{\vec{P}}{\epsilon_0 \vec{E}}$
32. ϵ_r is related to susceptibility as
 (a) $\epsilon_r = 1 + \chi_e$ (b) $\epsilon_r = 1 - \chi_e$
 (c) $\epsilon_r = \chi_e^2$ (d) $\epsilon_r = \frac{1}{\chi_e}$

Answers

- | | | | |
|--------|---------|---------|---------|
| 1. (a) | 9. (a) | 17. (d) | 25. (d) |
| 2. (c) | 10. (b) | 18. (c) | 26. (b) |
| 3. (b) | 11. (c) | 19. Yes | 27. (a) |
| 4. (d) | 12. (d) | 20. (a) | 28. (c) |
| 5. (a) | 13. (a) | 21. (d) | 29. (c) |
| 6. (b) | 14. (c) | 22. (a) | 30. (c) |
| 7. (c) | 15. (a) | 23. (b) | 31. (b) |
| 8. (b) | 16. (b) | 24. (c) | 32. (a) |

Micro-Assessment Questions

1. What are scalar and vector fields?
2. Give the similarities between Newton's law of universal gravitation and Coulomb's law.
3. Give the differences between Newton's law of universal gravitation and Coulomb's law.
4. An uncharged metallic sphere suspended from a thread is attracted to a charged rubber rod. After it touches the rod, the sphere experiences a repulsion. Why?
5. A student from India is studying in the United States of America. He experiences static shocks extensively during the winters unlike his country. Explain.
6. What are point functions?
7. What is nabla or grad operator?
8. Is gradient a scalar or vector quantity?
9. What do you understand by single-valued continuous functions?
10. Electric field is lamellar in nature. Explain.
11. Give the expression for divergence of vector A .
12. Is divergence a scalar or vector quantity?
13. List the difference between gradient and divergence.
14. What is solenoidal field?
15. What is the significance of positive divergence?
16. What do you understand by irrotational field?
17. Write down the expression for Laplacian operator.
18. Explain Gauss divergence theorem.
19. Explain Stoke's theorem.
20. What is the meaning of "charge"?
21. Explain the dielectric constant.
22. On what factors do dielectric constant depend?
23. Define 1V as electric potential.
24. What is polarization?
25. What do you understand by space-charge polarization?

Critical Thinking Questions

1. What do you understand by gradient? Give its physical significance.
2. Explain divergence along with its physical significance.
3. What do you infer from the negative divergence?
4. Give the expression for curl of vector quantity A ? Is curl vector or scalar quantity?
5. State and explain Coulomb's law.
6. Coulomb's forces are central in nature. Explain.
7. Show that Coulomb's forces obey Newton's third law.
8. What is charge? Define its unit.
9. Give important postulates about charge.
10. Describe the quantization of charge.
11. Why the magnitude of test charge is kept small?
12. Write down the mathematical expression of electric field in terms of position vectors.
13. Describe principle of superposition. Are the forces independent of each other or not?
14. Why the electric lines of force do not intersect?

15. What is the difference between continuous and discrete charge distribution?
16. The electric field inside a hollow, uniformly charged sphere is zero. Does this infer that the potential is zero inside the sphere?
17. Obtain the electric field for infinite charged plane sheet.
18. Show that electric field exists only between the plane sheets and is zero outside it.
19. What is Gauss's law?
20. What are dielectric materials? How they differ from insulators?
21. What is the difference between dielectric strength and the dielectric constant?
22. Show that polarization is equal to surface charge density of induced charges.
23. Obtain the relation between electric susceptibility and dielectric constant.
24. Why a water molecule is permanently polarized? Which molecules have no permanent polarization?
25. How does electronic and ionic polarization differ from each other?
26. What do you understand by orientation polarization?

Graded Questions

1. Define electric field? What is test and source charge?
2. Describe electric lines of force? Give their properties.
3. What is continuous charge distribution? Differentiate between linear, surface, and volume charge distributions.
4. Show that the electric charge distribution for uniformly charged infinite wire is inversely proportional to distance from the source.
5. Derive the expression for electric field for uniformly charged ring. How can the electric field for circular disc be treated as the special case?
6. Show that for circular disc, the center acts as point of discontinuity and electric field takes sudden jump.
7. State and prove Gauss's law. Deduce Coulomb's law from Gauss's law.
8. Obtain the differential form of Gauss's law using Gauss divergence form.
9. Define electric potential and potential difference. Express electric field as the gradient of potential.
10. Write down the potential for continuous charge distributions.
11. What do you understand by dielectric polarization? Explain using the schematic diagram.
12. What is displacement vector? How does it depend on polarization vector?
13. Write in detail the different types of polarizations.
14. What is the magnitude of the electric force between two protons separated by 2×10^{-15} m?

Remember and Understand

1. The vector field is said to be solenoidal when its divergence is zero.
2. The field is said to be irrotational when its curl is zero.
3. The bodies showing the properties of attraction and repulsion are charged bodies.
4. One coulomb is defined as the amount of charge passing per second through any section of wire carrying a current of 1A.
5. Principle of superposition and Coulomb's law are basic properties of electrostatics. Both deal with forces between charges at rest.

6. Electric field is the space property due to which the charge modifies its surroundings in such a way that the incoming test charge will experience force on it.
7. The magnitude of test charge should be small so that it should not affect position of source charge.
8. Theoretically, the space of electric field extends upto infinity. A point charge that produces electric field is called source charge and the point charge used to detect electric field is called test charge.
9. Consider a single fixed point charge or source q located at the position vector \vec{r}^1 . Let \vec{r} be the position vector of the observation point p . Place a test charge q_0 at the point p .

$$\vec{F} = \frac{1}{4\pi\epsilon_0} \frac{q q_0 (\vec{r} - \vec{r}^1)}{|\vec{r} - \vec{r}^1|^3}$$

$$\vec{E} = \frac{\vec{F}}{q_0} = \frac{q}{4\pi\epsilon_0} \frac{(\vec{r} - \vec{r}^1)}{|\vec{r} - \vec{r}^1|^3}$$

10. The electric line of force describes the path along which unit positive charge would travel when it is free.
11. The strength of field lines is determined by the density of field lines around the charge. Electric flux is defined as the number of electrical lines of force crossing through an area in a direction perpendicular to that area and is denoted by ϕ .
12. Dielectric materials are nonconducting materials that exhibit polarization under the effect of electric field.
13. The center of gravity of positive and negative charges coincides for polar molecules, whereas for nonpolar molecules they do not coincide.
14. The electric field due to infinite long wire along x -axis is given by:

$$\vec{E} = \frac{\lambda \hat{i}}{4\pi\epsilon_0 x}$$

15. The field between two infinite charge plane sheet is independent of distance and is given by $\frac{\sigma}{\epsilon_0}$.
16. According to Gauss theorem, the total electric flux emanating out of a closed surface is $\frac{1}{\epsilon_0}$ times total charge q enclosed inside the surface i.e.

$$\oint \vec{E} \cdot \vec{ds} = \frac{q}{\epsilon_0}$$

17. The displacement vector \vec{D} and polarization \vec{P} are related as

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

18. The relation between dielectric constant and susceptibility is

$$K = 1 + \chi_c$$

Statistical Physics

Keywords: probability, classical mechanics, quantum mechanics, Maxwell–Boltzmann statistics, Bose–Einstein and Fermi–Dirac Statistics, electron gas, photon gas

Learning Objectives

- ◆ To understand the probability, microstates, and macrostates
- ◆ To learn about arrangements of particles in boxes, and hence thermodynamic probability
- ◆ To understand the concept of phase space, that is, position and velocity space
- ◆ To get insight on the classification of statistics in classical and quantum regime
- ◆ To understand the Maxwell–Boltzmann statistics for ideal gas system where the collisions are considered to be elastic and noninteracting
- ◆ To understand about the most probable velocity, root-mean-square velocity and average velocity
- ◆ To learn about Bose–Einstein and Fermi–Dirac statistics
- ◆ To understand the occupation index and its significance
- ◆ To learn about Fermi energy
- ◆ To apply Bose–Einstein statistics to the photon gas where number of photons is not constant
- ◆ Application of Fermi–Dirac statistics to the electron gas
- ◆ Understanding the classical and quantum approach to obtain specific heat of solids
- ◆ To learn about Dulong–Petit’s law, which indicates that specific heat of solids is independent of temperature
- ◆ To understand the Einstein’s theory of specific heat
- ◆ To learn that at high temperatures, the specific heat is same as derived by Dulong–Petit’s law

Thermodynamics is dependent on microscopic as well as macroscopic properties of system. Statistical physics basically bridges the gap between microscopic and macroscopic properties of system. Using statistical physics, we can discuss whether the particles obey quantum or classical physics. But before we proceed for classical or quantum approach, we should be aware of phase space, probability, and states (micro/macro). These are discussed in the sections that follow.

11.1 Probability and States

When we toss a coin, the probability of a head or tail coming up is $\frac{1}{2}$. It can be understood as the ratio of number of ways leading to favorable way to total outcomes. The probability of getting head or tail are two independent events. When three coins are tossed simultaneous, and when the probability of head coming up has to be calculated, then it is given as $P = P_1 \cdot P_2 \cdot P_3$. $P_1, P_2,$ and P_3 represent individual probabilities for every coin. Then P can be written as $P = \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} = \frac{1}{8}$. Hence for simultaneous events, probability can be given by multiplicative law.

Let us consider two apartments that are identically equal and similar to each other such that all the physical properties are equal. Let us distribute three particles in these two compartments. As the compartments are same, the a priori probability for particles go in any compartment is equal. All the possible arrangements of distribution of particles in two compartments are called microstates. Macrostate is usually defined by (n_1, n_2) , where n_1 is the number of particle in the first compartment and n_2 is the number of particle in the second compartment. All the macrostates and microstates for the distribution of three particles in two equal-size compartment are given in Table 11.1. For three particles in two compartments, the total numbers of possible outcomes are eight.

Table 11.1 All possible macrostates and microstates

Microstates		Macrostates	Frequency (W)	Probability
Compartment 1	Compartment 2			
(1, 2, 3)	–	(3, 0)	1	1/8
(1, 2)	(3)			
(2, 3)	(1)	(2, 1)	3	3/8
(3, 1)	(2)			
(3)	(1, 2)			
(2)	(1, 3)	(1, 2)	3	3/8
(1)	(2, 3)			
–	(1, 2, 3)	(0, 3)	1	1/8

All eight possible macrostates have equal possibility of occurrence. Frequency of occurrence is defined as the total number of microstates for a given macrostate. This frequency highly depends on whether the particle is distinguishable or indistinguishable. This is the case when particles have to be distributed in two compartments. Let n be the total number of particles. Let n_1 and n_2 be particles in two compartments such that $(n_1 + n_2 = n)$. Total number of possible arrangement is $n!$. For compartment 1, n_1 could be arranged in $n_1!$ ways and n_2 could be arranged in $n_2!$ ways. Hence, the thermodynamic probability is given by

$$W(n_1, n_2) = \frac{n!}{n_1! n_2!} \tag{1}$$

$$\text{Total meaningful ways} = \sum_{i=1}^k \frac{n!}{n_i!} \tag{2}$$

Equation (2) specifies n number of particles is k compartments. Let g_k is the number of cells in k th compartment. It can be written as $\sum_{i=1}^k g_i = G$, G is the total number of cells.

If n_i particle could be arranged in g_i cells, the total number of ways could be g_i . All other particles could also be arranged in g_i ways. Hence, n_i particles could be arranged in $\sum_{i=1}^k g_i^{n_i}$ ways. Hence, we can summarise as

For $k \rightarrow$ compartments

$n_1 \cdots n_k \rightarrow$ total particles in respective compartments
i.e., n_1 in 1, n_2 in 2, and n_k in k .

$g_1 \cdots g_k \rightarrow$ number of cells in respective compartments
i.e., g_1 in 1, g_2 in 2, and g_k in k .

Hence, the probability could be written as follows:

$$W(n_1 \cdots n_k) = n! \prod_{i=1}^k \frac{(g_i)^{n_i}}{n_i!} n \quad (3)$$

11.2 Concept of Phase Space

For static systems, only position coordinates are required to define the position of atoms. But for dynamic system, the particles are in motion; hence, they have velocity coordinates in addition to position coordinate. Hence, for a moving particle, (x, y, z) are position coordinates and (v_x, v_y, v_z) are velocity coordinates. Therefore, a total of six coordinates are required to define the particle, that is, (x, y, z, v_x, v_y, v_z) . These six coordinates constitute the phase space.

The volume of position space is dV , that is, $dV = dx \cdot dy \cdot dz$, and the volume of momentum space is $d\Gamma$, that is, $d\Gamma = dp_x \cdot dp_y \cdot dp_z$

The volume of cell in phase space is $d\tau = dV \cdot d\Gamma$

$$d\tau = dV \cdot d\Gamma \quad (4)$$

Further,

$$d\tau = dV \cdot d\Gamma = h^3 \quad (\text{say}) \quad (5)$$

The dimension of h is mass \times velocity² \times sec according to classical mechanics. Classical mechanics do not put any restriction on the h ; but according to quantum mechanics,

$$dx \cdot dp_x \geq h, \quad h \text{ is Planck's constant with value } 6.634 \times 10^{-34} \text{ Js}$$

Hence, the volume of phase space cell can never be smaller than h^3 .

$$d\tau = dx \cdot dy \cdot dz \cdot dp_x \cdot dp_y \cdot dp_z \geq h^3 \quad (6)$$

11.3 Statistics

Statistics could be classified into two categories: classical statistics and quantum statistics (see Figure 11.1). Usually for quantum statistics, minimum cell size is defined. Moreover, the number of cells is small than number of particles. This leads to multiple occupancy of cell, and hence the particles cannot be distinguished. But for classical statistics, there is no restriction on the minimum volume of cell and hence there can be number of cells. The number of cells could be greater than the number of particles. The cells can be labeled, and hence which particle is in which cell can be easily determined. This makes the particles to be distinguished on the basis of cell numbers. When the number of particles is very small, that is, at low concentration of particles, the quantum statistics can be treated as classical statistics. We will discuss both the statistics in sections that follow.

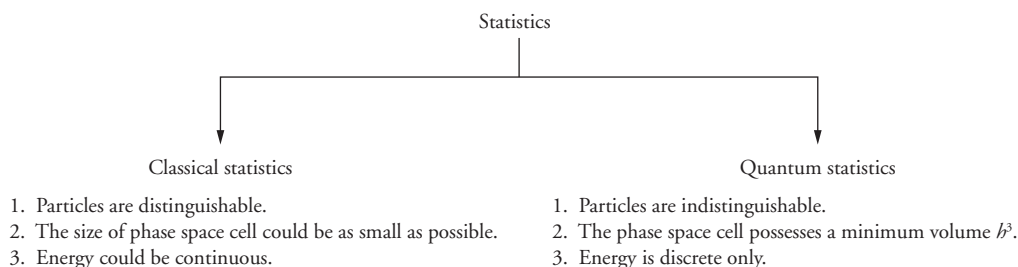


Figure 11.1 Classification of statistics

Maxwell gave a new insight toward understanding the theories. Maxwell had high interest in geometry. He wrote his findings about ovals and double foci ellipses at a very young age of 15 years. Maxwell's father was aware of his son's caliber. Hence, he presented the findings to a Professor Forbes who taught at Edinburgh Royal Society. Professor Forbes was amazed at the findings from such a young boy having very less experience, although some studies were reported also. Maxwell formulated mathematical models that answered all the questions, and hence no question was left. He further used statistics to explain the matter's behavior using projected laws. This laid the foundation to modern physics. This law was the main reason behind the relativity theory of Einstein. Maxwell calculated the exact velocity of molecule of gas using experiments. He found that faster molecule generates more heat, which meant that speed and heat evolved were directly proportional to each other. The experiment showed heat as a particle property, which could control the particles' movement.



J.C. CLARK WITH LADY CLARK

11.4 Classical Statistics (Maxwell–Boltzmann Statistics)

In 1800, three physicists, that is, J.C. Maxwell, L. Boltzmann, and J.W. Gibbs, gave the satisfactory explanation of thermodynamics. Clausius explained that there is range of molecular speeds for all gas molecules. The speed of gas molecules depends on temperature. Maxwell was very much inspired

from Clausius, and he calculated average molecular speed, dispersion, and most probable speed for these particles. Further, in 1872, Boltzmann wished to describe the time evolution for the gas toward Maxwellian distribution. For this purpose, Boltzmann used time-dependent speed distribution function and kinetic equations. Boltzmann committed suicide in 1908, when he was subjected to criticism over his theory and its acceptance. But Yale Professor, J.W. Gibbs, quietly established statistical mechanics, and his work was not recognized during his lifetime. This section emphasizes on Maxwell–Boltzmann theory. For an ideal gas, the concentration is small, and hence classical mechanics applies well. The collisions among gas molecule are considered to be elastic and non interacting. These collisions will not affect the interactions within system.

Let us consider ideal gas in volume V with n molecules. These molecules collide against the wall as well as among each other. Due to these collisions, the energy or momentum can change, but it remains conserved for the system. Let E be the total energy of system. Let for k compartments, the range of energy is from 0 to E_k . Hence, the energy can be divided as E_1, E_2, \dots, E_k . The particles are from 0 to n_k , that is, n_1, n_2, \dots, n_k particles are distributed in k compartments. The number of particles may belong to E_1, E_2, E_k energy. All the possible arrangements possess different energies, but only a certain arrangement corresponds to most probable state. Hence, it is important to find out the most probable state as it represents the actual energy distribution under equilibrium state. Let g_1, g_2, \dots, g_k be the number of cells corresponding to interval 1, 2, 3, \dots, k .

The thermodynamic probability is given by Eqn. (3) as follows:

$$W(n_1, n_2, \dots, n_k) = n! \prod_{i=1}^k \frac{(g_i)^{n_i}}{n_i!}$$

Take natural logarithms on both the sides:

$$\text{i.e.} \quad \ln W = \ln n! + \sum_{i=1}^k n_i \ln g_i - \sum_{i=1}^k \ln n_i!$$

Here, we have to use Sterling's formula, that is, when n is extremely large, then $\ln n! = n \ln n - n$

$$\ln W = n \ln n - n + \sum_{i=1}^k n_i \ln g_i - \left[\sum_{i=1}^k ((n_i \ln n_i) - n_i) \right]$$

$$\ln W = n \ln n - n + \sum_{i=1}^k n_i \ln g_i - \left[\sum_{i=1}^k n_i \ln n_i - n \right]$$

$$\ln W = n \ln n + \sum_{i=1}^k n_i \ln g_i - \sum_{i=1}^k n_i \ln n_i$$

W represents the most probable state; hence, the maximum value is expected for it, or $d(\ln W) = 0$. In addition to this, n and g_i are constant for system, but n_i can vary from cell to cell.

$$d(\ln W) = 0 + \sum_{i=1}^k dn_i \ln g_i - \sum_{i=1}^k \frac{n_i}{n_i} dn_i - \sum_{i=1}^k dn_i \ln n_i$$

$$0 = 0 + \sum_{i=1}^k dn_i (\ln g_i - \ln n_i) = 0$$

$$\Rightarrow \sum_{i=1}^k (\ln g_i - \ln n_i) dn_i = 0 \quad (7)$$

For an ideal isolated system, n is total particles and E is total energy and following conditions must be fulfilled:

$$dn = \sum_{i=1}^k dn_i = 0 \quad (8a)$$

$$dE = \sum_{i=1}^k E_i dn_i = 0, \quad E = E_1 n_1 + E_2 n_2 + E_3 n_3 \quad (8b)$$

Multiply Eqn. (8a) by $-\alpha$ and Eqn. (8b) by $-\beta$ and add both of them to Eqn. (7).

$$\begin{aligned} \sum_{i=1}^k (\ln g_i - \ln n_i) dn_i - \sum_{i=1}^k \alpha dn_i - \sum_{i=1}^k \beta E_i dn_i &= 0 \\ \sum_{i=1}^k (\ln g_i - \ln n_i - \alpha - \beta E_i) dn_i &= 0 \end{aligned} \quad (9)$$

Since $dn_i \neq 0$; hence for this equation to hold good, the bracketed term should be zero.

$$\ln g_i - \ln n_i - \alpha - \beta E_i = 0$$

$$\ln \frac{g_i}{n_i} = \alpha + \beta E_i$$

$$\frac{g_i}{n_i} = e^{\alpha + \beta E_i}$$

$$n_i = \frac{g_i}{e^{\alpha + \beta E_i}} \quad (10)$$

Equation (10) is Maxwell–Boltzmann energy distributions law rewriting Eqn. (10):

$$n_i = g_i e^{-\alpha} e^{-\beta E_i} \quad (11)$$

Where $e^{-\beta E_i}$ = Boltzmann factor and $\sum_{i=1}^k e^{-\beta E_i}$ is called partition function. We have to evaluate α and β

constants, as they are not known yet. We have to make following assumptions:

- (i) The energy interval lies b/w E and $E + dE$.
- (ii) The number of particles lying in energy interval $\left(E - \frac{1}{2}\right)$ and $\left(E + \frac{1}{2}\right)$ is $n(E)$.

Equation (11) can be written as follows:

$$n(E) = g(E) e^{-\alpha} e^{-\beta E} \quad (12a)$$

In terms of momentum,

$$\left[E = \frac{p^2}{2m} \right]$$

$$\text{Hence, } n(p) = g(p) e^{-\alpha} e^{-\frac{\beta p^2}{2m}} \quad (12b)$$

$$\left[\begin{array}{l} n(p) \rightarrow \text{number of particles in momentum interval } \left(p - \frac{1}{2} \right) \text{ to } \left(p + \frac{1}{2} \right) \\ g(p) \rightarrow \text{number of cells in phase space} \end{array} \right]$$

If the molecules lie between momentum interval band $p + dp$, then for interval dp , Eqn. (12b) becomes

$$n(p) dp = g(p) e^{-\alpha} e^{-\beta p^2 / 2m} dp \quad (12c)$$

Total phase volume for interval p to $p + dp$ is given by $g(p) dp h^3 = \int d\tau$

$$\begin{aligned} g(p) dp &= \frac{1}{h^3} \int d\tau = \frac{1}{h^3} \iiint dx dy dz \iiint dp_x dp_y dp_z \\ g(p) dp &= \frac{1}{h^3} V \iiint dp_x dp_y dp_z \end{aligned} \quad (12d)$$

As shown in Figure 11.2, the volume enclosed between two spheres of radii p and $p + dp$ is given by the following equation:

$$d\Gamma = 4\pi p^2 dp$$

Hence, Eqn. (12a) becomes

$$g(p) dp = \frac{4\pi p^2 dp \cdot V}{h^3} \quad (12e)$$

Substituting Eqn. (12e) in Eqn. (12c),

$$n(p) dp = \frac{4\pi V p^2 dp}{h^3} \cdot e^{-\alpha} \cdot e^{-\frac{\beta p^2}{2m}} \quad (13)$$

For calculating total number of molecules, we have to integrate Eqn. (13), that is,

$$\int_0^{p_{\max}} n(p) dp = n \quad (14a)$$

Any particle/molecule having momentum greater than 0 is outside the limit, that is, for $p > p_{\max}$, $n(p) = 0$. Hence, we can use limit (upper) to be ∞ .

$$n = \int_0^{\infty} n(p) dp$$

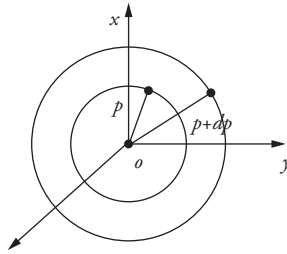


Figure 11.2 Momentum space for particles

$$\begin{aligned}
 n &= \int_0^{\infty} \frac{4\pi V p^2 dp}{h^3} e^{-\alpha} e^{-\beta p^2 / 2m} \\
 n &= \frac{4\pi V e^{-\alpha}}{h^3} \int_0^{\infty} p^2 e^{-\beta p^2 / 2m} dp \\
 n &= \frac{4\pi V e^{-\alpha}}{h^3} \left[\frac{1}{4} \frac{\sqrt{\pi}}{(\beta / 2m)^{3/2}} \right] \\
 &\quad \left[\text{Using standard intergral, } \int_0^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4} \frac{\sqrt{\pi}}{a^{3/2}} \right] \\
 n &= \frac{4\pi V e^{-\alpha}}{h^3} \left[\frac{1}{4} \frac{\sqrt{\pi}}{(\beta / 2m)^{3/2}} \right] \\
 e^{-\alpha} &= \frac{nh^3}{V} \left(\frac{\beta}{2\pi m} \right)^{3/2} \tag{14b}
 \end{aligned}$$

Substituting Eqn. (14b) in Eqn. (13),

$$\begin{aligned}
 n(p) dp &= \frac{4\pi V p^2}{h^3} \cdot \frac{nh^3}{V} \left(\frac{\beta}{2\pi m} \right)^{3/2} e^{-\beta p^2 / 2m} \cdot dp \\
 n(p) dp &= 4\pi n \left(\frac{\beta}{2\pi m} \right)^{3/2} p^2 e^{-\beta p^2 / 2m} dp \tag{15}
 \end{aligned}$$

Using Eqn. (15), further relation could be obtained using energy.

i.e.

$$\begin{aligned}
 p^2 &= 2mE \\
 dp &= \sqrt{\frac{m}{2E}} dE \tag{16a}
 \end{aligned}$$

Substituting Eqn. (16a) in Eqn. (12e),

$$g(E)dE = \frac{4\sqrt{2\pi}V}{h^3} m^{3/2} \cdot E^{1/2} dE \quad (16b)$$

Substituting Eqn. (16a) in Eqn. (15), and we obtain

$$n(E)dE = \frac{2n}{\sqrt{\pi}} \beta^{3/2} \sqrt{E} e^{-\beta E} dE \quad (17)$$

For evaluating β , we have to take into consideration average kinetic energy, that is, average KE = $3/2 k_B T$. This is valid for any system at thermal equilibrium and is known as law of equipartition of energy. Total energy of system for n particles is given by

$$\begin{aligned} E' &= \int_0^{\infty} E n(E) dE = \frac{3}{2} n k_B T \quad [k_B \text{ is Boltzmann's constant}] \\ \frac{3}{2} n k_B T &= \int_0^{\infty} E \cdot \frac{2n}{\sqrt{\pi}} \beta^{3/2} \sqrt{E} e^{-\beta E} dE \\ \frac{3}{2} n k_B T &= \frac{2n\beta^{3/2}}{\sqrt{\pi}} \int_0^{\infty} E^{3/2} e^{-\beta E} dE \\ &\quad \left[\text{Standard integral } \int_0^{\infty} x^{3/2} e^{-ax} dx = \frac{3}{4a^2} \sqrt{\frac{\pi}{a}} \right] \\ \frac{3}{2} n k_B T &= \frac{2n\beta^{3/2}}{\sqrt{\pi}} \left[\frac{3}{4\beta^2} \frac{\sqrt{\pi}}{\beta} \right] = \frac{3n}{2\beta} \\ \beta &= \frac{1}{k_B T} \end{aligned} \quad (18a)$$

Substituting this value in Eqn. (17), we get

$$n(E)dE = \frac{2\pi n}{(\pi k_B T)^{3/2}} \sqrt{E} e^{-E/k_B T} dE \quad (18b)$$

Similarly, we can find out $n(p)dp$ also as follows:

$$n(p)dp = \frac{\sqrt{2\pi}n}{(\pi m k_B T)^{3/2}} p^2 e^{-p^2/2m k_B T} dp \quad (18c)$$

The number of molecules/particles having speeds within range v and $v + dv$ is given by the following equation;

$$n(v)dv = \frac{\sqrt{2\pi}n(m)^{3/2} v^2 e^{-mv^2/2k_B T} dv}{(\pi k_B T)^{3/2}} \quad (18d)$$

Equation (18d) is Maxwell–Boltzmann's law for distribution of velocity.

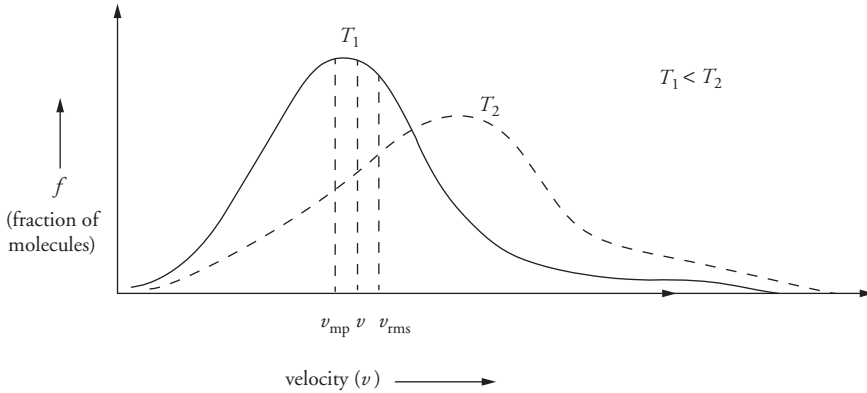


Figure 11.3 Velocity distribution of molecules at different temperatures

We have calculated all fundamental distributions, and they can be listed as follows:

$$\begin{aligned}
 n(p) dp &= \frac{\sqrt{2\pi n}}{(\pi m k_B T)^{3/2}} p^2 e^{-p^2/2mk_B T} dp \\
 n(E) dE &= \frac{2\pi n}{(\pi k_B T)^{3/2}} \sqrt{E} e^{-E/k_B T} dE \\
 n(v) dv &= \frac{\sqrt{2\pi n} m^{3/2} v^2 e^{-\frac{mv^2}{2k_B T}}}{(\pi k_B T)^{3/2}} dv
 \end{aligned} \tag{19}$$

Now, the further objective is to calculate the most probable speed. Figure 11.3 is the plot that gives the distribution of velocity as a function of fraction of molecules (f) lying in unit velocity interval around v , that is, $f = \frac{n(v)}{n}$.

The maximum value of velocity is most probable speed (v_{mp}), and hence the condition $\frac{\partial f}{\partial v} = 0$ holds well for it. From Eqn. (19),

$$\begin{aligned}
 n(v) dv &= \frac{\sqrt{2\pi n} (m)^{3/2} v^2 e^{-mv^2/2k_B T} dv}{(\pi k_B T)^{3/2}} \\
 f &= \frac{n(v)}{n} = \frac{\sqrt{2\pi} \pi (m)^{3/2} v^2 e^{-mv^2/2k_B T}}{(\pi k_B T)^{3/2}} \\
 f &= C v^2 e^{-mv^2/2k_B T}
 \end{aligned} \tag{20}$$

C is a constant with value $\frac{\sqrt{2\pi} m^{3/2}}{(\pi k_B T)^{3/2}}$ for given temperature.

Taking derivation of f w.r.t. v and putting it equal to zero, we obtain most probable speed (mps),

$$v_{\text{mp}} = \sqrt{\frac{2k_B T}{m}} \quad (21)$$

The average speed could be obtained as follows:

$$\begin{aligned} \bar{v} &= \frac{\int_0^{\infty} v n(v) dv}{\int_0^{\infty} n(v) dv} \\ \bar{v} &= \sqrt{\frac{8k_B T}{m\pi}} \end{aligned} \quad (22)$$

[For obtaining Eqn. (22), the standard integral is used, that is, $\int_0^{\infty} x^3 e^{-ax^2} dx = \frac{1}{2a^2}$.]

Root-mean-square velocity is given by

$$\begin{aligned} v_{\text{rms}} &= \left(\bar{v^2} \right)^{1/2} = \frac{1}{n} \int_0^{\infty} v^2 n(v) dv \\ v_{\text{rms}} &= \sqrt{\frac{3k_B T}{m}} \end{aligned} \quad (23)$$

From Eqs (20)–(23), we obtain the ratios as follows:

$$\frac{v_{\text{rms}}}{v_{\text{mp}}} \approx 1.22 \quad \text{and} \quad \frac{\bar{v}}{v_{\text{mp}}} \approx 1.13$$

Hence, following two points are concluded:

- (i) Root-mean-square velocity is 22 percent greater than most probable speed for given temperature.
- (ii) Average speed is 13 percent greater than mps for given temperature.

Ludwig Boltzmann was born in Vienna on February 20, 1844. His father was a tax official. He obtained his PhD degree in 1866 at the University of Vienna. Boltzmann made contributions to statistical mechanics. Along with it, he made detailed calculations in the kinetic theory of gases. He was probably the first person to get an insight and understanding of Maxwell's theory of electromagnetism, and he wrote a two-volume treatise. Boltzmann worked on black-body radiation using Stefan's law, which was later termed by Hendrik Antoon Lorentz as "a true pearl of theoretical physics." Wilhelm Ostwald vocally criticized his work on statistical mechanics and other contemporaries, who disregarded atoms and physical science exclusively based on energy conditions. They could not understand the statistical nature of Boltzmann's ideas and theories. Ludwig Boltzmann got very much demoralized due to the harsh and blunt criticism of his work. At the age of 62 years, he hanged himself to death on September 5, 1906, at Duino, Italy.



LUDWIG BOLTZMANN

11.5 Quantum Statistics (BE and FD Statistics)

We have seen that MB distribution is valid when the average particle distance d is quite large as compared to uncertainty in particle position, that is,

$$d \gg \Delta x \quad (24a)$$

We know from equipartition theory that at thermal equilibrium temperature T , $\bar{p} = 0$ and $\overline{p^2} = \frac{3k_B T}{2}$

if we take momentum for one degree of freedom, then

$$\overline{p^2} = \frac{1}{2} k_B T$$

$$\text{Hence, } \Delta p_x = \sqrt{\overline{p_x^2} - \overline{p_x}^2} = \sqrt{mk_B T}$$

We know from Heisenberg's uncertainty principle that

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

$$\Delta x \geq \frac{\hbar}{2\sqrt{mk_B T}} \quad (24b)$$

Put $d = \left(\frac{N}{V}\right)^{1/3}$, where N is number of particles and V is volume for Eqn. (24a)

$$\frac{\hbar}{2\sqrt{mk_B T}} \ll \left(\frac{V}{N}\right)^{1/3}$$

$$\frac{N}{V} \frac{\hbar^3}{8(mk_B T)^{3/2}} \ll 1 \quad (24c)$$

Hence, MB statistics holds good for low concentration of particles as is evident from Eqn. (24c). When N is large, then we shift to quantum approach, where multiple occupancy is valid. Two types of quantum approaches have been given as illustrated in Figure 11.4.

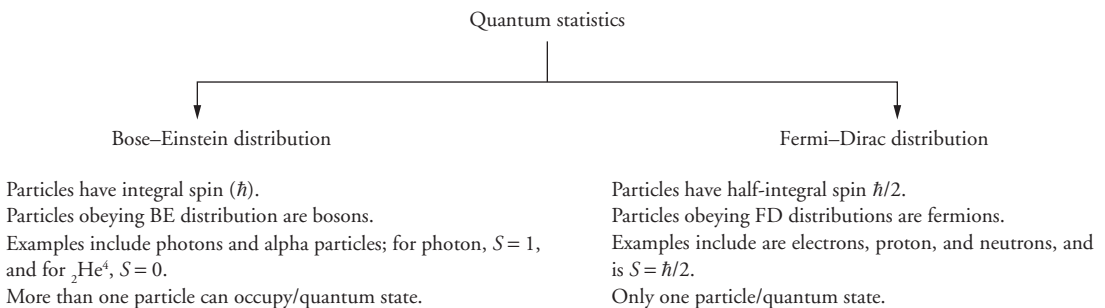


Figure 11.4 Distribution of quantum statistics.

11.6 Bose–Einstein Statistics

Consider a system with n -identical particles in k number of compartments. Each compartment has many cells with minimum h^3 volume. Let us suppose for k -compartment, g_k be the total number of cells, and n_k is number of particles to be distributed in g_k cells. Bosons/particles have multiple occupancy; hence, one cell can be occupied by more than one particle.

The total number of objects in j th compartment is $(n_j + g_j - 1)$. Hence, $(g_j - 1)$ partitions are separating them total number of particles are n , for j th compartments, n_j particles are present, and total number of arrangements can be given by $n_j!$. The partitions could be arranged in $(g_j - 1)!$ ways as demonstrated in Figure 11.5. All of these arrangements do not affect the distribution. Hence, the number of different arrangement for j th compartment is

$$\frac{(n_j + g_j - 1)!}{(n_j)!(g_j - 1)!}$$

For all the k compartment, all different arrangements could be given as follows:

$$W(n_1, n_2, \dots, n_k) = \prod_{j=1}^k \frac{(n_j + g_j - 1)!}{(n_j)!(g_j - 1)!} \tag{25}$$

Taking natural logarithm and differentiating it [g_j and n are constant]:

$$d(\ln W) = \sum_{j=1}^k (\ln(n_j + g_j - 1) - \ln n_j) dn_j$$

$n_j \gg 1$, hence 1 could be neglected.

$$d(\ln W) = \sum_{j=1}^k (\ln(n_j + g_j) - \ln n_j) dn_j$$

Also $d(\ln W) = 0$ at thermal equilibrium:

$$\sum_{j=1}^k (\ln(n_j + g_j) - \ln n_j) dn_j = 0 \tag{26a}$$

As discussed in Section 11.5, using Lagrange’s multipliers condition, we obtain

$$\sum dn_j = 0 \tag{26b}$$

$$\sum E_j dn_j = 0 \tag{26c}$$

Multiply Eqn. (26b) by $-\alpha$ and Eqn. (26c) by $-\beta$ and adding to Eqn. (26a).



Figure 11.5 Particle in cell and partitions

$$\sum_{j=1}^k \left[\left(\ln(n_j + g_j) - \ln n_j \right) - \alpha - \beta E_j \right] dn_j = 0$$

As dn_j could not be zero, only the bracket part is zero:

$$\ln(n_j + g_j) - \ln n_j = \alpha + \beta E_j$$

$$\ln \frac{(n_j + g_j)}{n_j} = \alpha + \frac{1}{k_B T} E_j \quad \left[\text{as} \quad \beta = \frac{1}{k_B T} \right]$$

$$\frac{n_j + g_j}{n_j} = e^{\alpha + \frac{1}{k_B T} E_j}$$

$$1 + \frac{g_j}{n_j} = e^{\alpha + \frac{E_j}{k_B T}}$$

$$\frac{g_j}{n_j} = e^{\alpha + \frac{E_j}{k_B T}} - 1$$

$$n_j = \frac{g_j}{e^{\alpha} e^{\frac{E_j}{k_B T}} - 1}$$

For i th compartment, we can write

$$n_i = \frac{g_i}{e^{\alpha} e^{\frac{E_i}{k_B T}} - 1} \quad (27)$$

Equation (27) is the Bose–Einstein distribution junction

Satyendra Nath Bose presented several papers in theoretical physics and pure mathematics along with Saha. In 1924, Bose wrote a paper deriving Planck's quantum radiation law without any reference to classical physics. He used novel way of counting states with identical particles. He was working as a Reader at the Physics Department of the University of Dhaka at that time. This paper originated very important field of quantum statistics. This paper was not accepted at once for publication. Saha sent the article directly to Albert Einstein in Germany. Einstein, found the paper to be of great importance, and he translated it into German. He submitted the paper on Bose's behalf to the prestigious *Zeitschrift für Physik*. As a result of this recognition, Bose could work for two years in European X-ray and crystallography laboratories. During this time, he worked with Louis de Broglie, Marie Curie, and Einstein.



S.N.BOSE

11.7 Fermi–Dirac Statistics

The particles that obey Pauli exclusion principle also obey Fermi–Dirac statistics. Hence, the multiple occupancy of cells is completely ruled out. Let n particles be distributed in k compartments. Let E_1, E_2, \dots, E_k be the energy corresponding to 1, 2, 3, ..., k compartment. Let n_1, n_2, \dots, n_k be the number of particles corresponding to 1, 2, 3, ..., k compartments, g_j be the number of cells corresponding to j th compartment. In Fermi–Dirac distribution, $g_j > n_j$ and $(g_j - n_j)$ cells are vacant. g_j cells can be arranged in $g_j!$ ways, but all the particles are indistinguishable, and hence $n_j!$ are meaningless. $(g_j - n_j)!$ arrangement are also meaningless as they are empty cells.

Total number of different ways of arranging particles is

$$\frac{g_j!}{(g_j - n_j)!n_j!}$$

The thermodynamic probability is given by (for all the macrostates)

$$W(n_1, n_2, \dots, n_k) = \prod_{j=1}^k \frac{g_j!}{(g_j - n_j)!n_j!} \quad (28a)$$

Taking natural logarithm and differentiating it, applying the condition $d(\ln W) = 0$ and n and g_j are constant.

$$d(\ln W) = \sum_j (\ln(g_j - n_j) - \ln(n_j)) dn_j \quad (28b)$$

$$\Rightarrow \sum_j (\ln(g_j - n_j) - \ln n_j) dn_j = 0 \quad (28c)$$

Usually, $\sum dn_j = 0$ and $\sum E_j dn_j = 0$ as per Lagrange's multiplier method (as discussed in Sections 11.5 and 11.6).

$$\sum_j (\ln(g_j - n_j) - \ln n_j - \alpha - \beta E_j) dn_j = 0$$

As $dn_j \neq 0$, hence equating the bracket to zero.

$$(\ln(g_j - n_j) - \ln n_j) - \alpha - \beta E_j = 0$$

$$\ln \frac{(g_j - n_j)}{n_j} = \alpha + \beta E_j$$

$$\frac{g_j - n_j}{n_j} = e^{\alpha + \frac{E_j}{k_B T}} \quad \left[\beta = \frac{1}{k_B T} \right]$$

$$\frac{g_j}{n_j} - 1 = e^\alpha e^{E_j/k_B T}$$

$$\frac{g_j}{n_j} - 1 = e^\alpha e^{E_j/k_B T} + 1$$

$$n_j = \frac{g_j}{e^\alpha e^{E_j/k_B T} + 1}$$

For i th compartment,

$$n_j = \frac{g_j}{e^\alpha e^{E_j/k_B T} + 1} \quad (29)$$

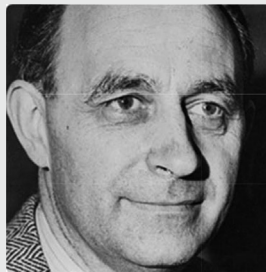
Equation (29) is called Fermi–Dirac distribution.

Conclusively, we can say

$$\left. \begin{array}{l} \text{MB statistics} \quad n_i = \frac{g_i}{e^\alpha e^{E_i/k_B T}} \\ \text{BE statistics} \quad n_i = \frac{g_i}{e^\alpha e^{E_i/k_B T} - 1} \\ \text{FD statistics} \quad n_i = \frac{g_i}{e^\alpha e^{E_i/k_B T} + 1} \end{array} \right\} \quad (30)$$

$\frac{n_i}{g_i}$ = occupation index, which is less than or equal to 1 for FD. It is ≥ 1 for BE statistics.

Fermi's historic and unique accomplishments caused him to be recognized as one of the great scientists of the twentieth century. Enrico Fermi was born in Rome, Italy, on September 29, 1901, to Alberto Fermi (a Chief Inspector of the Ministry of Communications) and mother Ida de Gattis (school teacher). His primary education was from a local school. Fermi's

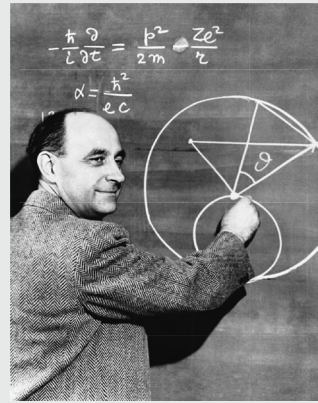


"There are two possible outcomes: if the result confirms the hypothesis, then you've made a measurement. If the result is contrary to the hypothesis, then you've made a discovery."

Enrico Fermi

aptitude and interest for physics and mathematics was highly encouraged by one of his father's friends Adolfo Amidei. Adolfo gave him several books on physics and mathematics.

Fermi joined the Scuola Normale Superiore in Pisa in 1918 where he spent four years and got his PhD in physics under the guidance of Professor Puccianti in 1922. Under Italian Government scholarship, he spent few months with Professor Max Born in Göttingen. In 1924, he got Rockefeller Fellowship, and he moved to Leyden to work with P. Ehrenfest. Fermi discovered the statistical laws in 1926, nowadays known as the Fermi statistics. From 1927 to 1938, Fermi was the professor of theoretical physics at the University of Rome. In 1934, Fermi carried out his experiments during which he bombarded a variety of elements with neutrons. Further, he discovered that slow-moving neutrons were quite effective in producing radioactive atoms. He was not aware of the fact that he split the uranium atom into different atoms. In 1938, Fermi won the Nobel Prize for Physics for his work on nuclear processes. He was employed as the professor of physics at Columbia University, New York, during 1939 where he continued until 1942. He accepted professorship at the Institute for Nuclear Studies at the University of Chicago in 1946. He worked in this Institute until his death. He died of cancer at the University of Chicago on November 28, 1954.



E. FERMI

11.8 Application of FD Statistics

The free electron model of metals demonstrates that metals have sea of free electrons into which the ions are immersed. These free electrons are responsible for high conductivities of metals. But these free electrons collide among themselves, as well as fixed ions. In other words, it is known as an electron gas. Fermi–Dirac statistics could be applied to find the energy distribution of electron sea.

Let n number of electrons be enclosed inside a conductor volume V , and the total energy of electrons is E . From Eqn. (30), the energy distribution for these electrons could be given as follows:

$$n_j = \frac{g_j}{e^\alpha e^{E_j/k_B T} + 1}$$

For a continuous range of energy from E to $E + dE$:

$$n(E)dE = \frac{g(E)dE}{e^\alpha e^{E/k_B T} + 1} \quad (31a)$$

In Section 11.4, Eqn. (12e), we found out

$$g(p)dp = \frac{4\pi V p^2 dp}{h^3}$$

We are taking the case of electron gas, and electrons exist in two spin states, that is, $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$.

Hence, $g(p)dp$ becomes

$$g(p)dp = \frac{8\pi V p^2 dp}{h^3} \quad (31b)$$

We know that energy and momentum are related to each other by $E = p^2/2m$. Hence, Eqn. (31b) could be written as follows:

$$g(E)dE = \frac{8\pi V \sqrt{2} m^{3/2} E^{1/2} dE}{h^3} \quad (31c)$$

Substituting Eqn. (31c) in Eqn. (31a),

$$n(E) dE = \frac{8\pi \sqrt{2} \pi V m^{3/2}}{h^3} \frac{E^{1/2} dE}{e^{\alpha} e^{E/k_B T} + 1} \quad (32)$$

Equation (32) is FD distribution for electron gas. As the temperature (T) of system is decreased, the energy also decreases. Upon cooling a system, the electron will occupy lower states. This implies that at absolute zero, that is, $T = 0$ K, all the lower energy states are occupied. Along with that, Pauli's exclusion principle is obeyed, according to which one energy state will contain only one electron. Hence, the entire n electrons are accommodated in different energy states. But above certain energy level, all the energy levels are vacant. This marks the Fermi level. Hence, the Fermi level corresponds to level above which all the levels are empty, and the energy E_F corresponding to Fermi level is called Fermi energy.

At $T = 0$ K, $n(E) dE = 0$ from Eqn. (32), also we have to put $\alpha = -\frac{E_F}{k_B T}$.

$$\text{Hence, we obtain } n(E) dE = \frac{8\sqrt{2} \pi V m^{3/2}}{h^3} \frac{E^{1/2} dE}{e^{(E-E_F)/k_B T} + 1} \quad (33)$$

$$\frac{n(E)}{g(E)} = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

At $T = 0$ K,

$$\begin{aligned} \frac{n(E)}{g(E)} &= 1 \\ n(E) &= g(E) \end{aligned} \quad (34a)$$

But at $T = 0$ K, for $E > E_F$

$$\frac{n(E)}{g(E)} = 0$$

or

$$n(E) = 0 \quad (34b)$$

Hence, above Fermi level, all energy levels are empty at absolute zero. Let us find total number of electrons up to Fermi level, that is,

$$n = \int_0^{E_F} g(E) dE = \frac{2}{3} \left[\frac{8\sqrt{2}\pi V m^{3/2} E_F^{3/2}}{h^3} \right]$$

$$\frac{3}{2} n h^3 = 8\sqrt{2}\pi V m^{3/2} E_F^{3/2}$$

$$E_F^{3/2} = \frac{3 n h^3}{2 \times 8\sqrt{2}\pi V m^{3/2}}$$

$$E_F = \frac{h^2}{2m} \left[\frac{3n}{8\pi V} \right]^{2/3} \tag{35}$$

(n/V) represents the concentration of electrons. Eqn. (35) portrays that Fermi energy is independent of shape and size of material, and it is constant for particular metal.

The average energy at 0 K, and for $E < E_F$ is given by

$$\bar{E} = \frac{\int_0^{E_F} E n(E) dE}{n} = \frac{\int_0^{E_F} E \left(\frac{3}{2} n E_F^{-3/2} \right) E^{1/2} dE}{n} \quad \text{[using Eqs (33) and (35)]}$$

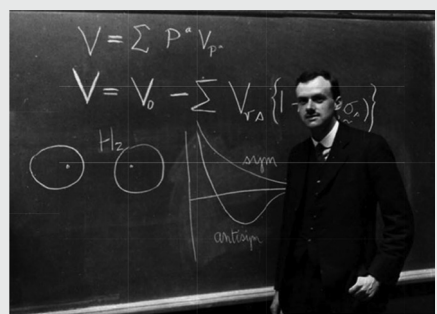
$$\bar{E} = \frac{3}{2} \int_0^{E_F} E^{3/2} dE = \frac{3}{2} E_F$$

$$\bar{E} = \frac{3}{5} E_F \tag{36}$$

Hence, average energy is 0.6 times the Fermi energy.

Paul Adrien Maurice Dirac was an English theoretical physicist and mathematician who is widely regarded to be one of the founders of quantum mechanics and quantum electrodynamics. Noted for his 1928 relativistic quantum theory of the electron, and for predicting of the existence of antiparticles, Dirac shared the 1933 Nobel Prize for Physics with Erwin Schrödinger.

Paul Dirac is known as one of the greatest physicists in history. His contributions laid the backbone for quantum mechanics and quantum electrodynamics. Dirac was the first physicist to formulate quantum electrodynamics. In addition to this, he also discovered the magnetic monopole solutions. He formulated quantum field theory after reworking on his own Dirac equation. The work described the existence of annihilation of matter–antimatter.



P.A.M. DIRAC

The work described the existence of annihilation of matter–antimatter.

Paul was born on August 8, 1902, in Bristol, England. Dirac's father used to teach French and was an immigrant from Saint-Maurice, Switzerland. Paul attended the Bishop Road Primary School. Later on, he went to Merchant Venturers' Technical College where his father was a French teacher. Dirac obtained his degree in electrical engineering from University of Bristol in 1921. In 1923, Dirac joined the University of Cambridge as a research student, where he further worked on unpublished hypothesis of Heisenberg's quantum mechanics.

In 1932, Dirac was made Lucasian professor of mathematics at the University of Cambridge where he taught for almost 37 years and did his independent research. Paul Dirac died on October 20, 1984, in Tallahassee, Florida, at the age of 82.

11.9 Application of BE Statistics

11.9.1 Photon Gas

We have gone through the Planck's approach of black-body radiations. Now this section emphasizes on quantum approach to discuss black-body radiation. The electromagnetic radiations carry energy in discrete packets also known as photons. The energy of photon is hf and momentum is $\frac{hf}{c}$. If we take a hollow cavity, such that large number of photons is there, then we can use BE statistics to evaluate energy distribution, BE is applicable on integral spin particles; hence, it is valid for photon gas. Photons are subject to creation and destruction; hence, their number is not constant, that is, $\sum dn_i \neq 0$. Hence, the Lagrange multiplier α cannot be considered and only β is valid. Therefore, the BE statistics can be written as Eqn. (30).

$$n_j = \frac{g_j}{e^{E_j/k_B T} - 1} \quad (37a)$$

In terms of frequency, the relation Eqn. (37a) could be written down as follows:

$$n(f) = \frac{g(f)}{e^{E/k_B T} - 1} = \frac{g(f)}{e^{hf/k_B T} - 1} \quad (37b)$$

For calculating the function $g(f)$, we need to calculate $g(p) dp$ [as obtained in Eqn. (8)]. From Eqn. (12e), the $g(p) dp$ is given as follows:

$$g(p) dp = \frac{4\pi V p^2 dp}{h^3}$$

Photons also have two states of polarization, that is, "left handed and right handed." Hence, the photons are distinguishable on the basis of their polarization state that yields above relation to be

$$g(p) dp = \frac{8\pi V p^2 dp}{h^3} \quad (38)$$

$$\text{Now } p = \frac{hf}{c} \quad \Rightarrow \quad dp = \frac{h}{c} df$$

Therefore, Eqn. (38) could be written as follows:

$$g(f)df = \frac{8\pi V}{h^3} \frac{h^2 f^2}{c^2} \frac{h}{c} df = \frac{8\pi V f^2 df}{c^3} \quad (39)$$

Substituting Eqn. (39) in Eqn. (37b), we get

$$n(f)df = \frac{8\pi V f^2 df}{c^3} \times \frac{1}{e^{hf/k_B T} - 1} \quad (40a)$$

The energy density b/w (f and $f + df$) is given by following equation:

$$E(f)df = \frac{hf n(f)df}{V} = \frac{8\pi h f^3 df}{c^3 (e^{hf/k_B T} - 1)} \quad (40b)$$

Equation (40b) is Planck's law for black-body radiation.

Equation (40b) can be written in terms of wavelength as follows:

$$E(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5} \frac{d\lambda}{(e^{hc/\lambda k_B T} - 1)} \quad (41)$$

Equation (41) turns to Rayleigh–Leans law in low-temperature regime, that is, $hf \gg k_B T$

$$E(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5} \left(\frac{\lambda k_B T}{hc} \right) d\lambda = \frac{8\pi f^2 k_B T df}{c^3} \quad (42)$$

Equation (42) is regarded as ferrous Rayleigh–Jeans law.

11.9.2 Specific Heat of Solids (Classical and Quantum Approach)

Specific heat of a substance is the ratio of differential thermal energy dE for a mole of substance to the differential increase in temperature, that is,

$$C = \frac{dE}{dT} \quad (43)$$

C has units of cal/mole/K. For obtaining specific heat, we need to calculate E , that is, internal thermal energy of solid, as a function of temperature T . The variation of specific heat vs. temperature for solids is shown in Figure 11.6.

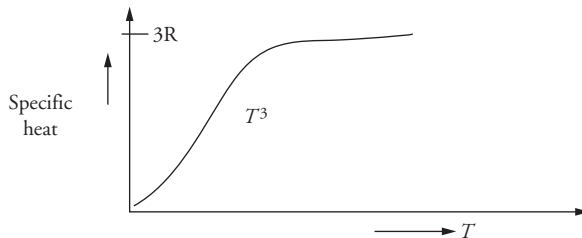


Figure 11.6 Variation of specific heat with temperature

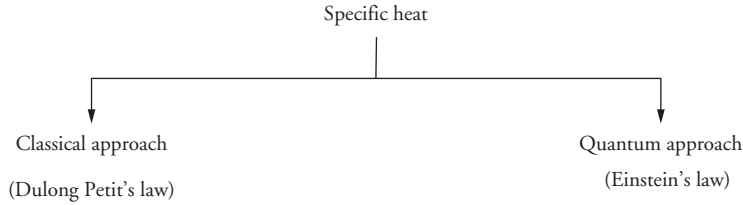


Figure 11.7 Classification of theories to calculate specific heat

From Figure 11.6, it is clear that specific heat tends to zero at absolute zero. At high temperatures, the specific heat varies as T^3 and then approaches almost a constant value of $3R$, where R is universal gas constant. There are basically two approaches for calculating specific heat as demonstrated in following section and also Figure 11.7.

11.9.2.1 Dulong and Petit Law

This model assumes the solid to be a collection of atoms that are vibrating, independently having equal force constant. Each atom is represented as three one-dimensional harmonic oscillator. The particle is executing the simple harmonic motion with same frequency but different amplitudes. If the total number of atoms is N , then the total energy of solid is N times average energy of each atomic oscillator. Let the particle be simple harmonic oscillator; hence, it will obey Hook's law as differential equation of motion:

i.e. Along z -direction, K is the force constant z is displacement and m is mean.

$$\frac{d^2 z}{dt^2} + \left(\frac{k}{m}\right)z = 0 \quad (44)$$

$$[\text{where } |F| = kz \Rightarrow ma = +kz \Rightarrow w^2 z = \frac{+k}{m}z \Rightarrow w^2 = \frac{+k}{m}]$$

The total energy of system is sum of potential and kinetic energy,

i.e.

$$E = \text{KE} + \text{PE}$$

$$E = \frac{p_z^2}{2m} + \int F \cdot dz$$

$$E = \frac{p_z^2}{2m} + \int_z^0 -(kz) dz = \frac{p_z^2}{2m} + \frac{mw^2 z^2}{2} \quad (45)$$

The average energy could be given as follows:

$$\bar{E} = \frac{\int_0^\infty E dN}{\int_0^\infty dN} \quad (46a)$$

For calculating Eqn. (46a), we should bear the following points in mind:

- (i) Although the atomic oscillators have same frequency, the amplitude is different; hence, energies are different.
- (ii) dN is the number of oscillators whose energy lie between energy interval E and $E + dE$.
- (iii) The dN oscillators are proportional to Boltzmann's exponential factor $e^{-\frac{E}{k_B T}}$.

$$\begin{aligned} \bar{E} &= \frac{\int_0^{\infty} E e^{-E/k_B T} dE}{\int_0^{\infty} e^{-E/k_B T} dE} \\ \bar{E} &= \frac{\int_0^{\infty} \left(\frac{p_z^2}{2m} + mw^2 z^2 \right) \exp \left[-\left(\frac{p_z^2}{2m} + \frac{mw^2 z^2}{2} \right) / k_B T \right] dE}{\int_0^{\infty} \exp \left[-\left(\frac{p_z^2}{2m} + \frac{mw^2 z^2}{2} \right) / k_B T \right] dE} \\ \bar{E} &= \frac{\frac{1}{2m} \int_{-\infty}^{\infty} p_z^2 e^{-\left(\frac{p_z^2}{2mk_B T} dp_z \right)} dE}{\int_{-\infty}^{\infty} e^{-\left(\frac{p_z^2}{2mk_B T} dp_z \right)} dE} + \frac{m\omega^2}{2} \frac{\int_{-\infty}^{\infty} z^2 e^{-\left(\frac{m\omega^2 z^2}{2k_B T} dz \right)} dE}{\int_{-\infty}^{\infty} e^{-\left(\frac{m\omega^2 z^2}{2k_B T} dz \right)} dE} \\ &\quad \downarrow \qquad \qquad \qquad \downarrow \\ &\quad \text{Potential energy} \qquad \qquad \text{Kinetic energy} \\ \bar{E} &= \frac{k_B T}{2} + \frac{k_B T}{2} = k_B T \end{aligned} \tag{46b}$$

[Equation (46b) has been calculated using special integral $\int_0^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4} \frac{\sqrt{\pi}}{a^{3/2}} \infty$ or simple integral could also be used.]

As per assumption, every oscillator possesses three degrees of freedom, hence

$$E = 3N_A \bar{E} = 3N_A k_B T \quad (N_A \text{ is Avogadro's number}) \tag{46c}$$

and

$$C = \frac{dE}{dT} = 3N_A k_B = 3R \tag{46d}$$

$$C = (3 \times 1.99) \text{ Kcal/Kmol K} \tag{46e}$$

$$C = (5.97) \text{ Kcal/Kmol K} \tag{46f}$$

Equation (46d) is Dulong–Petit’s law. This law shows independence of temperature. But the law is no longer valid for lighter elements and higher temperatures. The specific heat of solids drops to zero at absolute zero, which could not be explained on the basis of Dulong–Petit’s law. Hence, this law was to be modified. Then Einstein gave quantum approach, which explained everything.

11.9.2.2 Einstein’s Theory of Specific Heat

In 1907, Einstein assumed the oscillators to be $3N_A$ independent harmonic oscillators vibrating with frequency f . Classical theory assumed the energy to be continuous, but Einstein’s quantum approach assumed the energy to be in discrete packets. He used Planck’s formula, that is, $E = nhf = n\hbar\omega$.

The average energy for dN oscillators in energy range E and $E + dE$ is given by the following equation:

$$\bar{E} = \frac{\sum E dN}{\sum dN} \quad (47)$$

$$\bar{E} = \frac{\sum nhf \left[e^{-(E/k_B T)} \right]}{\sum \left[e^{-(E/k_B T)} \right]}$$

$$\bar{E} = \frac{hf \left[e^{-hf/k_B T} + 2e^{-2hf/k_B T} + \dots \right]}{\left[1 + e^{-hf/k_B T} + e^{-2hf/k_B T} + \dots \right]}$$

$$\bar{E} = hf \left[\frac{d}{dx} \log \left[1 + e^{-hf/k_B T} + e^{-2hf/k_B T} + \dots \right] \right]$$

$$\bar{E} = hf \left[\frac{d}{dx} \log \left[\frac{1}{1 - e^{-hf/k_B T}} \right] \right]$$

$$\bar{E} = hf \left[\frac{d}{dx} \left[\log 1 - \log \left(1 - e^{-(hf/k_B T)} \right) \right] \right]$$

$$\bar{E} = \frac{hf}{e^{hf/k_B T} - 1} \quad (48)$$

The total energy is given by the following equation:

$$E = 3N_A \bar{E} = \frac{3N_A hf}{e^{hf/k_B T} - 1}$$

$$C = \left(\frac{dE}{dT} \right) = \frac{d}{dT} \left(\frac{3N_A hf}{e^{hf/k_B T} - 1} \right) = \frac{3N_A k_B \left(\frac{hf}{k_B T} \right)^2 e^{hf/k_B T}}{\left[e^{hf/k_B T} - 1 \right]^2}$$

$$C = 3R \left[\left(\frac{hf}{k_B T} \right)^2 \frac{e^{hf/k_B T}}{\left(e^{hf/k_B T} - 1 \right)^2} \right] \quad (49a)$$

The following cases may arise:

- (i) For low temperatures $hf \gg k_B T$

$$C = 3R \left(\frac{hf}{k_B T} \right)^2 e^{-hf/k_B T} \quad (50)$$

Relation (50) clearly demonstrates that as the temperature decreases the specific heat drops exponentially and at absolute zero $C \rightarrow 0$.

- (ii) At high temperatures, $hf \ll k_B T$

$$C = 3R \left(\frac{hf}{k_B T} \right)^2 \frac{\left(1 + \frac{hf}{k_B T} \right)}{\left(1 + \frac{hf}{k_B T} - 1 \right)^2} \quad [\text{as } T \text{ as large}]$$

$$C = 3R \left(1 + \frac{hf}{k_B T} \right) \approx 3R \quad (51)$$

Hence, at high temperatures, the specific heat is same as derived by classical Dulong–Petit’s law.

SUMMARY

This unit deals with the probability and states. Probability is the ratio of number of ways leading to favorable way to total outcomes. For independent events, the probability is multiplicative in nature. The thermodynamic probability deals with the possible microstates in the macrostate. The concept of phase space deals with position coordinates (x, y, z) and velocity coordinate (v_x, v_y, v_z) for the moving particle. The statistics is divided into classical and quantum statistics. In classical statistics, the particles are distinguishable with continuous energy and small-phase space cell. Maxwell–Boltzmann statistics follow classical mechanics. According to quantum mechanics, the particles are indistinguishable with discrete energy and minimum phase space volume h^3 . Bose–Einstein and Fermi–Dirac statistics follow the quantum statistics. Using Maxwell–Boltzmann statistics, the most probable, root-mean-square and average velocity have been obtained. Root-mean-square velocity is 22 percent greater than most probable speed for given temperature, whereas average speed is 13 percent greater than the most probable speed for given temperature. FD statistics have been applied to free electron model of metals.

The free electrons are responsible for high conductivities of metals. When the temperature of system decreases, the energy also decreases and upon cooling, the electrons occupy lower states. Bose–Einstein statistics has been applied to photon gas. As photons are subject to creation and destruction, hence their number is not constant. Specific heat of solids has been calculated using classical (Dulong and Petit law) and quantum (Einstein’s theory of specific heat) approach.

SOLVED PROBLEMS

Q.1: Two six-faced dice are thrown together obtain the probability that face 4 comes up in both.

Ans: These dices are independent of each other, hence the events are considered independent.

The probability for 4 to come is $\frac{1}{6}$.

The total probability for two dices will become

$$= \frac{1}{6} \times \frac{1}{6} = \frac{1}{36}$$

Q.2: How could four distinguishable particles be arranged in three compartments?

Ans: The distributions could be given as follows:

$$\begin{aligned} & [0, 0, 4] \quad [4, 0, 0] \quad [0, 4, 0] \\ & [0, 1, 3] \quad [0, 3, 1] \quad [3, 1, 0] \\ & [1, 0, 3] \quad [1, 3, 0] \quad [3, 0, 1] \\ & [0, 2, 2] \quad [2, 0, 2] \quad [2, 2, 0] \\ & [1, 1, 2] \quad [1, 2, 1] \quad [2, 1, 1] \end{aligned}$$

The number of arrangements is given by thermodynamic probability, according to which

$$W(n_1, n_2 \dots n_k) = \frac{n!}{n_1! n_2! \dots n_k!}$$

Here, $n = 4$

$$\text{For } W(0, 4, 0) = \frac{4!}{0!0!4!} = 1$$

$$W(3, 1, 0) = \frac{4!}{3!1!0!} = 4$$

$$W(0, 2, 2) = \frac{4!}{0!2!2!} = 6$$

$$W(1, 1, 2) = \frac{4!}{1!1!2!} = 12$$

[**Note:** In the above thermodynamic probability, only one representative is taken, that is, $W(0, 2, 2) = W(2, 0, 2) = W(2, 2, 0)$. For all these arrangements W is 6.]

Total number of possible arrangements become

$$\begin{aligned} &= 3 \times 1 + 4 \times 6 + 3 \times 6 + 3 \times 12 \\ &= 3 + 24 + 18 + 36 \\ &= 81 \end{aligned}$$

Q.3: A card is drawn from well-shuffled pack. Obtain the probability of the card to be either a king or queen.

Ans: The total number of kings and queens are 8 for a pack of card.

Total number of cards are 52.

Hence, the P (for either king or queen) = $\frac{8}{52}$.

Q.4: If a coin is tossed, what would be the probability of tail not coming up?

Ans: Total number of outcomes are 2.

For head/tail, the probability is $\frac{1}{2}$.

Hence, the probability for tail not coming up is $1 - \frac{1}{2} = \frac{1}{2}$.

Q.5: Two coins are tossed simultaneously. Obtain the probability for heads to be coming up in both coins.

Ans: For two coins, the total number of ways is given by 4.

i.e. $(H, H), (T, T), (H, T), (T, H)$

Hence, the probability for heads coming up in both coins is $\frac{1}{4}$.

Q.6: A pair of six-faced dice is thrown simultaneously. Obtain the probability for which the sum of numbers showing up is 6?

Ans: There are 36 ways in which the outcome can come.

(1, 1) (2, 1) (3, 1) (4, 1) (5, 1) (6, 1)
 (1, 2) (2, 2) (3, 2) (4, 2) (5, 2) (6, 2)
 (1, 3) (2, 3) (3, 3) (4, 3) (5, 3) (6, 3)
 (1, 4) (2, 4) (3, 4) (4, 4) (5, 4) (6, 4)
 (1, 5) (2, 5) (3, 5) (4, 5) (5, 5) (6, 5)
 (1, 6) (2, 6) (3, 6) (4, 6) (5, 6) (6, 6)

There are five ways in which the dices can show up 6, that is,

(5, 1) (4, 2) (3, 3) (2, 4) (1, 5)

Hence, the probability = $\frac{5}{36}$.

Q.7: Obtain the percentage error in Stirling formula if (i) $n = 5$ and (ii) $n = 6$

Ans: (i) According to Stirling's formula,

$$\log_e n! = n \log_e n - n$$

for $n = 5$

$$\log_e 5! = \log_e (120) = 2.303 \times \log_{10} (120) = 4.788$$

According to Stirling formula,

$$\begin{aligned} \log_e n! &= 5 \log_e 5 - 5 \\ &= 3.048 \end{aligned}$$

Hence, the error comes out to be

$$\begin{aligned} &= 4.788 - 3.048 \\ &= 1.74 \end{aligned}$$

$$\% \text{ error in Stirling's formula} = \frac{1.74}{4.788} \times 100$$

$$= 36.34\%$$

(ii) For $n = 6$,

$$\begin{aligned} \log_e n! &= \log_e 6! \\ &= 2.303 \times \log_{10} (6!) \\ &= 2.303 \times \log_{10} (720) \\ &= 6.5804 \end{aligned}$$

According to Stirling's formula,

$$\begin{aligned} \log_e n! &= n \log_e n - n \\ &= 6 \times 2.303 \times \log_{10} (6) - 6 \\ &= 6 \times 2.303 \times 0.778 - 6 \\ &= 4.752 \end{aligned}$$

Hence, error comes out to be

$$\begin{aligned} &= 6.5804 - 4.752 \\ &= 1.8284 \end{aligned}$$

% error is equal to

$$= \frac{1.8284}{6.5804} \times 100$$

$$\% \text{ error} = 27.78\%$$

Q.8: For nitrogen gas at NTP, obtain the most probable and rms velocity.

Ans: For nitrogen, the mass is given by

$$\text{Mass } (m) = \frac{\text{Molecular weight}}{\text{Avogadro's number}}$$

$$\text{Mass } (m) = \frac{28}{6.023 \times 10^{23}} = 4.66 \times 10^{-23} \text{ gm}$$

Here, $T = 273 \text{ K}$, $k_B = 1.38 \times 10^{-16} \text{ ergs/K}$

$$\begin{aligned} v_{\text{mp}} &= \sqrt{\frac{2k_B T}{m}} \\ &= \sqrt{\frac{2 \times 1.38 \times 10^{-16} \times 273}{4.66 \times 10^{-23}}} \\ &= \sqrt{161.69 \times 10^7} \\ &= \sqrt{1616.9 \times 10^6} = 40.2 \times 10^3 \\ &= 4.02 \times 10^4 \text{ cm/sec} \end{aligned}$$

$$\begin{aligned} v_{\text{rms}} &= \sqrt{\frac{3k_B T}{m}} \\ &= \sqrt{\frac{3 \times 1.38 \times 10^{-16} \times 273}{4.66 \times 10^{-23}}} \\ &= \sqrt{242.53 \times 10^7} \\ &= \sqrt{2425.3 \times 10^6} \\ &= 49.247 \times 10^3 \\ &= 4.92 \times 10^4 \text{ cm/sec} \end{aligned}$$

Q.9: What would be the temperature, where average speed of hydrogen gas molecular is double the average speed of oxygen at 300 K.

Ans: The average velocity is given by

$$v_{\text{avg}} = \sqrt{\frac{8k_B T}{m\pi}}$$

where k_B is Boltzmann's constant and T is absolute temperature.

Let the mass of hydrogen atom is M and of oxygen is m .

For average speed of oxygen at $T = 300$ K

$$(v_{\text{avg}})_{\text{Oxygen}} = \sqrt{\frac{8k_B(300)}{m\pi}}$$

$$\text{and } (v_{\text{avg}})_{\text{Hydrogen}} = \sqrt{\frac{8k_B T}{M\pi}}$$

According to the given condition,

$$(v_{\text{avg}})_{\text{Hydrogen}} = 2(v_{\text{avg}})_{\text{Oxygen}}$$

$$\sqrt{\frac{8k_B T}{M\pi}} = 2\sqrt{\frac{8k_B(300)}{m\pi}}$$

$$\frac{8k_B T}{M\pi} = 4\left(\frac{8k_B \times 300}{m\pi}\right)$$

$$\frac{T}{M} = \frac{4 \times 300}{m}$$

$$T = \frac{4 \times 300 \times M}{m}$$

$$T = \frac{4 \times 300 \times 2}{32}$$

$$T = 75^\circ\text{K}$$

Q.10: Obtain the average velocity and root-mean-square velocity for hydrogen atom at 27°C .

Ans:

$$T = 27^\circ\text{C} = 300 \text{ K}$$

$$k_B = 1.38 \times 10^{-16} \text{ ergs/k}$$

$$N = 6 \times 10^{23} \text{ mol/mole}$$

$$m = \frac{\text{Molecular weight}}{\text{Avogadro number}}$$

$$m = \frac{2}{6.023 \times 10^{23}} = 3.3 \times 10^{-24} \text{ gm}$$

We will obtain average velocity first.

$$v_{\text{avg}} = \sqrt{\frac{8k_B T}{m\pi}}$$

$$\begin{aligned}
 &= \sqrt{\frac{8 \times 1.38 \times 10^{-16} \times 300}{3.3 \times 10^{-24} \times 3.14}} \\
 &= \sqrt{319.629 \times 10^{+8}} \\
 &= 17.878 \times 10^4 \\
 &= 1.78 \times 10^5 \text{ cm/sec}
 \end{aligned}$$

Now for root-mean-square velocity,

$$\begin{aligned}
 v_{\text{rms}} &= \sqrt{\frac{3k_B T}{m}} \\
 V_{\text{rms}} &= \sqrt{\frac{3 \times 1.38 \times 10^{-16} \times 300}{3.3 \times 10^{-24}}} \\
 &= \sqrt{376.36 \times 10^8} \\
 &= 19.4 \times 10^4 = 1.94 \times 10^5 \text{ cm/sec}
 \end{aligned}$$

Q.11: What would be the probability that the speed of hydrogen molecule at 300 K lies between 148 and 149 m/sec.

Ans: The probability of molecule possessing speed between v and $v + dv$ is given by

$$n(v) dv = \frac{\sqrt{2\pi n} m^{3/2} v^2 e^{-mv^2/2k_B T} dv}{(\pi k_B T)^{3/2}}$$

$$\begin{aligned}
 \text{Mass of Hydrogen} &= \frac{\text{Molecular mass}}{\text{Avogadro number}} \\
 &= \frac{2}{6 \times 10^{23}} = 3.3 \times 10^{-24} \text{ gm}
 \end{aligned}$$

$$k_B = 1.38 \times 10^{-23} \text{ J/K}$$

$$T = 300 \text{ K}$$

$$v = 148 \text{ m/sec}$$

$$dv = 149 - 148 = 1 \text{ m/sec}$$

The probability is given by the following relation:

$$P(v)dv = \frac{\sqrt{2\pi} m^{3/2} v^2 e^{-mv^2/2k_B T} dv}{(\pi k_B T)^{3/2}}$$

$$P(v)dv = 1.41 \times 3.14 \times \left(\frac{3.3 \times 10^{-24}}{3.14 \times 1.38 \times 10^{-23} \times 300} \right)^{3/2} (148)^2 e^{-\left(\frac{3.3 \times 10^{-24} \times (148)^2}{2 \times 1.38 \times 10^{-23} \times 300} \right)} \times 1$$

$$P(v)dv = 4.4274 \times (2.538 \times 10^{-3} \times 10^{-1})^{3/2} \times 21904 e^{-(87.298 \times 10^{-1})}$$

$$P(v)dv = 96977.76 \times (1.593 \times 10^{-2}) \times (2.538 \times 10^{-4}) \times e^{-8.7298}$$

$$P(v)dv = 96977.76 \times 4.043 \times 10^{-6} \times 1.6169 \times 10^{-4}$$

$$P(v)dv = 633955.9042 \times 10^{-10}$$

$$P(v)dv = 6.339 \times 10^{-5}$$

Q.12: Calculate the most probable speed for oxygen molecule at NTP, given that $k_B = 1.38 \times 10^{-16}$ ergs/K and Avogadro's number (N) = 6.023×10^{23} .

Ans: The most probable speed is given by

$$v_{mp} = \sqrt{\frac{2k_B T}{m}}$$

$$T = 273 \text{ K}$$

and

$$\text{Mass}(m) = \frac{\text{Molecular mass}}{\text{Avogadro number}}$$

$$= \frac{32}{6.023 \times 10^{23}} = 5.312 \times 10^{-23} \text{ gm}$$

$$v_{mp} = \sqrt{\frac{2 \times 1.38 \times 10^{-16} \times 273}{5.312 \times 10^{-23}}}$$

$$v_{mp} = \sqrt{\frac{753.48 \times 10^7}{5.312}}$$

$$v_{mp} = \sqrt{141.84 \times 10^7}$$

$$v_{mp} = \sqrt{1418.4 \times 10^6}$$

$$v_{mp} = 37.66 \times 10^3 = 3.76 \times 10^4 \text{ cm/sec}$$

Q.13: Calculate the different arrangements for 7 indistinguishable particles among 4 cells with a priori probability for Bose–Einstein statistics.

Ans: For BE statistics, the distinct arrangements could be given by

$$= \frac{(n_j + g_j - 1)!}{n_j!(g_j - 1)!}$$

Here, $n_j = 7$ and $g_j = 4$

$$= \frac{(7 + 4 - 1)!}{7!(4 - 1)!} = \frac{10!}{7!3!}$$

$$= \frac{10 \times 9 \times 8 \times 7!}{7!3!} = \frac{10 \times 9 \times 8}{3 \times 2} = 5 \times 3 \times 8$$

$$= 120$$

Hence, there are 120 different arrangements for 7 particles in four cells.

Q.14: For the particles obeying BE statistics, 7 particles are arranged in 2 compartments. The first compartment has 8 cells and the second compartment has 9 cells of equal size. Obtain the microstates for macrostate (3, 4).

Ans: In this case,

$$g_1 = 8 \text{ and } g_2 = 9$$

$$n_1 = 3 \text{ and } n_2 = 4$$

The thermodynamic probability is given by

$$\begin{aligned} W(n_1, n_2) &= \frac{(n_1 + g_1 - 1)!}{n_1!(g_1 - 1)!} \times \frac{(n_2 + g_2 - 1)!}{n_2!(g_2 - 1)!} \\ &= \frac{(8 + 3 - 1)!}{3!(8 - 1)!} \times \frac{(9 + 4 - 1)!}{4!(9 - 1)!} \\ &= \frac{10!}{3!7!} \times \frac{12!}{4!8!} \\ &= \frac{10 \times 9 \times 8 \times 7!}{3!7!} \times \frac{12 \times 11 \times 10 \times 9 \times 8!}{4!8!} \\ &= \frac{10 \times 9 \times 8}{3 \times 2} \times \frac{12 \times 11 \times 10 \times 9}{4 \times 3 \times 2 \times 1} \\ &= 5 \times 3 \times 8 \times 11 \times 5 \times 9 \\ &= 59,400 \end{aligned}$$

Hence, the thermodynamic probability is given by 59,400.

Q.15: Calculate the different arrangements for 5 particles among 6 cells with a priori probability for Fermi–Dirac statistics.

Ans: For FD statistics, the arrangements are given by

$$\frac{g_j!}{(g_j - n_j)!n_j!}$$

Here $g_j = 6$ and $n_j = 5$

Here, the number of arrangements is $\frac{6!}{1!5!}$

$$= \frac{6!}{1!5!} = 6$$

Hence, there are six different arrangements.

Q.16: For particles obeying FD statistics, 6 particles are arranged in two compartments. The first compartment has 7 cells and the second compartment has 8 cells, all of equal size. Obtain the microstates for macrostate (2, 4).

Ans: Here,

$$g_1 = 7 \text{ and } g_2 = 8$$

$$n_1 = 2 \text{ and } n_2 = 4$$

Hence, the thermodynamic probability is given by

$$\begin{aligned} W(n_1, n_2) &= \frac{g_1!}{(g_1 - n_1)!n_1!} \times \frac{g_2!}{(g_2 - n_2)!n_2!} \\ &= \frac{7!}{5!2!} \times \frac{8!}{4!4!} \\ &= \frac{7 \times 6 \times 5!}{2 \times 1 \times 5!} \times \frac{8 \times 7 \times 6 \times 5 \times 4!}{4 \times 3 \times 2 \times 1 \times 4!} \\ &= 7 \times 3 \times 7 \times 5 \times 2 \\ &= 1470 \end{aligned}$$

Hence, there are 1470 different microstates for 6 particles in two cells (with a priori probability).

Q.17: Calculate the number of modes in a body of volume 50 cc in the wavelength range 5890 – 5896 Å.

Ans: For, the frequency range f and $f + df$, the number of modes are given by

$$\frac{8\pi f^2}{c^3} df$$

$$f = \frac{c}{\lambda}$$

$$df = -\frac{c}{\lambda^2} d\lambda$$

Hence, the number of modes in range λ and $\lambda + d\lambda$ is given by

$$\frac{8\lambda}{\lambda^4} d\lambda$$

Here, $\lambda = 5890 \text{ \AA}$ and $d\lambda = 6 \text{ \AA}$

Number of modes in 50 cc ($\approx 50 \times 10^{-6} \text{ m}^3$)

$$\begin{aligned} &= \frac{8 \times 3.14 \times 6 \times 10^{-10}}{(5890 \times 10^{-10})^4} \times 50 \times 10^{-6} \\ &= \frac{7536 \times 10^{-16}}{1.20354 \times 10^{15} 10^{-40}} \\ &= \frac{7536 \times 10^{-16}}{1.2035 \times 10^{-25}} \\ &= 6261.74 \times 10^9 \\ &= 6.26 \times 10^{12} \end{aligned}$$

Q.18: 40 Fermi particles are distributed in three compartments having energy $2E$, E , $-E$ Obtain the energy of macrostate (20, 5, 15).

Ans: Total energy of macrostate is given by

$$E = \sum_{j=1}^k n_j E_j$$

For $k = 3$, with energy $2E$, E , and $-E$.

$$\begin{aligned} E &= n_1 E_1 + n_2 E_2 + n_3 E_3 \\ &= 20 \times 2E + 5 \times E + 15 \times (-E) \\ &= 40E + 5E = 15E \\ &= 30E \end{aligned}$$

Q.19: Obtain the Fermi energy for silver metal. Given density of silver = 10.5 gm/cm^3 and atomic weight is 1.08 gm. Silver atom has 1 free electron / atom

Ans: The Fermi energy, $E_F = \frac{h^2}{8m} \left[\frac{3n}{\pi V} \right]^{2/3}$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$\text{Volume} = \frac{\text{mass}}{\text{density}} = \frac{108}{10.5 \times 10^6} \text{ m}^3$$

$$E_F = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31}} \left[\frac{3 \times 10.5 \times 10^6}{3.14 \times 108} \right]^{2/3}$$

$$E_F = 8.78 \times 10^{-19} \text{ J}$$

In eV, we get

$$E_F = \frac{8.78 \times 10^{-19}}{1.6 \times 10^{-19}} = 5.48 \text{ eV}$$

Q.20: The Fermi velocity of an electron is 7.3×10^5 m/sec for cesium atom. Also obtain the Fermi energy of cesium metal.

Ans: The Fermi energy is given by

$$\begin{aligned} E_F &= \frac{1}{2} m v_F^2 \\ &= \frac{1}{2} \times 9.1 \times 10^{-31} \times 7.3 \times 10^5 \\ &= 2.41 \times 10^{-19} \text{ J} \end{aligned}$$

In eV,

$$\begin{aligned} E_F &= \frac{2.41 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 1.506 \text{ eV} \end{aligned}$$

According to the Fermi temperature,

$$\begin{aligned} k_B T_F &= E_F \\ T_F &= \frac{E_F}{k_B} \\ T_F &= \frac{1.506 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23}} \\ &= 1.748 \times 10^4 \text{ K} \end{aligned}$$

OBJECTIVE QUESTIONS

1. The probability for two independent events with probability P_1 and P_2 is

(a) $\frac{P_1}{P_2}$

(b) $\frac{P_2}{P_1}$

(c) $P_1 + P_2$

(d) $P_1 \cdot P_2$

2. Frequency of occurrence is defined as total number of _____ for a given macrostate.

- (a) particles (b) microstates
(c) cells (d) compartments

3. The thermodynamic probability for n number of particles in k compartments is

- (a) $\frac{n_k}{n}$ (b) $\frac{n}{n_k}$
(c) $\prod_{i=1}^k \frac{n!}{n_i!}$ (d) $\sum \frac{n!}{n_i!}$

4. The probability for the distribution of n particles in g_k compartments is

- (a) $n! \prod_{i=1}^k \frac{(g_i)^{n_i}}{n_i!}$ (b) $\prod_{i=1}^k \frac{g_i}{n_i!}$
(c) $n! \prod_{i=1}^k (g_i)^{n_i}$ (d) $\prod_{i=1}^k \frac{n_i!}{g_i}$

5. Phase space is constituted by

- (a) 8 coordinates (b) 6 coordinates
(c) 3 coordinate (d) 9 coordinates

6. The volume dc of phase space is given by

- (a) $dV \cdot d\Gamma$ (b) $\frac{dV}{d\Gamma}$
(c) $dV + d\Gamma$ (d) $\frac{d\Gamma}{dV}$

7. In classical mechanics, the dimension of h is

- (a) erg. sec. (b) mass \times velocity² \times sec
(c) both of them (d) none of these

8. According to quantum mechanics, the volume of phase space is

- (a) $\leq h^3$ (b) $\leq h^2$
(c) $> h$ (d) $\geq h^3$

9. Classical mechanics assumes the energy to be

- (a) discrete (b) continuous
(c) impackets (d) all of these

10. In quantum mechanics, the particles are

- (a) distinguishable (b) indistinguishable
(c) of the same mass (d) of the same velocity

11. According to Sterling's formula when n is extremely large, then

- (a) $\ln n! = n \ln n - n$ (b) $\ln n = n \ln n!$
(c) $n = n \ln n - n^2$ (d) $\ln n! = n \ln n! - n!$

12. The MB energy distribution law is given by

- (a) $n_i = g_i (e^{\alpha + \beta E_i})$ (b) $n_i = g_i e^{\beta E_i}$
(c) $n_i = g_i (e^{-\alpha - \beta E_i})$ (d) $g_i = n_i (e^{-\alpha - \beta E_i})$

13. The Boltzmann factor is given by

- (a) $e^{\beta E_i}$ (b) $\sum e^{\beta E_i}$
(c) $e^{-\beta E_i}$ (d) $\sum e^{-\beta E_i}$

14. The partition function is given by

- (a) $e^{\beta E_i}$ (b) $\sum e^{-\beta E_i}$
(c) $e^{-\beta E_i}$ (d) $\sum e^{\beta E_i}$

15. The factor $e^{-\alpha}$ in MB statistics is given by

- (a) $\frac{n}{V} \left(\frac{\beta}{2\pi m} \right)^{1/2}$ (b) $\frac{nh^3}{V} \left(\frac{2\pi m}{\beta} \right)^{3/2}$
(c) $\frac{nh^3}{V} \left(\frac{2\pi m}{\beta} \right)^{1/2}$ (d) $\frac{nh^3}{V} \left(\frac{\beta}{2\pi m} \right)^{3/2}$

16. The value of β is given by

- (a) $k_B T^2$ (b) $k_B T$
(c) $\frac{1}{k_B T}$ (d) $\frac{1}{k_B T^2}$

17. The most probable velocity is given by

- (a) $\sqrt{\frac{2k_B T}{m}}$ (b) $\sqrt{\frac{8k_B T}{\pi m}}$
(c) $\sqrt{\frac{3k_B T}{m}}$ (d) \sqrt{v}

18. The root-mean-square velocity is given by

(a) $\sqrt{\frac{2k_B T}{m}}$

(b) $\sqrt{\frac{3k_B T}{m}}$

(c) $\sqrt{\frac{8k_B T}{\pi m}}$

(d) $\sqrt{\frac{k_B T}{m}}$

19. The ratio of rms and most probable velocity is

(a) 1.22

(b) 1.13

(c) 1.45

(d) 1.52

20. In BE statistics, the number of different arrangements is given by

(a) $\frac{n_j!}{(n_j)(g_j - 1)!}$

(b) $\frac{n_j!(g_j - 1)!}{(n_j + g_j - 1)!}$

(c) $\frac{n_j!}{(g_j - n_j)!}$

(d) $\frac{(n_j + g_j - 1)!}{n_j!(g_j - 1)!}$

21. The Bose–Einstein distribution function is given by

(a) $n_i = \frac{g_j}{e^\alpha e^{\beta E_j}}$

(b) $n_j = \frac{g_j}{e^\alpha e^{\beta E_j} + 1}$

(c) $n_j = \frac{g_j}{e^\alpha e^{\beta E_j} - 1}$

(d) $g_j = \frac{n_j}{e^\alpha e^{\beta E_j} - 1}$

22. The Thermodynamic probability for FD statistics is

(a) $\frac{g_j!}{(g_j - n_j)!}$

(b) $\frac{g_j!}{(g_j - n_j)! n_j!}$

(c) $g_j!(g_j - n_j)!$

(d) $g_j!$

23. The Fermi–Dirac distribution is given by

(a) $n_j = \frac{g_j}{e^\alpha e^{\beta E_j} + 1}$

(b) $n_j = \frac{g_j}{e^\alpha e^{\beta E_j} - 1}$

(c) $n_j = \frac{g_j}{e^\alpha e^{\beta E_j}}$

(d) $g_j = \frac{n_j}{e^\alpha e^{\beta E_j} + 1}$

24. The Fermi energy is given by

(a) $\frac{h^2}{2m} \left(\frac{8\pi V}{3n} \right)^{2/3}$

(b) $\frac{2m}{h^2} \left(\frac{8\pi V}{3n} \right)^{1/2}$

(c) $\frac{h^2}{2m} \left(\frac{3n}{8\pi V} \right)^{2/3}$

(d) $\left(\frac{3n}{8\pi V} \right)^{2/3}$

25. The average energy at 0K is given by

- (a) $\frac{1}{4}E_F$ (b) $\frac{3}{5}E_F$
 (c) $\frac{1}{2}E_F$ (d) 0

26. According to Dulong and Petit's law, the C_v is

- (a) $5R$ (b) $3R$
 (c) $2R$ (d) R

27. According to Einstein's theory of solids, at low temperatures the specific heat is

- (a) $3R\left(\frac{hf}{k_B T}\right)^2$ (b) $3R\left(\frac{hf}{k_B T}\right)e^{-hf/k_B T}$
 (c) $3R\left(\frac{hf}{k_B T}\right)^2 e^{-\frac{hf}{k_B T}}$ (d) 0

ANSWERS

- | | | |
|--------|---------|---------|
| 1. (d) | 10. (b) | 19. (a) |
| 2. (b) | 11. (a) | 20. (d) |
| 3. (c) | 12. (c) | 21. (c) |
| 4. (a) | 13. (c) | 22. (b) |
| 5. (b) | 14. (b) | 23. (a) |
| 6. (a) | 15. (d) | 24. (c) |
| 7. (c) | 16. (c) | 25. (b) |
| 8. (d) | 17. (a) | 26. (b) |
| 9. (b) | 18. (b) | 27. (c) |

Micro-assessment Questions

1. What are the basic assumptions of Fermi–Dirac statistics?
2. Explain the thermodynamic probability.
3. What is difference between microstate and macrostate?
4. How will you define cells in compartments?
5. What are fermions?
6. Describe the bosons with examples.
7. Which particles obey Pauli exclusion principle?
8. What do you understand by constraints on system?
9. What do you understand by most probable state for a system?
10. Which factor describes the distribution of molecular speeds for ideal gas?
11. Define momentum space. How does it differ from phase space?
12. What are fermions?
13. What are bosons?
14. How did the concept of phase space come into existence?
15. What is partition function?
16. What is Boltzmann factor?
17. What is the main application for FD statistics?
18. What is Rayleigh–Jeans law?
19. What is specific heat of solid?

Critical Thinking Questions

1. Give any two laws of probability.
2. Calculate the percentage error in Sterling formula when $n = 3$.
3. What do you understand by phase space?
4. What should be the minimum size for a phase space cell according to quantum and classical mechanics?
5. Give the various microstates and macrostates for system with two distinguishable particles.
6. Describe briefly the two main classifications for statistics.
7. What are the assumptions for Bose–Einstein statistics?
8. Explain how Fermi–Dirac statistics could be applied to electron gas?
9. Give the derivation for Maxwell–Boltzmann statistics.
10. What do you understand by photon gas?
11. The identical gas molecules are treated distinguishable classically. Explain.
12. Define cells for a compartment.
13. What is the meaning and importance of “a priori probability”?
14. What is the difference between BE and FD statistics?
15. Why hydrogen escapes the earth atmosphere and oxygen cannot?
16. Discuss the distribution of three particles in two boxes classically and quantum mechanically.
17. Explain the common approach for dealing with MB, BE, and FD statistics.
18. State and explain the Maxwell–Boltzmann statistics for the distribution of molecular speeds.
19. Give the distribution of three particles in three boxes according to MB, BE, and FD statistics.

20. Obtain the expression for phase space cells in the kinetic energy interval E and $E + dE$.
21. Prove that for MB distribution, $\beta = 1/k_B T$.
22. Show that MB distribution holds good for low concentration of particles.
23. How does MB and BE distribution differ from each other?
24. What do you understand by Dulong and Petit law?

Graded Questions

1. Assuming that low-energy neutrons are in thermal equilibrium with the surroundings without absorption and that the Maxwellian distribution for velocities is valid, deduce their energy distribution.
2. Show that for Maxwellian distribution of velocities of gas molecules, the root mean square of speed $\langle v_{rms} \rangle = (3 k_B T/m)^{1/2}$.
3. Show that the average speed of gas molecule $\langle v_{avg} \rangle = 8 k_B T/\pi m$.
4. Show that the most probable speed of the gas molecules $v_p = (2 k_B T/m)^{1/2}$. Also show that the ratio $v_p : \langle v_{avg} \rangle : \langle v_{rms} \rangle :: \sqrt{2} : \sqrt{8/\pi} : \sqrt{3}$.
5. Assuming that the hydrogen molecules have a root-mean-square speed of 1,270 m/s at 300 K, calculate the rms at 600 K.
6. Calculate the fraction of the oxygen molecule with velocities between 199 m/s and 201 m/s at 27°C.
7. In the quantum theory of black-body radiation, Planck assumed that the oscillators are allowed to have energy, 0, E , $2E$, Show that the mean energy of the oscillator is $E_{avg} = E/[\exp(E/k_B T) - 1]$ where $E = hf$.
8. A black-body has its cavity of cubical shape. Determine the number of modes of vibration per unit volume in the wavelength region 4,990–5,010 Å.
9. Estimate the temperature of the earth, assuming that it is in radiation equilibrium with the sun (assume the radius of sun $R = 7 \times 10^8$ m, the earth–sun distance $r = 1.5 \times 10^{11}$ m, the temperature of solar surface $T = 5,800$ K).
10. The mass of the sun is 2×10^{31} kg, its radius 7×10^8 m, and its effective surface temperature 5,700 K. Then
 - (a) obtain the mass of the sun lost per second by radiation.
 - (b) obtain the time necessary for the mass of the sun to diminish by 1 percent.
11. Prove that the specific heat is constant and is independent of temperature.
12. State and explain Einstein theory of specific heat. Show that at high temperatures, the specific heat is same as derived by Dulong and Petit's law.

Remember and Understand

1. The macroscopic behavior of a system is identified by the compartments. Each compartment has definite energy, momentum, velocity, and specific volume.
2. Thermodynamic probability depends upon nature of particles. In other words, it treats the particles to be distinguishable or indistinguishable.
3. All the distinct arrangements of particles are termed macrostates for the particles.
4. When the particle is at rest, only three position coordinates are required to define the particle, that is, x , y , z . But when the particle is moving, then momentum coordinates are also taken

into account due to velocity. Hence, six coordinates are required to define the particle. This six-dimensional space is termed as phase space.

5. The phase space can be divided into small compartments (k). Further, the particles are divided into these compartments.
6. The state with maximum thermodynamic probability corresponds to most probable macrostate.
7. The statistics are categorized into classical and quantum. Maxwell–Boltzmann statistics is classical and treats particles as distinguishable. Quantum statistics is further classified as Bose–Einstein and Fermi–Dirac, and both of them treat particles as indistinguishable.
8. At low-density limit and high-temperature limit, the quantum statistics become identical to classical mechanics.
9. The Dulong–Petit law states that the specific heat is independent of temperature.

Superconductors and Semiconductors

Keywords: superconductor, Meissner effect, Silsbee effect, soft and hard superconductors, BCS theory, semiconductors, p–n junction diode, forward biasing and reverse biasing, rectifiers, transistors, amplifiers

Learning Objectives

- ◆ To understand the phenomena of superconductivity
- ◆ To learn about the critical field and Meissner effect
- ◆ To learn about the classification of superconductors into type I and type II
- ◆ To learn about the properties of superconductors, that is, entropy, heat capacity, energy gap, and thermal conductivity
- ◆ To study about the isotope effect
- ◆ To gain insight over flux quantization and thermodynamics of superconducting transitions
- ◆ To understand the Bardeen, Cooper, and Schrieffer theory for the explanation of superconductivity
- ◆ To understand the classification of materials into conductors, insulators, and semiconductors
- ◆ To know about intrinsic and extrinsic semiconductors
- ◆ To learn about different dopings in semiconductors, that is, p-type and n-type semiconductors
- ◆ To understand about the forward biasing and reverse biasing of p–n junction diode
- ◆ To know about junction diode as a half- and full-wave rectifier
- ◆ To know about zener diode as a voltage regulator
- ◆ To gain insight into the transistors and its components, that is, base, collector, and emitter.
- ◆ To understand the working of p–n–p and n–p–n transistors
- ◆ To learn about the input characteristics of n–p–n and p–n–p transistors in common base and common emitter configurations
- ◆ To understand the working of a transistor as an amplifier
- ◆ To learn about voltage and power gain in common base and common emitter configurations

H. Kamerlingh Onnes was the first to liquefy helium, and he discovered the phenomena of superconductivity in 1911. He observed how resistance varies with temperature for mercury. At a temperature of 4.15 K, the resistance of mercury falls down sharply and reached almost zero as shown in the Figure 12.1. The temperature at which the resistance abruptly falls to zero (in the absence of magnetic field) is called critical temperature.

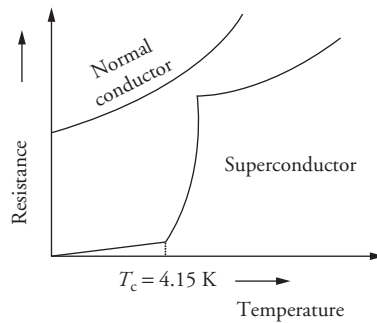


Figure 12.1 Variation of resistance with temperature.

Hence, the phenomena in which the resistivity of conductor approaches zero, when the temperature of conductor is reduced below critical temperature, is called superconductivity, and the materials that exhibit this property are known as superconductors.

Many elements in the periodic table—intermetallic compounds, semiconductor, and other alloys—show the phenomena of superconductivity. Many thallium cuprates have critical temperature of 125 K. The alloys of niobium (Nb) and germanium (Ge) have critical temperature of 23.2 K. Y–Ba–Cu–O system have the critical temperature of 90 K. The superconductors whose critical temperature is greater than 25 K are known as high-temperature superconductors. Many superconductors have been obtained, which have transition temperature of almost 138 K, and they have composition Hg–Ba–Ca–Cu–O.

12.1 The Critical Field

Superconductivity gets destroyed when strong magnetic field is applied to superconductors. The superconductor behaves as normal conductor. The magnetic field at which the superconductor starts behaving as normal conductor is known as critical field, and it is denoted by H_c . The following equation gives the relation between critical field and critical temperature:

$$H_c = H_0 \left(1 - \left(\frac{T}{T_c} \right)^2 \right) \quad (1)$$

H_0 is the critical field at 0 K, and it is material property of every element. High value of T_c represents low value of H_c . At $T = T_c$, H_c becomes zero.

The curve between H_c and T is a parabolic curve (Figure. 12.2). Beyond the boundary of parabola, the material behaves as normal conductor; and inside the boundary, it is superconducting.

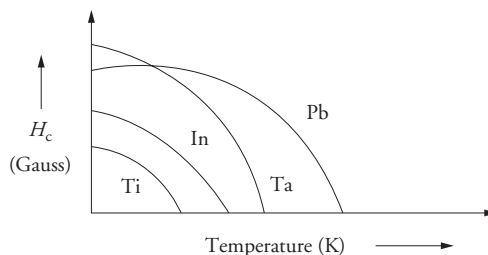


Figure 12.2 H_c – T curves for superconductors.

Onnes found that the superconductivity gets destroyed when the current exceeds the critical value. At the same time, current is also the cause of magnetic field [$B = \mu_0 I/2\pi r$]. Hence, these two phenomena are interrelated. According to Silsbee, the superconductivity gets destroyed by the magnetic field associated with current rather than the current itself.

12.2 Meissner Effect (Flux Exclusion)

In 1933, Meissner and Ochsenfeld found that if a superconductor is cooled below the critical temperature in magnetic field, then the magnetic field lines are pushed out of the superconductor. This phenomenon is called the Meissner effect (Figure 12.3). For the Meissner effect, the sample should be free from strain and impurities. In case the sample contains some impurities, then the flux may remain trapped inside the specimen. Perfect superconductors behave as perfect diamagnet. Meissner effect could be attained in either of the following two ways:

- (i) T_c is reached first, and then the magnetic field is applied.
- (ii) The magnetic field is applied, and then the sample is cooled up to critical temperature(T_c).

Mathematically, the explanation could be given as follows:

As there is no field inside the superconductor,

$$B = \mu_0 (H + M) = 0 \quad (\text{M is the magnetization and H is magnetic field}) \quad (2)$$

$$H = -M \quad (3)$$

Magnetic susceptibility is given by the following equation:

$$\chi = \frac{M}{H} \quad (4)$$

$$\chi = -1 \quad (5)$$

Equation (5) signifies the perfect diamagnetic substances. But, it is contradictory to Maxwell's equations.

From Ohm's Law,

$$J = \sigma E \quad (6a)$$

For superconductor, charge density $\rho = 0$, and hence $E = 0$.

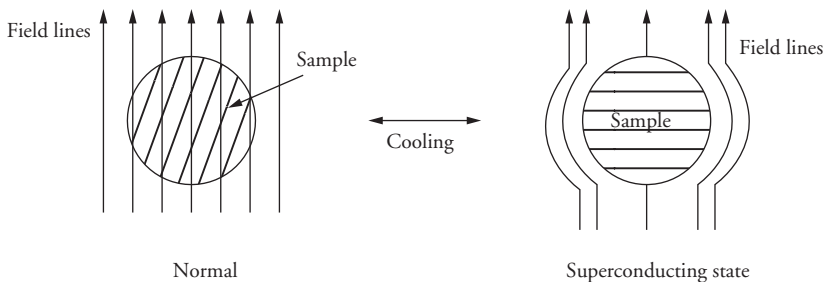


Figure 12.3 Meissner effect indicating the exclusion of field lines from the superconductor.

Therefore, from Maxwell's equation,

$$\nabla \times E = \frac{-d\vec{B}}{dt} \quad (6b)$$

$$\frac{dB}{dt} = 0$$

$$B = \text{constant} \quad (6c)$$

This equation signifies that for a perfect superconductor, the magnetic field is constant even if it is cooled below transition temperature. Hence, according to Maxwell equation, the magnetic field is not expelled, but it is constant inside the superconductor. Therefore, $E = 0$ and $B = 0$ are mutually independent of each other.

12.3 Type-I and Type-II Superconductors

There are two groups of superconductors as shown in Figure 12.4(a)–(b). These two types are discussed as follows:

1. Type-I Superconductors (Soft)

Figure 12.4(a) represents type-I superconductors. They follow Meissner's effect, and they are perfect diamagnets. The flux is completely excluded from their body. Moreover, these are also pure specimens (impure specimens may have some flux trapped inside them). The critical field is very low for these samples. Hence, they do not have much technical applications.

2. Type-II Superconductors (Hard)

Figure 12.4(b) represents type-II superconductors. These superconductors do not have very sharp value of critical field H_c . These superconductors do not follow Meissner's effect strictly. Below H_{c1} , the specimen is diamagnetic, that is, no magnetic field lines exist inside the body. H_{c1} is also known as lower critical field. At fields $H > H_{c1}$, the field lines penetrate inside the specimen that increases up to $H = H_{c2}$. H_{c2} is the upper critical field. Large field is required to destroy the superconductivity of specimen. Hence, these superconductors are called hard superconductors. For these superconductors, magnetization does not vanish abruptly. It vanishes gradually unlike soft superconductors. Type-II superconductors can be divided into three regions:

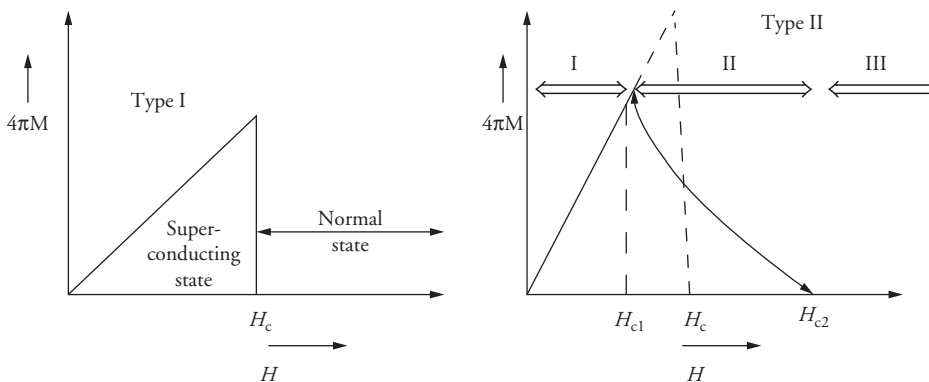


Figure 12.4 Magnetization curve for (a) Type-I and (b) Type-II superconductors.

- (i) Region I: It is the superconducting state ($H < H_{c1}$).
- (ii) Region II: It is the vortex/intermediate state ($H_{c1} < H < H_{c2}$).
- (iii) Region III: It is the normal state ($H > H_{c2}$).

These superconductors have many practical applications, for example, high field magnets for particle accelerators and magnetic levitation trains.

12.4 Properties of Superconductors

The following are some of the important properties of superconductor.

12.4.1 Entropy and Heat Capacity

For superconductors, the entropy decreases sharply as the temperature decreases below critical temperatures (Figure. 12.5). Entropy represents the randomness and disorder of the system. Hence, decrease in entropy indicates decreased randomness or increased order of the system. Therefore, superconducting state is more ordered than the normal state. In normal state, there are many thermally excited electrons. These electrons get ordered in the superconducting state. In type-I superconductors, the length of the order of 10^{-6} m has been obtained and this length is called coherence length.

The specific heat consists of two components, that is,

$$C = C_e + C_l = A_1 T + A_2 T^3 \quad (7)$$

Equation (7) indicates the contribution of specific heat from electrons and lattice. A_1 and A_2 are constants. The changes in specific heat of specimen occur due to the change in C_e . The electronic specific heat varies with temperature as follows:

$$C_e \propto \exp\left[-\frac{\Delta}{k_B T}\right] \quad (8)$$

$\Delta = 1.4 k_B T_c$ and k_B is Boltzmann's constant. Δ is also known as energy gap parameter. Figure 12.6(a)–(b) represents variation of $\frac{C}{T}$ vs T^2 and $\frac{C_e}{A_1 T_c}$ vs $\frac{T}{T_c}$.

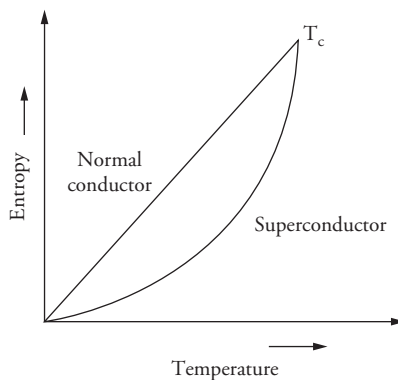


Figure 12.5 Entropy vs. temperature for normal and superconductor.

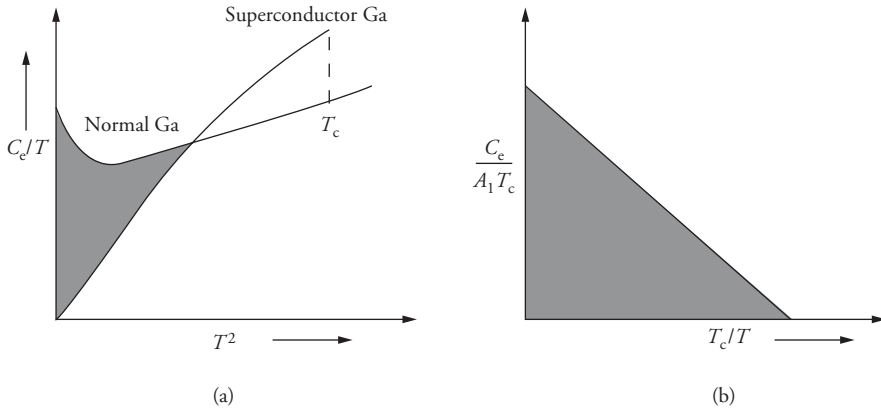


Figure 12.6 (a) Temperature variation of heat capacity in normal as well as superconducting state for Ga and (b) variation of electronic specific heat vs T_c/T .

12.4.2 Energy Gap

The heat capacity varies in exponential manner for superconductors as $C_e \propto \exp\left[-\frac{\Delta}{k_B T}\right]$. This relation goes in accordance with the thermal excitation for energy gap (Figure 12.7(a)–(b)) for superconductors.

The energy gap in superconductor is different from the semiconductors or insulators. For superconductors, the energy gap separates the normal electron states from the superconducting electronic states. As the temperature becomes T_c , the gap decreases continuously. For semiconductors or insulators, the band gap separates valence and conduction bands. Moreover, for insulators, the band gap is independent of temperature. For superconductors, the electrons in the excited state behave as normal electrons and they are above the energy gap. Below the energy gap, the electrons behave as superconducting electrons.

Δ is the energy gap parameter and is equal to $1.4 k_B T_c$ for Ga, we obtain energy gap as

$$E_g = 2\Delta \approx 10^{-4} \text{ eV} \tag{9}$$

Photons of energy less than 2Δ are not absorbed. For measuring band gap, microwave radiations are passed through superconductors. The absorption will take place only when $hf \geq E_g$.

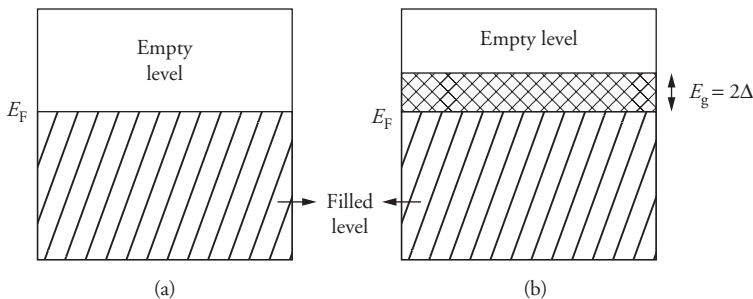


Figure 12.7 (a) Energy band for normal state and (b) for superconductors.

12.4.3 Thermal Conductivity

The thermal conductivity decreases when the specimen changes from normal to superconductor. There is no electronic contribution when the material becomes superconductor. For impure superconductors, the thermal conductivity increases. Hulm suggested that increase in thermal conductivity of impure superconductors is due to decrease in scattering of lattice waves by electrons.

12.5 Isotope Effect

The superconducting critical temperature is different for isotopes of elements. This effect is known as isotope effect and was discovered by Maxwell and Reynolds in 1950. If M is the mass of superconductor and T_c is the critical temperature, then

$$M^\alpha \propto \frac{1}{T_c}$$

$$M^\alpha T_c = \text{constant} \quad (10)$$

For most of the semiconductor, $\alpha = 1/2$, hence

$$M^{1/2} T_c = \text{constant} \quad (11)$$

As per this relation, when M decreases, then T_c increases. Maxwell and Serine obtained $T_c = 4.185$ K and 4.146 K for mercury, and the mass was found to be 199.5 and 203.4 a.m.u, respectively. The variation of $\log T_c$ and $\log M$ for mercury is given by Figure 12.8.

From the lattice vibrations, we know that θ_D is Debye temperature is inversely proportional to square root of mass of atom, that is,

$$\theta_D \propto \frac{1}{\sqrt{M}}$$

$$\theta_D M^{1/2} = \text{constant} \quad (12a)$$

Comparing Eqs (11) and (12a),

$$\frac{T_c}{\theta_D} = \text{constant} \quad (12b)$$

From Eqn. (12b), it is evident that superconducting state of specimen is related to the phonon vibrations. Hence, the phonon interactions might be playing a crucial role in superconductivity. Bardeen, Cooper, and Schrieffer gave a new theory of superconductivity based on phonon interaction.

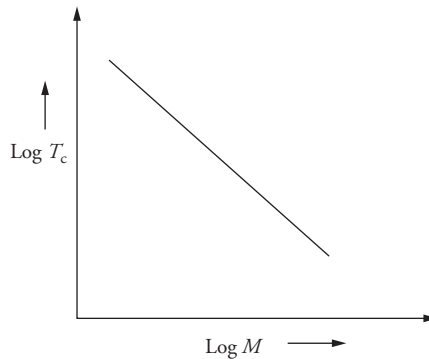


Figure 12.8 Variation of $\log T_c$ vs $\log M$.

12.6 Flux Quantization

When a superconductor ring or hollow sphere is placed in magnetic field that is perpendicular to the plane of ring, and the temperature is reduced below transition temperature, then there is no magnetic flux density inside it and the superconductor behaves like a perfect diamagnet. The current flows through the surface. Current continues to flow even when the external field is made zero. This current produces a flux ϕ , given by

$$\phi = \frac{nh}{2e} \quad (13)$$

$n = 1, 2, 3$ and h is Planck's constant ($h=6.63 \times 10^{-34}$ J s). The state of flux quantisation is shown in Figure. 12.9.

For $n = 1$,

$$\phi = \frac{h}{2e} = 2.07 \times 10^{-13} \text{ Wb} \quad (14)$$

Equation (14) gives the minimum value of flux associated with the ring, and it is known as fluxoid.

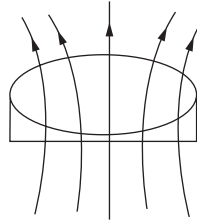


Figure 12.9 Flux quantization.

12.7 The Thermodynamics of Superconducting Transitions

According to Meissner effect, the transition between superconductor and normal state is thermodynamically reversible. Van Laer and Keesom gave the experimental demonstration of the transition. We will obtain an expression for the entropy difference of normal and superconducting state. We will obtain the expression for type-I superconductor (with $B = 0$). The Gibbs free energy/volume in magnetic field is

$$G = U - TS - HM \quad (15a)$$

Where $M \rightarrow$ Magnetization induced due to magnetic field H.

$S \rightarrow$ Entropy.

$U \rightarrow$ Internal energy.

The energy density in the presence of magnetic field is given by

$$dU = TdS + H dM \quad (15b)$$

For gaseous systems, where P and V are pressure and volume respectively

$$dU = TdS - PdV \quad (15c)$$

The Gibbs energy for gaseous system is

$$G = U - TS + PV \quad (15d)$$

Comparing Eqs (15b) and (15c), we get $H \leftrightarrow P$ and $M \leftrightarrow V$.
Differentiating Eqn. (15a), we obtain

$$dG = dU - TdS - SdT - HdM - MdH \quad (16)$$

Use Eqn. (15b) in Eqn. (16), then

$$dG = -SdT - MdH \quad (17a)$$

In case of constant temperature, $dT = 0$

$$dG = -MdH \quad (17b)$$

Equation(17b) has to be solved for normal and superconducting state as follows:

1. Normal State

Normal state is nonmagnetic along with zero magnetic susceptibility, which makes $M = 0$

$$(dG)_N = 0 \quad (18a)$$

Hence,

$$G_N(T, H) = G_N(T, 0) \quad (18b)$$

Therefore, application of magnetic field does not alter the free energy.

2. Superconducting State

In superconducting state, $B = 0$ or $M = \frac{-H}{4\pi}$

$$(dG)_s = -MdH = \frac{H}{4\pi}dH \quad (19a)$$

$$G_s(T, H) = G_s(T, 0) + \frac{H^2}{8\pi} \quad (19b)$$

Hence, on increasing the magnetic field, the Gibbs free energy increases.

When $H > H_c$, then

$$G_N(T, H_c) = G_s(T, H_c) \quad (20)$$

From Eqs (19a–b) and (20),

$$G_N(T, 0) - G_s(T, 0) = \frac{H_c^2}{8\pi} \quad (21)$$

$\frac{H_c^2}{8\pi}$ gives stabilization energy density of superconductor and its value may be 10^4 ergs/cm³

The entropy can be given by $S = -\left(\frac{\partial G}{\partial T}\right)_H$

$$\text{Hence from Eqn. (21),} \quad S_N = S_s - \frac{1}{8\pi} \left(\frac{dH_c^2}{dT} \right) \quad (22)$$

Where $S_N \rightarrow$ Entropy in normal state

$S_s \rightarrow$ Entropy in superconducting state

$\left(\frac{dH_c^2}{dT}\right)$ is always negative, hence entropy in normal state is more than the superconducting state.

This signifies that, superconducting state is more ordered than the normal state. Difference in heat capacity could be given by the following equation

$$C_S - C_N = \frac{Td}{dT} (S_S - S_N) = \frac{TH_c d^2 H_c}{4\pi dT^2} + \frac{T}{4\pi} \left(\frac{dH_c}{dT} \right)^2 \quad (23)$$

For $T = T_c$ and $H_c = 0$

$$C_S - C_N = \frac{T_c}{\pi} \left(\frac{dH_c}{dT} \right)^2 \quad (24)$$

Equation (24) is known as Rutgers Formula. The difference in heat capacity depends on critical temperature.

12.8 BCS Theory

Many theories were proposed to explain the phenomena of superconductivity. London and London, Ginzburg also proposed theory to put forward their postulates for superconductivity. But, the theory given by Bardeen, Cooper, and Schrieffer (BCS) is the most successful theory to explain superconductivity. Although this theory could explain the properties of low-critical-temperature superconductors, it could not explain the properties of high-temperature superconductors. The theory by Bardeen–Cooper and Schrieffer could be explained as follows:

12.8.1 Interaction of Electron and Phonon

As discussed in Section 12.5, it is clear that the critical temperature and Debye temperature are related to each other. This idea was first given by Frohlich in 1950. Hence, the electrons cannot be treated as independent entities. They are supposed to interact with the lattice via quanta of lattice vibrations or phonons. When the current carrying electrons interact with the phonons, of lattice, then it gives rise to resistance in the conductors. When electron moves through the lattice, then there is interaction between electron and ions in the vicinity of electrons. The lattice gets distorted as shown in Figure 12.10. This distortion leads to lattice vibrations, and hence energy is quantized in the form of phonon.

Due to elastic behavior of lattice, the momentum is imparted to the ions. The positive charge density gets increased in that region. Furthermore, this region of positive density propagates as waves carry momentum through the lattice. Momentum transfer takes place between phonon and electron. Whenever the momentum gets transferred from one electron to another via phonon, then it is said to be electron–phonon–electron interaction. The mathematical demonstration is given in Figure 12.11.

In electron having wave vector \vec{k} interacts with the lattice producing virtual photon of momentum $m\vec{v}$. Then, it is observed by another electron of wave vector k' . As shown in Figure 12.11, the first electron possesses momentum of $\vec{k} - m\vec{v}$ and second electron exhibits momentum of $k' + m\vec{v}$, keeping one thing in consideration that the process is virtual; hence, no energy conservation is required. The two electrons possessing wave vector \vec{k} and k' , respectively, exchange their momentum via interaction involving phonon as intermediary. Moreover, the force of repulsion between two negative charged electrons have been suppressed by the positive interaction via phonons. The pair of these two electrons is called Cooper's pair.

Therefore, lattice vibrations play imperative role in superconductivity. Hence, the materials that have large amplitude of lattice vibrations tend to be good superconductors although they may not be good conductors at room temperatures. Therefore, some metals such as copper and silver are not good superconductors because the amplitude of lattice vibrations is small for them. In contrast to them, lead, tin, mercury, etc, have larger amplitude of vibrations, hence having good superconductivity.

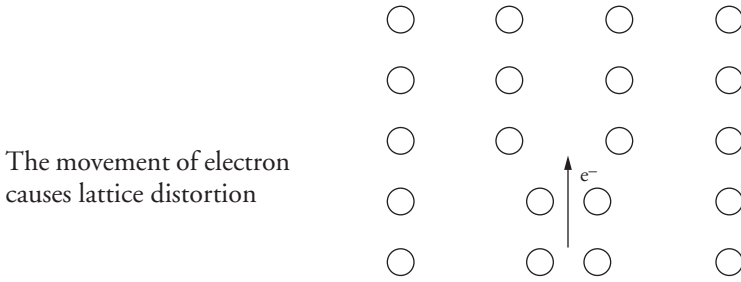


Figure 12.10 Motion of electron through lattice causes electrostatic interaction.

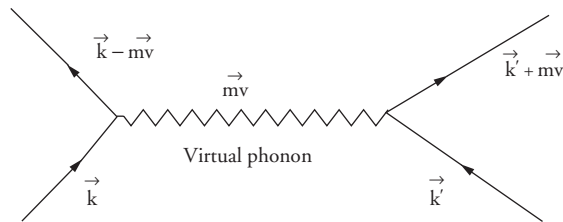


Figure 12.11 Interaction of electron and phonon.

Cooper pair is formed when two electrons overcome Coulomb's repulsive force via interaction of phonon. Energy gap E_g corresponds to binding energy of Cooper pair and is of the order of 10^{-3} eV. Free electrons have more energy than the binding energy of Cooper pair. This binding energy corresponds to temperature of 10 K. Hence, superconductivity is regarded as low-temperature phenomena. Cooper pairs can be treated as a single quantum state despite the fact that these electrons normally repel each other due to electrostatic interaction. When the temperature falls below transition temperature, these Cooper pairs condensate. This can be interpreted as a single macroscopic quantum state that flows without resistance. These pairs of electrons exhibit coupled motion up to certain distance, which is called coherence length. In other words, coherence length is the distance up to which the pairs behave as a single entity.

The electrons in Cooper pair are loosely bound [$E_g = 10^{-3}$ eV]. Hence, they keep on changing partners. The Cooper electrons behave as bosons as they have opposite spins leading to total spin of zero. Cooper pairs obey Bose–Einstein statistics. The current in superconductor is attributed to single large system of Cooper pairs. To break this current, the correlation of Cooper pair must be broken, which requires large amount of energy. Hence, the current persists if the system is undisturbed.

12.8.2 BCS Ground State

For normal conductors, there is no interaction between electrons (Fermi gas) unlike superconductors. For Fermi gas, all the states above Fermi level are vacant and below it, all the states are filled. According to BCS theory, there exists an energy gap E_g between the ground state and very first excited state. This energy gap is the binding energy of Cooper pairs, which is dependent on temperature.

At $T = T_c$, the pairing vanishes; and at $T = 0$ K, the pairing is complete, leading to maximum band-gap (Fig. 12.12).

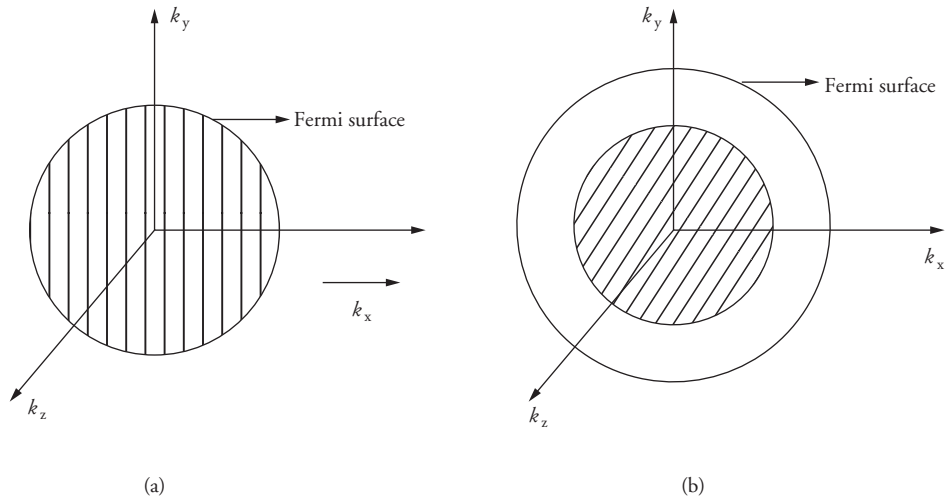


Figure 12.12 (a) Free electron gas (b) BCS ground state.

John Bardeen, Leon Cooper, and Robert Schrieffer studied superconductivity in metals and alloys in 1957. They gave a new theory known as BCS theory and won Nobel Prize for it in 1972. The BCS theory has been confirmed for more than 60 years in most superconductors. Schrieffer was the PhD student of Bardeen. Leon Cooper joined his group in 1955 where they worked on the underlying principle of superconductivity. Cooper significantly explained the pairing of electrons at low temperatures, that is, electrons move in pairs known as Cooper pairs. In 1957, their work was published as “theory of superconductivity” in *Physical Review*, which is highly cited till date. The work describes the collective wavefunction of Cooper pairs and its behavior. However, this theory fails to explain certain phenomena in new superconductors. Hence, scientists are working on it to give its explanation.



**BARDEEN, COOPER AND SCHRIEFFER
(LEFT TO RIGHT)**

12.9 Semiconductos

Electronics deals with the flow of current through semiconductors, vacuum, inert gases, or conductors. Earlier, vacuum tubes were used as the electronic devices, for example, diode, triode, pentode, etc. Later on, the vacuum tubes were replaced by semiconductors as semiconductors have small size and require low voltage for their operation. Moreover, semiconductors do not produce humming voice and no heating is required to turn on the circuit. Solids can be classified into the following categories depending on energy bands and conductivity.

1. Metals

These have low values of resistivity of the order of 10^{-8} ohm-m. For example, Ag, Cu, W, Hg, Al, etc. In terms of band gap, Figure 12.13(a) demonstrates the band gap for metals. For metals or conductors,

the valence and conduction band overlaps. Hence, there is no forbidden energy gap. The electrons in the valence bands require very less energy to move to the conduction band.

2. Insulators

Insulators have very high value of resistivity of the order of 10^8 – 10^{17} ohm-m, for example, wood, and glass. The valence band is completely filled with electron, whereas conduction band is empty. The band gap between valence and conduction band is ≈ 6 eV. The electrons require large amount of energy to jump to the conduction band (Figure. 12.13(b)).

3. Semiconductors

The resistivity of semiconductor lies in between that of metals and insulators, that is, 10^0 – 10^5 ohm.

The forbidden energy gap between conduction and valence band is of the order of 1 eV (Figure. 12.13(c)). For Si, the energy gap is 1.2 eV; and for Ge, it is 0.72 eV. At 0 K, the semiconductor behaves as insulator because the electrons in valence band do not have enough energy to jump to the conduction band. But at room temperature, some electrons may jump to the conduction band. Therefore, semiconductors may conduct at room temperature.

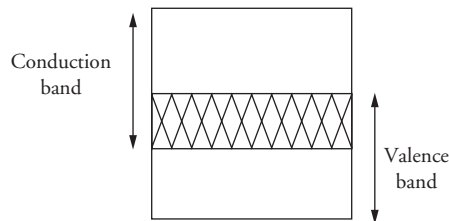


Figure 12.13(a) Band gap for metals.

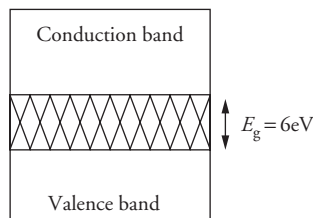


Figure 12.13(b) Band gap for insulator.

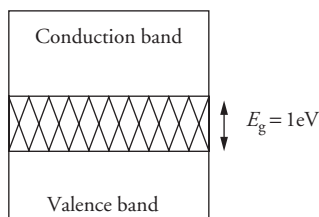


Figure 12.13(c) Band gap for semiconductor.

12.10 Types of Semiconductors

There are two types of semiconductors: intrinsic semiconductors and extrinsic semiconductors as discussed below.

12.10.1 Intrinsic Semiconductors

These are pure semiconductors that have thermally generated current carriers. Germanium and silicon are intrinsic semiconductors. Each atom of silicon or germanium has four valence electron, and each atom shares its electron via covalent bond with the neighboring atom Figure. 12.14(a).

At 0 K, no free electron is available as all the covalent bonds are complete. Hence at 0 K, the semiconductor behaves as insulators. At room temperature, some covalent bands get broken due to thermal energy. The electron gets free and leaves the bond, leaving a hole behind as shown in Figure 12.14(b). The hole is equivalent to positive electron (+e). Some electrons from neighboring bonds will move to fill the vacancy created by electron, and hence another hole in the neighborhood is created. Hence, the conduction mechanisms for intrinsic semiconductor constitute movement of electrons and holes. The intrinsic concentration is given by the following equation:

$$n_c = n_n = n_i \quad (25)$$

At room temperature, the electrons gain thermal energy, and hence jump from the valence band to the conduction band. Hence, holes are created in the valence band as demonstrated in Figure 12.15. Furthermore, the nearby electrons jump to fill that empty holes. Therefore, the conduction phenomenon is basically due to thermal excitations.

12.10.2 Extrinsic Semiconductors

In order to increase the conductivity of pure intrinsic semiconductors, some suitable dopants are added to it. The process of adding impurities to intrinsic semiconductor is called doping. The impurity atoms that are added to intrinsic semiconductors are called dopants. The semiconductor having dopants to increase the conductivity is called extrinsic semiconductor. Sometimes, the impurity atom is diffused into molten material. The impurity atom can also be bombarded with the intrinsic semiconductor and the doping concentration is $1:10^6$. Two types of impurities can be added in the intrinsic semiconductor as described below:

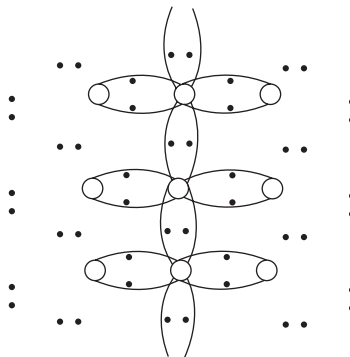


Figure 12.14(a) Intrinsic semiconductor.

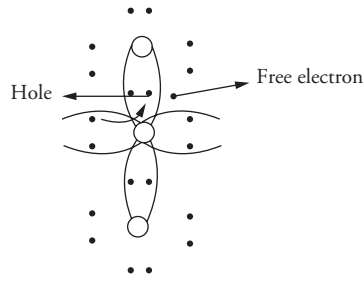


Figure 12.14(b) Conduction in intrinsic semiconductors.

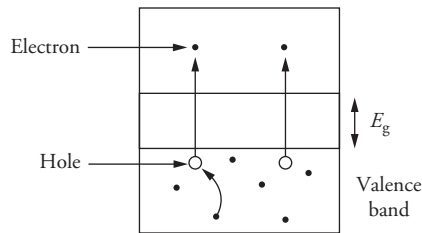


Figure 12.15 Band gap diagram for intrinsic semiconductors.

1. P-type Semiconductors

When trivalent impurity is added to the pure intrinsic semiconductor, we obtain p-type extrinsic semiconductors. In Figure 12.16(a), trivalent indium atom is added to the silicon atom, then it replaces silicon atom from its lattice. The indium atom has three atoms in its outermost shell. Hence, it can form bonds with three neighboring atom, and the fourth bond has deficiency of one electron (known as hole). Neighboring electrons jump to that void, and a hole is created at its own place. Such type of semiconductor having excess positive charge (holes) is known as p-type semiconductor. For p-type semiconductors, holes are majority carriers and electrons are minority carriers. Figure 12.16(b) shows the bandgap of p-type semiconductor.

For p-type semiconductors, the energy level corresponding to holes lie near to the valence band, and this energy level is known as acceptor level. At room temperature, the electrons that are thermally generated jump easily to acceptor level, and hence holes are created in valence band. For p-type semiconductors, holes act as current carriers.

2. N-type Semiconductors

When pentavalent impurity is added to the intrinsic semiconductor, then it is n-type extrinsic semiconductor. When pentavalent impurity atom (As) is added to the silicon crystal, then it replaces the silicon atom and settles down at its position. Arsenic atom shares its four electrons with silicon lattice, and one extra electron is unaccommodated and loosely bound to parent nucleus. It moves freely through the lattice as demonstrated in Figure 12.17(a). Hence, the crystals have large number of free electrons. Therefore for n-type semiconductor, electrons are majority charge carriers. The fifth extra electron occupies a discrete level known as donor level which lies near to conduction band.

For Si, donor energy level $E_d = 0.05$ eV (Figure 12.17(b)) and for Ge, $E_d = 0.01$ eV. At room temperature, the electrons from donor level can jump to conduction band.

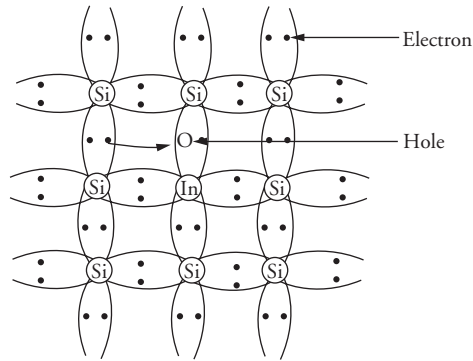


Figure 12.16(a) p-type semiconductor.

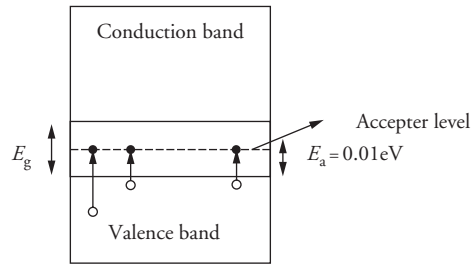


Figure 12.16(b) Energy band diagram for p-type semiconductor. (E_a -acceptor level energy)

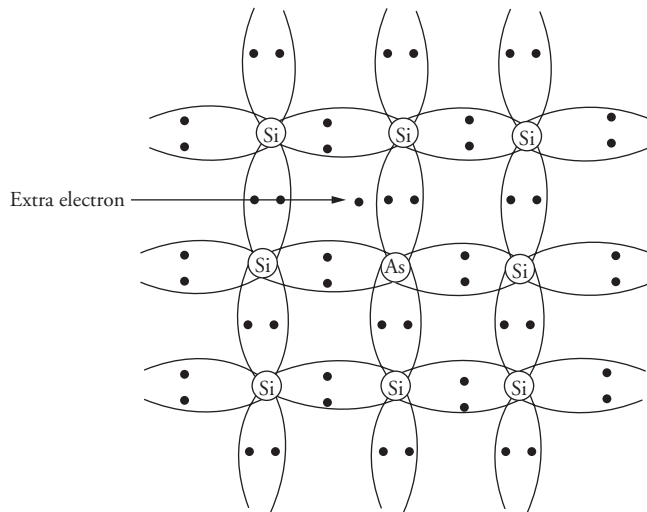


Figure 12.17(a) n-type extrinsic semiconductor.

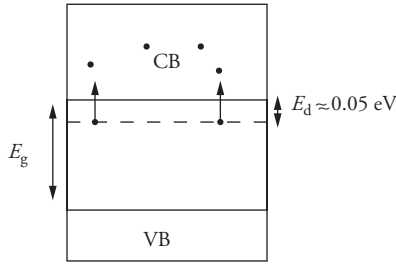


Figure 12.17(b) Energy band diagram for p-type (E_d -donor-level energy).

12.11 p-n Junction

When a Si or Ge material is doped in such a way that one part is doped with trivalent impurity and other part is doped with pentavalent impurity, then it forms p-n junction. In the p-region, holes are majority charge carriers where as in n-region, electrons are majority carriers. Hence, there is concentration gradient in the two sides. Therefore, the holes will diffuse toward n-region and electrons will diffuse toward p-region. The electron and holes will combine at the junction. Furthermore, there will be no mobile charge carriers around the junction region; hence, this region is known as depletion layer or depletion region. This is also known as space-charge region and is about 10^{-6} m . The p-n junction diode is represented by $\rightarrow\text{||}$ where arrowhead represents p-type semiconductor and bar is negative n-type semiconductor. The depletion layer consists of negative as well positive immobile ions. Hence, the ions on p and n regions are separated by distance that is equal to the depletion layer.

Further diffusion of electrons and holes is stopped as a potential difference gets set up across the junction. This potential difference is referred to as potential barrier (V_B). For Si, $V_B = 0.7\text{V}$ and Ge, $V_B = 0.4\text{V}$. Due to this potential barrier, an electric field is set up across the junction, that is,

$$E = \frac{V_B}{d} \tag{26}$$

The direction of electric field is from positive to negative (in Figure 12.18, from right to left across the junction). Hence, this gives rise to drift current across the junction whose direction is opposite to the flow of diffusion current. At the stage of equilibrium, drift current is equal to diffusion current. This leads to the formation of p-n junction diode.

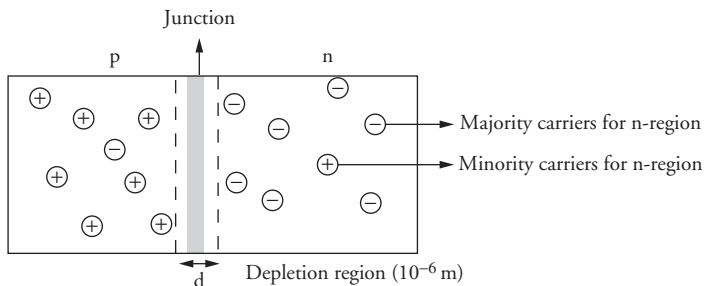


Figure 12.18 p-n junction.

12.12 Biasing of p–n Junction

When dc voltage is applied across the p–n junction, then the barrier voltage gets changed and p–n junction is said to be biased. Depending upon which terminal of battery is connected to the p-side or n-side, following are the two types of biasing.

1. Forward Biasing

When the positive terminal of battery is connected to the p-side and negative terminal is connected to the n-side, then the p–n junction is said to be forward biased as shown in Figure 12.19(a). If V is the applied voltage, then the net voltage is given by $V - V_B$ where V_B is the barrier potential. The effective height of barrier potential increases. Hence, small resistance is offered at the junction to the flow of majority carriers and the depletion region decreases. When the external voltage is sufficient to overcome the barrier potential, then the electrons and holes recombine with each other. Whenever an electron recombines with hole, then an electron from negative terminal of battery enters the n-region subsequently drifting toward the junction region. At the same time, a covalent bond breaks near the junction region producing an electron and hole. The hole drifts toward p–n junction and the electron enters positive terminal of the battery. The current is not due to minority carriers in this case.

2. Reverse Biasing

When the negative of battery is connected to the p-region and positive terminal of battery is connected to n-region, then the p–n junction is said to be reverse biased as shown in Figure 12.19(b). The depletion region in this case increases because the electrons get attracted to positive terminal and holes are attracted to negative terminal. The total net potential in this case is $V + V_B$. Hence, the resistance to the flow of majority carriers increases in this case. Therefore, the flow of current almost stops, but minority carriers, that is, holes in n-region and electrons in p-region move across the junction. Hence, small current of order of microamperes flow across the junction due to minority carriers. The flow of minority carriers depends on the temperature and is independent of the external applied voltage. This current is also known as the reverse saturation current. But there is a breakdown voltage at which the current increases abruptly. As the breakdown voltage distorts the crystal structure, this condition is not suitable for many practical applications.

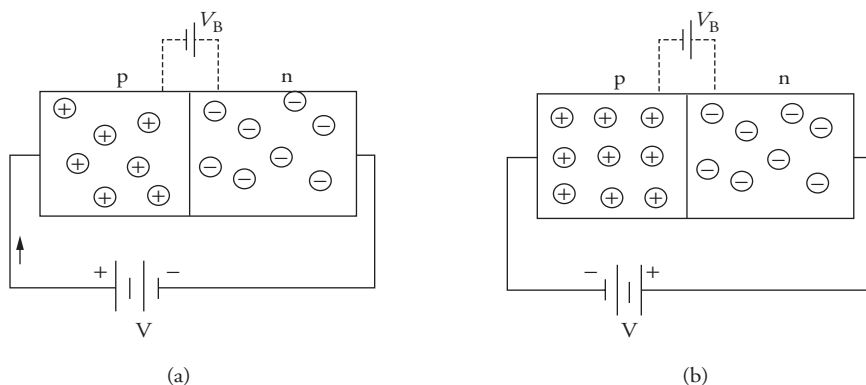


Figure 12.19 (a) Forward biasing and (b) reverse biasing of p–n junction diode.

12.13 Junction Diode as a Rectifier

The electric power is generated, transmitted, and then distributed in the form of alternating current. The alternating current (A.C.)/voltage can be easily transmitted with low losses. Some of the devices require direct current (D.C.) for their operation. This implies that A.C. current or voltage needs to be rectified in the form of direct current or voltage. Any electrical device that offers high resistance to current in one-direction and then low resistance in the opposite direction is called rectifier. p–n junction diode is used as a rectifier because it offers high resistance when it is reverse biased and low resistance when it is forward biased.

The rectifiers usually have power dissipation in the range of 0.1–10 W and breakdown voltage of 50–250 V. Some of high power rectifies have switching time of 500 ns. Two main rectifiers are given below:

12.13.1 Half-Wave Rectifier

The principle of half-wave rectifier (HWR) states that the current will flow through p–n junction diode, if it is forward biased and very small or negligible current flows through it when it is reversed biased.

Working

The circuit of HWR is shown in Figure 12.20(a). Ac input is given and transformer is there at input. The transformer is a device that can step up or down the voltage. Hence, desired level of D.C. could be obtained. The A.C. supply is applied to the primary coil (P) of transformer. The secondary coil (S) is connected to the load resistance through junction diode. At load resistance, output signal is obtained. When the positive half cycle of A.C. input flows through primary coil of transformer, then induced emf is set up across the coil due to phenomena of mutual induction. The induced emf is set up in such a way that the lower end of the secondary coil becomes negative and the upper end of the secondary coil becomes positive. The upper end of the secondary coil is connected to the p-region of p–n diode. Hence, the diode gets forward biased and current starts flowing in the circuit as indicated by arrows in Figure 12.20(a). During the negative half cycle of A.C., the induced emf is set up in the secondary coil in such a way that the upper end of S-coil becomes negative and the lower end becomes positive. Hence, the diode gets reverse biased, and almost negligible output is obtained across the load resistance.

The output voltage waveform is shown in Figure 12.20(b). Only half of the input waveform is obtained; hence, the name of this rectifier is given as HWR. As the discontinuous output signal is obtained, hence efficiency of HWR is small. Moreover, the output may contain some ripples of A.C.

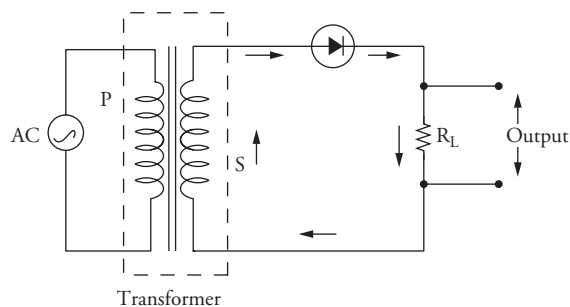


Figure 12.20(a) Half-wave rectifier.

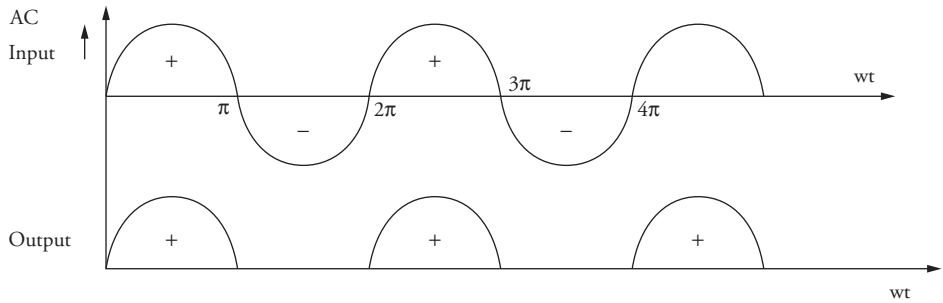


Figure 12.20(b) Waveform for input and output voltage.

12.13.2 Full-Wave Rectifier

The principle of full-wave rectifier (FWR) is the same as that of HWR, that is, when the p–n junction diode is forward biased, then current flows through the circuit. Hence, two diodes are connected, so that when one p–n diode gets forward biased then the other gets reverse biased, and vice versa.

Working:

The circuit of FWR is shown in Figure 12.21(a). The A.C. input signal is fed to the primary coil of the transformer and the p–regions are connected to the ends of the transformer. The load resistance is connected between the two diodes and central tapping of the secondary coil. During positive half-cycle of input A.C., diode D_1 gets forward biased and D_2 gets reverse biased. The direction of flow of conventional current is shown by arrows in Figure 12.21(a). During the negative half-cycle, the diode D_2 is forward biased and D_1 gets reverse biased. The output of both the cycles is obtained at load resistance R_L . The output waveform is shown in Figure 12.21(b). Both the halves of input waveform are rectified, hence the name is full-wave rectifier. The output waveform is continuous, therefore the efficiency of FWR is more than HWR. The disadvantage of FWR is pulsating output. By using filter circuits, the output can be smoothed.

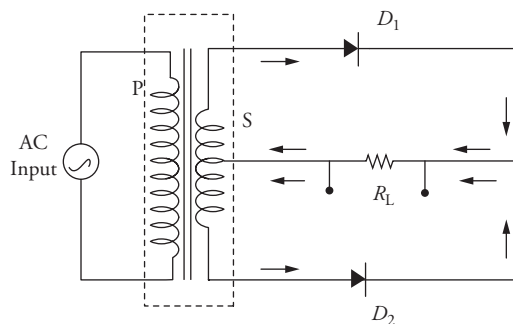


Figure 12.21(a) Full-wave rectifier.

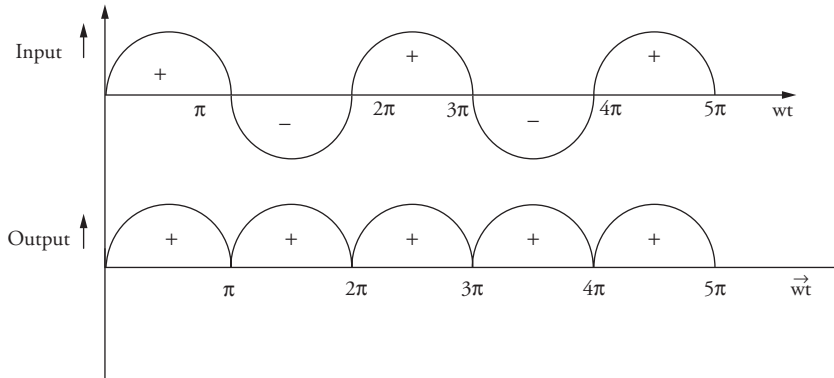


Figure 12.21(b) Output waveform of FWR.

12.14 Different Types of p–n Diodes

The ideal diode is the one that offers infinite resistance during reverse biasing and zero resistance during forward biasing. In other words, ideal p–n diode can be regarded as automatic switch. But for practical purposes, it is hard to obtain the ideal diode. Some common diodes that do not follow the ideal characteristics are described as below. But they have a wide range of practical applications.

12.14.1 Zener Diode

Zener diode is a specially designed p–n junction diode with sharp breakdown voltage. Its symbol is $\rightarrow|$

When the current flows for reverse breakdown, then it should be in safe limit. In other words, we can say that the diode should not be overheated as overheating may lead to permanent damage. The breakdown voltage of zener diode is made sharp by properly doping the p and n regions of diode. The current voltage characteristics for zener diode are shown in Figure 12.22(a) where V_z is zener voltage that is dependent upon the doping concentration. V_z is high, if the diode is lightly doped or vice versa. This could be attributed to the fact that the depletion layer for heavily doped p–n diode is thin. Zener diode is always reverse biased and when it is forward biased, it behaves like conventional p–n junction diode. For voltage stabilization, zener diode is the most commonly used device.

From Figure 12.22(b), it is clear that resistance is connected in series with input voltage. The load resistance (R_L) and zener diode are connected in parallel. Input voltage (V_{input}) is to be regulated by connecting zener diode in reverse biasing. When the input voltage increases or decreases, the resistance of zener diode decreases or increases, respectively. But the output voltage always remains constant.

When reverse voltage is increased beyond the breakdown voltage V_z , large I_z flows through zener diode. The output obtained across R_L is constant. Hence, V_{output} is constant.

Hence, voltage drop across R .

$$\begin{aligned} V &= V_{\text{input}} - V_z \\ IR &= V_{\text{input}} - V_z \end{aligned} \quad (27a)$$

and

$$(I_z + I_R)R = V_{\text{input}} - V_z$$

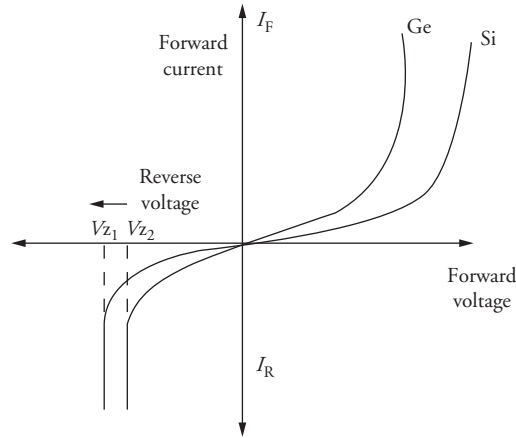


Figure 12.22(a) Characteristics of zener diode.

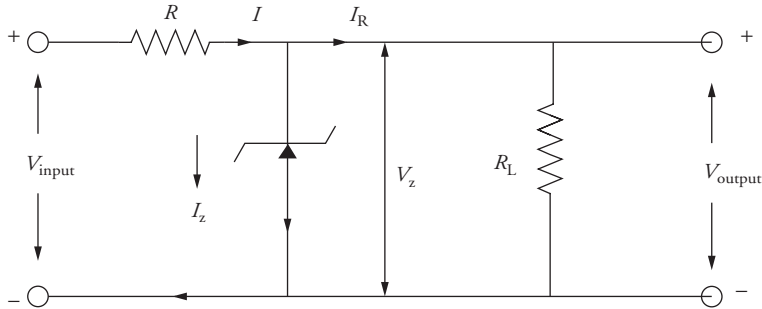


Figure 12.22(b) Zener diode as voltage regulator.

$$R = \frac{V_{\text{input}} - V_z}{I_z + I_R}$$

As $V_{\text{output}} = V_z$ and output is maintained constant,

$$R = \frac{V_{\text{input}} - V_{\text{output}}}{I_z + I_R} \tag{27b}$$

From Eqn. (27b) gives drop resistance for zener diode.

12.14.2 Light-Emitting Diode(LED)

It is a p–n junction diode in which current flows in forward direction and visible light is emitted. In the forward biasing of p–n junction diode, the potential barrier is lowered. During forward biasing, the flow of current is due to majority carriers. The majority carriers recombine at the depletion region. When electron falls into hole, then energy is radiated in the form of visible radiations. The photons emitted are given by energy $hf = E_g$. Hence,

$$\lambda = \frac{hc}{E_g} \tag{28}$$

For GaAsP, the band gap E_g is 1.0 eV, which corresponds to wavelength of 6500Å. Hence, by choosing different materials, LEDs are produced which emit different colors. The LEDs are used in digital watches, calculators, burglar alarms, and millimeters. LEDs have long life, and they do not require any warm-up time. They consume very less power and can be switched OFF and ON in ≈ 1 sec.

12.15 Transistors

A transistor is analogous to vacuum triode and has three terminals. J. Bardeen and W. Brattain developed transistor in Bell laboratories in 1947. Transistors have several advantages over the vacuum diodes as they have no filament, are small in size, and have long operating life. Actually, the word transistor compiles of two words “transfer resistor.” Transistors consists of two p–n junctions, that is, either p semiconductor is sandwiched in two n-type regions or n-semiconductor is sandwiched within two p-type regions (Figure.12. 23(a)). There are two types of transistors: (i) p–n–p and (ii) n–p–n transistors. The symbolic representation of both the transistors is given in Figure 12.24(a)–(b).

The transistor has three important parts:

- (i) **Emitter:** This part is heavily doped, and it supplies charge carriers. It is always forward biased w.r.t. base; hence, it supplies majority carriers.
- (ii) **Collector:** This part is moderately doped, and it collects the charge carriers. It is always reverse biased w.r.t. base.
- (iii) **Base:** It is in the center of collector and emitter region. It is lightly doped so that most of majority carriers should pass through it.

The width of three parts varies in order of collector > emitter > base. Thicker collector helps in dissipating higher energy.

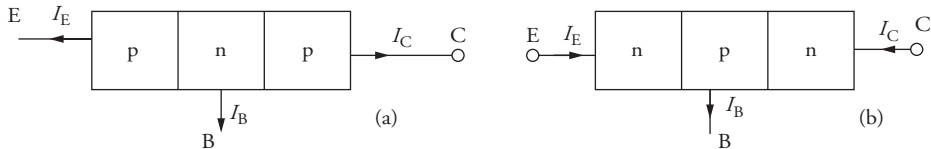


Figure 12.23 (a) p–n–p transistor and (b) n–p–n transistor.

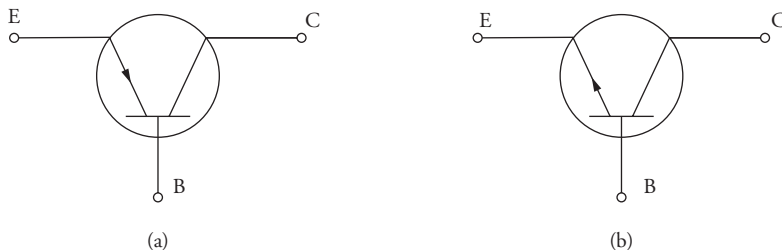


Figure 12.24 Symbolic representation of (a) p–n–p and (b) n–p–n (Direction of arrow represents direction of current).

John Bardeen was an eminent and renowned American physicist, who won the Nobel Prize twice, and he is the only person in history to receive two prizes in the same domain. John Bardeen was born in Wisconsin in 1908. He acquired an MS degree in electrical engineering from University of Wisconsin in 1929. He obtained PhD in 1936 from Princeton University. Bardeen revolutionized the fields of electronics (by inventing transistors) and magnetic resonance imaging (by inventing superconductivity). He invented the transistor along with coworkers William B. Shockley and Walter H. Brattain. In 1956, they received the Nobel Prize for the invention of transistor. Then, he formulated the theory of superconductivity along with Leon N. Cooper and John R. Schrieffer. He received the second Nobel Prize for discovering the principle of superconductivity in 1972. He did extensive research work at the universities of Minnesota and Harvard. He also worked at the Naval Ordnance Lab in Washington, DC. In 1945, he joined the solid state physics group at Bell Labs in New Jersey. In 1951, he left Bell Labs and started teaching at University of Illinois, where he worked with Cooper and Schrieffer to formulate the BCS theory. The invention of transistors revolutionized the field of electronics and regarded as the strongest discovery in the field of electronics. Bardeen died on January 30, 1991, in Boston, Massachusetts, due to heart trouble.

12.16 Action and Working of Transistor

There are two p–n junctions in transistor. The junction between collector and base is called collector–base junction and the junction between emitter and base is called emitter–base junction. We will discuss the action of both p–n–p and n–p–n transistors.

1. n–p–n Transistor

The emitter–base junction is forward biased and collector base junction is reverse biased (Figure 12.25). The emitter–base voltage is V_{EB} and collector–base voltage is V_{CB} . The emitter junction is forward biased; hence, electrons drift toward the base region. Electrons are majority charge carriers in emitter regions. Holes in base region also drift toward the junction region. Some of electrons recombine with the holes, but as the base region is very thin, most of electrons pass through the base region, that is, only 5 percent of electrons undergo recombination and rest pass through the base region to reach collector. Hence, collector current is smaller than emitter current. Therefore, emitter current can be divided into two parts i.e.

$$I_E = I_B + I_C \quad (29)$$

where I_E is emitter current, I_B is base current, and I_C is collector current.

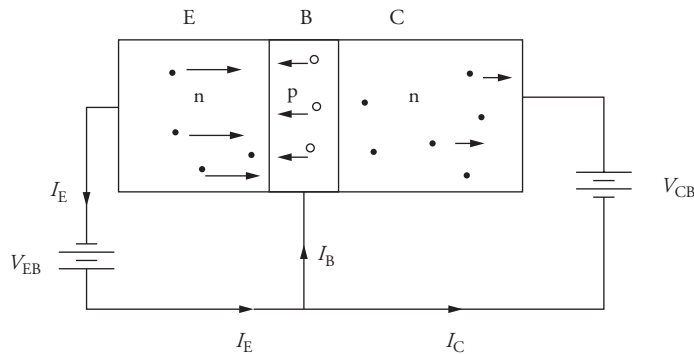


Figure 12.25 n–p–n transistor.

2. p–n–p Transistor

Similar to n–p–n transistor, the emitter base is forward biased and collector-base is reverse biased for p–n–p transistor (Figure. 12.26).

In this case, holes are the majority carriers and as the emitter junction is forward biased, the holes move toward the base region recombining with some electrons of the base region. Subsequently, the remaining holes reach the collector region and again $I_C < I_E$, and we can write down.

$$I_E = I_B + I_C$$

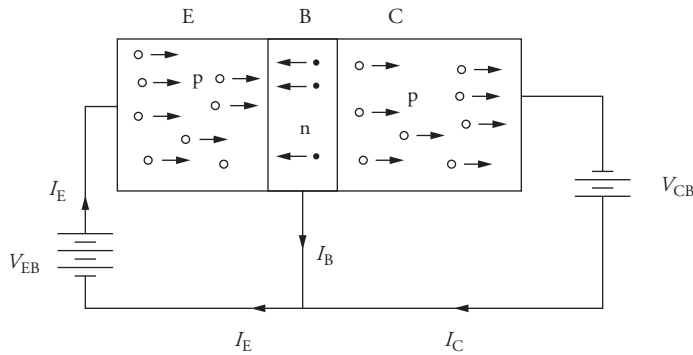
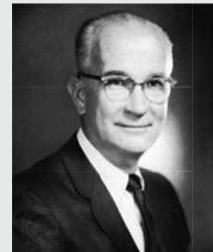


Figure 12.26 p–n–p transistor.

12.17 Characteristics of Transistors

The relation between current and voltage for p–n–p or n–p–n transistor is represented in the form of graphs. Such curves are known as characteristic curves. There are three types of characteristic curves, that is, common base (CB), common collector (CC), and common emitter (CE) characteristics. On the basis of operation of voltage, the characteristics can be of two types: static and dynamic. When transistor operates under the effect of D.C. only, it displays static characteristics, and when the transistor operates under the effect of D.C. as well as A.C. voltage, it displays the dynamic characteristics. The slopes of characteristic curve display certain parameters. The noteworthy point is that collector is always reverse biased and emitter is always forward biased.

William Shockley was born on February 13, 1910, in London. He was the son of William Hillman Shockley who was a mining engineer and Mary who was also working in mining. In 1932, William Shockley obtained his BSc degree at the California Institute of Technology. He obtained his PhD in 1936 on the energy band structure of sodium chloride. In 1936, he joined Bell Telephone Laboratories under the supervision of Dr C.J. Davisson. He became Director of the Shockley Semiconductor Laboratory of Beckman Instruments, in California. In 1946, he received the Medal for Merit, for his work with the War Department. In 1952, he also received the Morris Leibmann Memorial Prize of the Institute of Radio Engineers. He shared the Nobel Prize for Physics in 1956, jointly with his two former colleagues at the Bell Telephone Laboratories. He has obtained honorary science doctorates from the University of Pennsylvania, Rutgers University, and Gustavus Adolphus Colleges.



WILLIAM SHOCKLEY

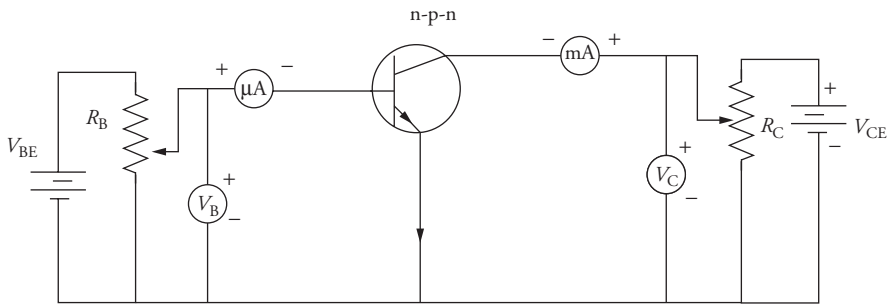


Figure 12.27 Circuit diagram for common emitter configuration.

12.17.1 CE Characteristics

Figure 12.27 demonstrates for the circuit diagram for n-p-n CE configuration. In CE configuration, emitter is common is between base and collector. Input voltage is applied across the emitter-base and output is collected at collector-base. Following are the input and output characteristics of n-p-n transistor.

1. Input Characteristics

The graph depicting the relationship curves between base current and (I_B) base-emitter voltage (V_{BE}) at constant collector emitter voltage (V_{CE}) is known as input characteristics.

The input characterizations are quite similar to the forward-biased diode characteristics. From Figure 12.28(a), it is clear that the base current varies in nonlinear manner with the base emitter voltage. Moreover, the input characteristics depend on V_{CE} . The input resistance is given by

$$R_{input} = \left. \frac{\Delta V_{BE}}{\Delta I_B} \right|_{V_{CE}} = \text{Constant} \tag{30}$$

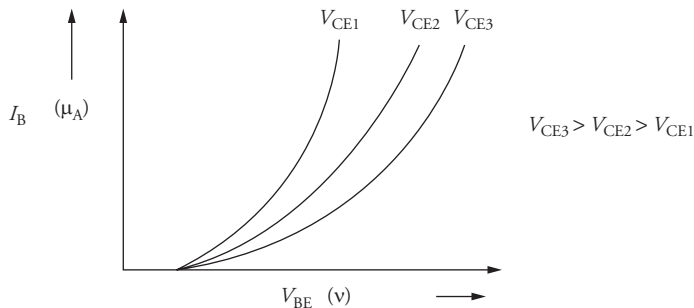


Figure 12.28(a) Input characteristics of n-p-n transistor.

2. Output Characteristics

The graphical depiction between collector current and current-emitter voltage at constant base current is called output characteristics of CE transistor. The output characteristics can further be divided in three regions: active region, cut-off region, and saturation region.

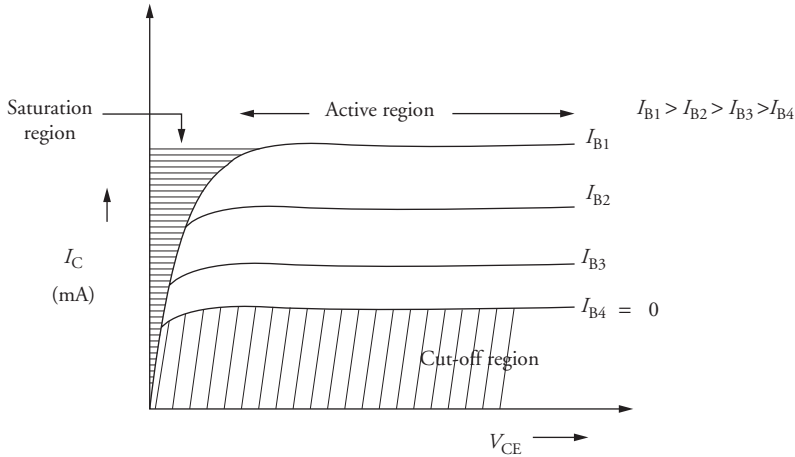


Figure 12.28(b) Output characteristics of n-p-n transistor.

(a) **Active Region**

This region lies above $I_B = 0$ and the collector current do not increase very sharply with collector emitter voltage. The emitter junction is forward biased and collector region is reverse biased. As clear from Figure 12.28(b), initially the collector current increases with the increase in collector-emitter voltage. For the purpose of amplification, the transistor is operated in active region.

(b) **Cut-Off Region**

The cut-off region lies below $I_B = 0$ as shown in Figure 12.28(b). To obtain the cut-off condition, slight reverse bias is applied to collector-emitter junction. The collector current has finite but small value.

(c) **Saturation Region**

The saturation region is shown in Figure 12.28(b). It lies in between the origin and the knees of the curve. To obtain the saturation region emitter and collector regions are forward biased. In saturation region, the collector current is independent of the base current. The saturation region lies close to zero voltage axis.

From Figure 12.28(b), it is clear that large value of base current corresponds to large collector current. Even when the base current is zero, the collector current is not zero, which could be attributed to the intrinsic conduction. The output resistance is given by

$$R_{\text{output}} = \left. \frac{\Delta V_{\text{CE}}}{\Delta I_{\text{C}}} \right|_{I_{\text{B}}} = \text{Constant} \quad (31)$$

12.17.2 CB Characteristics

For the CB characteristics, the emitter base is forward biased and collector base is reverse biased as shown in the Figure. 12.29(a). Following are the input and output characteristics for n-p-n CE transistor:

1. Input Characteristics

The graphs depicting the variation between emitter current (I_E) and base emitter voltage (V_{BE}) at constant collector base voltage are called input characteristics (Fig. 12.29(b)). The characteristics are same as that of forward biased p-n junction diode.

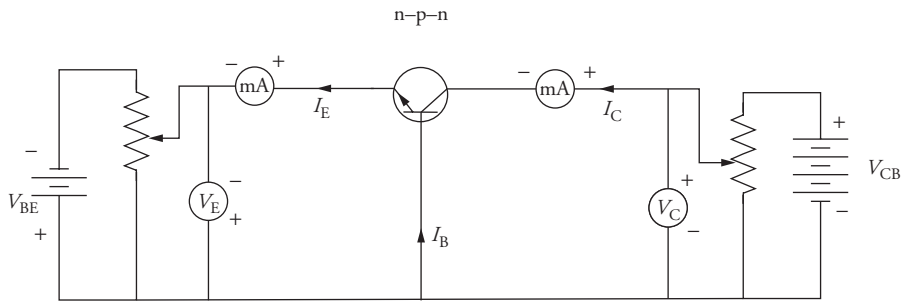


Figure 12.29(a) CB characteristics for n-p-n transistor.

Increasing V_{CB} means increasing the depletion region around collector–base junction. When the depletion region increases, then the thickness of base region decreases. Furthermore, decrease in base region thickness increases emitter current. This phenomenon is known as early effect. Hence, increase in V_{CB} reverse biasing leads to increase in emitter current.

The input resistance is given by

$$R_{\text{input}} = \left. \frac{\Delta V_{BE}}{\Delta I_E} \right|_{V_{CB}} = \text{Constant} \quad (32)$$

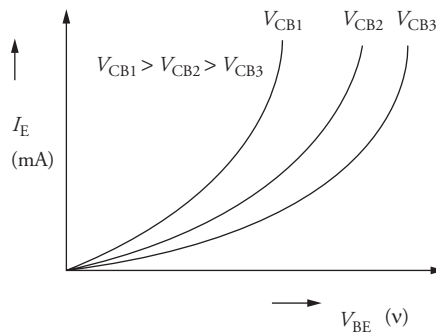


Figure 12.29(b) Input characteristics for n-p-n transistor.

2. Output Characteristics

The graphical depiction of collector current and collector base voltage at constant collector base voltage is known as output characteristics. Like CB configuration, CE output characteristics are divided into three regions as explained below (Figure 12.29(c)).

(a) Active Region

The emitter junction is forward biased and collector junction is reverse biased. The curves are almost flat. When $I_E = 0$, the transistor exhibits characteristics like p-n junction diode (base–collector region), then I_C is constituted due to minority carriers and is known as reverse saturation current (I_{CO}).

(b) Cut-Off Region

Both the collector and emitter are reverse biased for this region. The region below $I_E = 0$ constitutes cut-off region (Figure 12.29(c)).

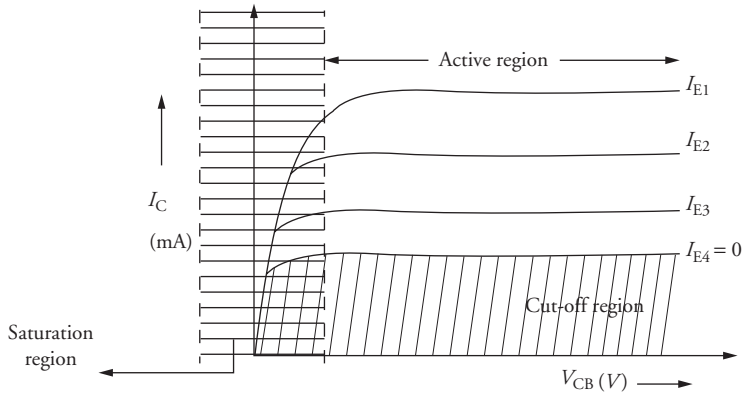


Figure 12.29(c) Output characteristics of n-p-n transistor.

(c) Saturation Region

Both the emitter and collector are forward biased. This region is situated toward the left of $V_{CB} = 0$.

The output resistance is given by

$$R_{\text{output}} = \left. \frac{\Delta V_{CB}}{\Delta I_C} \right|_{I_E} = \text{Constant} \quad (33)$$

12.18 α and β of a Transistor

The current gain of transistor can be calculated using various characteristic curves (CB and CE).

For CB configuration, $I_C \approx I_E$ as I_B is very small. The ratio of collector current to emitter current is called D.C. current gain.

$$\alpha_{\text{D.C.}} = \frac{I_C}{I_E} \quad (34)$$

The A.C. current gain is given by

$$\alpha_{\text{A.C.}} = \left. \frac{\Delta I_C}{\Delta I_E} \right|_{V_{CB}} = \text{Constant} \quad (35)$$

Hence, the ratio of change of collector current to change of emitter current at constant collector base voltage is ac current gain for CB configuration. For an ideal transistor $\alpha = 1$, but usually some current is lost in recombination. In order to decrease the base currents, appropriate doping must be done.

For CE configuration, the D.C. current gain is given by

$$\beta_{\text{D.C.}} = \frac{I_C}{I_B} \quad (36)$$

That is, the ratio of collector current to base current.

Similarly, the A.C. current gain is given by

$$\beta_{\text{A.C.}} = \left. \frac{\Delta I_C}{\Delta I_B} \right|_{V_{CE}} = \text{Constant} \quad (37)$$

We know that

$$I_E = I_B + I_C$$

For small currents,

$$\Delta I_E = \Delta I_B + \Delta I_C$$

$$\frac{\Delta I_E}{\Delta I_C} = \frac{\Delta I_B}{\Delta I_C} + 1$$

$$\frac{1}{\alpha} = \frac{1}{\beta} + 1$$

$$\beta = \frac{\alpha}{1 - \alpha} \quad (38)$$

If $\alpha \approx 1$, then β tends to infinity; hence, the current gain is higher in CE configuration. Therefore for most of practical applications, CE configuration is used.

Walter H. Brattain was born on February 10, 1902, in Amoy, China. He was the son of Ross R. Brattain and Otilie Houser. He received a BS degree from Whitman College in 1924. He was awarded the PhD degree by the University of Minnesota in 1929. He worked on the thermionic emission of tungsten. Dr Brattain got the honorary Doctor of Science degree from Portland University in 1952 and from the University of Minnesota in 1957.



W.H. BRATTAIN

12.19 Transistor as an Amplifier

Amplification is the process of strengthening a weak signal by increasing its magnitude. Transistor helps in amplifying the signals as described in the following section.

12.19.1 CB Transistor Amplifier

The circuit diagram for CB p–n–p transistor is shown in Figure 12.30. The base is common for emitter and collector. The base is grounded, emitter is forward biased (V_{EE}) and the collector is reverse biased (V_{CC}). Hence, the resistance at output is more than at the input due to reverse biasing of collector. The output is obtained at load resistance (R_L). Load resistance is connected in between collector and base.

As
$$I_E = I_B + I_C$$

I_C passes through the load resistance R_L ; hence, potential drop occurs across the load resistance given by $I_C R_L$.

Therefore,

$$V_{CB} = V_{CC} - I_C R_L \quad (39)$$

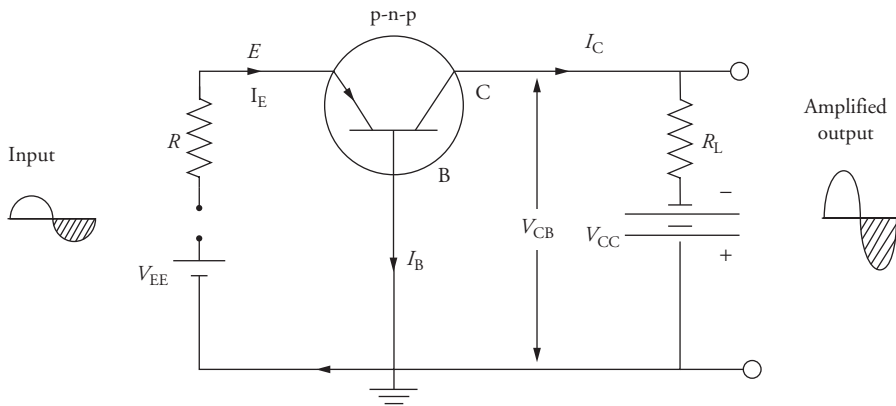


Figure 12.30 p-n-p amplifier.

Let the positive half cycle be fed to the input circuit, then emitter will become more positive and hence emitter current increases (Figure 12.30). If emitter current increases, then the collector current also increases. Therefore, $I_C R_L$ or potential drop along load resistance also increases. From Eqn. (39), the V_{CB} decreases more; hence, “-ve” terminal will become more positive and “+ve” will become more negative. Therefore, correspondingly, we obtain amplified output of A.C. wave. The input circuit has approximately $30\text{--}70\ \Omega$ of resistance and output can go up to $(500\text{--}700\ \text{k}\Omega)$. Hence, large load is produced across R_L .

The voltage gain for CB transistor is given by

$$A_v = \frac{\text{Output voltage}}{\text{Input voltage}} = \frac{I_C R_L}{I_E R} = \alpha \frac{R_L}{R} \quad (40)$$

$$A_v = \alpha \times \text{resistance gain} \quad (41)$$

A_v is very high because R_L is very high.

Similarly, Power gain = VI

$$= (\text{Voltage gain}) \times \text{Current gain}$$

$$A_v = \alpha^2 \times \text{Resistance gain} \quad (42)$$

12.19.2 CE Amplifier

The base emitter is forward biased and collector emitter is reverse biased for CE amplifier as shown in Fig. 12.31. The Emitter is common junction and grounded. As I_C flows through R_L , hence potential drop $I_C R_L$ occurs and net potential if given by

$$V_{CE} = V_{CC} - I_C R_L \quad (43)$$

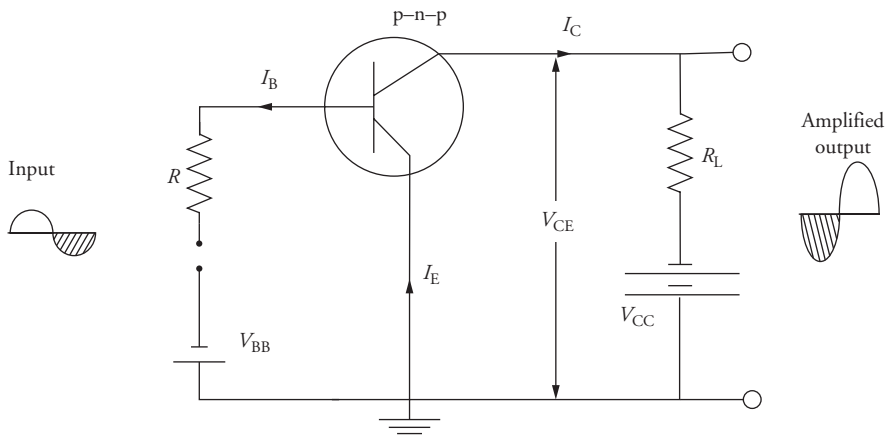


Figure 12.31 p–n–p amplifier.

When “+ve” cycle is set at the input, then V_{BB} decreases, which decreases base current I_B . Hence, I_C and I_E also decrease. Correspondingly, the potential drop also decreases and from Eqn. (43) V_{CE} also increases. Hence, negative becomes more negative and positive becomes more positive. Hence, corresponding to positive half cycle, “-ve” cycle is obtained. Hence, the output and input are out of phase with each other. Input resistance is between (1 and 5 K) and output goes up to (30–50 K).

The voltage gain is given by

$$A_v = \frac{\text{Output voltage}}{\text{Input voltage}} = \frac{I_C R_L}{I_B R}$$

$$A_v = \beta \times \text{Resistance gain} \quad (44)$$

and power gain is given by

$$\text{Power gain} = \text{Voltage gain} \times \text{Current gain}$$

$$\text{Power gain} = \beta^2 \times \text{Resistance gain} \quad (45)$$

Therefore, transistors show better gain and amplification in CE configuration because $\beta > \alpha$.

SUMMARY

This chapter gave the insight of superconductivity as a low-temperature phenomena. Meissner and Ochsenfeld demonstrated that the magnetic field times are pushed out of superconductor, when it is cooled below critical temperature in magnetic field. The superconductors are classified into type I (soft) and type II (hard) superconductors. Type I superconductors follow Meissner’s law strictly, whereas type II superconductors do not follow Meissner’s law. Entropy and thermal conductivity decreases when the temperature decreases below critical temperature. The superconducting critical temperature is different for isotopes of elements. The BCS theory could explain the properties of low critical temperature superconductors. The electrons move as Cooper pairs by overcoming Coulomb’s repulsive force via interaction of phonon. The classification of solids is also given as metals, insulators,

and semiconductors. Semiconductors, especially transistors revolutionized the field of electronics. The semiconductors are classified as intrinsic and extrinsic semiconductors. The extrinsic semiconductors are formed by doping the intrinsic semiconductor either with trivalent or pentavalent atoms. When a Si or Ge material is doped in such a way that one part is doped with trivalent impurity and other part is doped with pentavalent impurity, then it forms p–n junction. The diode gets biased when dc voltage is applied across p–n junction. The diodes can be used as half-wave/full-wave rectifies to rectify ac signal to dc signal. The transistors, which are analogous to vacuum triodes are used as amplifiers. The characteristics of transistors decide its working regime.

SOLVED PROBLEMS

Q. 1: The critical temperature T_c for mercury with isotopic mass 199.5 is 4.185 K. Obtain the critical temperature, when the isotopic mass changes to 203 K.

Ans: According to isotope effect,

$$M^{1/2}T_c = \text{Constant}$$

$$T_c = \frac{\text{Constant}}{M^{1/2}}$$

Hence,

$$T_{c_1} = \frac{\text{Constant}}{M_1^{1/2}} \quad (\text{a})$$

and

$$T_{c_2} = \frac{\text{Constant}}{M_2^{1/2}} \quad (\text{b})$$

Dividing (a) and (b),

$$\frac{T_{c_1}}{T_{c_2}} = \sqrt{\frac{M_2}{M_1}}$$

Here $T_{c_1} = 4.185\text{K}$ and $M_1 = 199.5$; $M_2 = 203$,

$$T_{c_2} = T_{c_1} \sqrt{\frac{M_1}{M_2}}$$

$$T_{c_2} = 4.185 \times \sqrt{\frac{199.5}{203}} = 4.1487$$

Hence $T_{c_2} = 4.149\text{K}$

Q 2: For a superconducting alloy, the critical fields at 4 K and 6 K are 5.234 and 3.942 MAm⁻¹. Obtain the critical field and critical temperature at 0 K.

Ans: According to critical field,

$$H_c = H_o \left(1 - \left(\frac{T}{T_c} \right)^2 \right)$$

For $T = 4$ K and $H_c = 5.234$ MAm⁻¹,

$$5.234 = H_o \left(1 - \left(\frac{4}{T_c} \right)^2 \right) \quad (a)$$

For $T = 6$ K and $H_c = 3.942$ MAm⁻¹,

$$3.942 = H_o \left(1 - \left(\frac{6}{T_c} \right)^2 \right) \quad (b)$$

Dividing (a) and (b),

$$\frac{5.234}{3.942} = \frac{T_c^2 - 16}{T_c^2 - 36}$$

$$1.3277 = \frac{T_c^2 - 16}{T_c^2 - 36}$$

$$T_c^2 - 16 = 1.3277 T_c^2 - 47.799$$

$$0.3277 T_c^2 = 31.799$$

$$T_c^2 = 97.0369$$

$$T_c = 9.8507 \text{ K}$$

The field at 0 K can be obtained by using the following equation:

$$H_c(4 \text{ K}) = H_o \left(1 - \left(\frac{4}{9.8507} \right)^2 \right)$$

$$5.234 = H_o (1 - 0.16488)$$

$$5.234 = H_o (0.83512)$$

$$H_o = 6.267 \text{ MAm}^{-1}$$

Q 3: The rating of a zener diode is given to be 360 mW at $V_z = 12$ V . Obtain the maximum current, which could be passed through it without damaging it.

Ans:

$$\text{Power} = \text{Voltage} \times \text{Current}$$

$$\text{Current} = \frac{\text{Power}}{\text{Voltage}}$$

Here, power = 360 mW and voltage = 12 V

$$\begin{aligned}\text{Current}(I_z) &= \frac{360 \times 10^{-3}}{12} \\ &= 30 \times 10^{-3} \text{ A} \\ &= 30 \text{ mA}\end{aligned}$$

Q.4: A 10 V Zener diode is used to regulate the voltage across a load resistor. The load current varies b/w 20 and 75 mA, whereas input voltage varies b/w 20 and 25 V. The minimum zener current is 10 mA. Obtain the series resistance R_s .

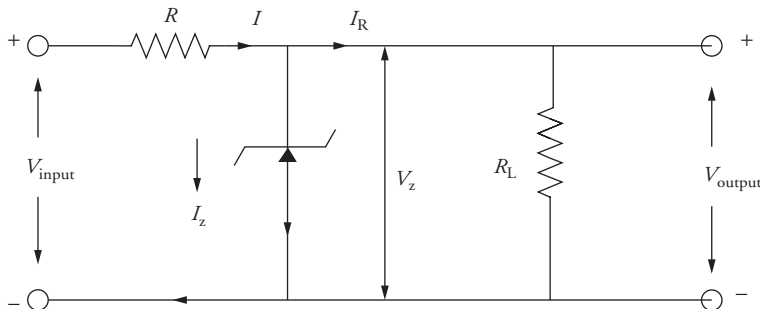
Ans:

$$V_{\text{input}} = 20 \text{ V} \quad V_z = 10 \text{ V}$$

$$I_R = 10 \text{ mA} \quad \text{and} \quad I_L = 75 \text{ mA}$$

$$\begin{aligned}R &= \frac{V_{\text{input}} - V_z}{I_z + I_R} \\ R &= \frac{20 - 10}{10 + 75} = \frac{10}{85 \text{ mA}} \\ R &= \frac{10 \times 1000}{85} \Omega \\ R &= 117.647 \\ R &\approx 117 \Omega\end{aligned}$$

Q.5: In the circuit given below, $R = 40 \Omega$ and $I_R = 15 \text{ mA}$. The voltage rating of the 1 W diode is 10 V. Give the range of voltage regulation for the Zener diode.



Ans: $R = 40 \Omega$ and $I_R = 15 \text{ mA}$

$$V_z = 10 \text{ V} \quad \text{and} \quad \text{power} = 1 \text{ W}$$

$$\text{Current } I_z = \frac{\text{power}}{\text{voltage}} = \frac{1}{10} = 0.1 \text{ A}$$

$$= 100 \text{ mA}$$

$$\begin{aligned} \text{Maximum current} &= I_{\max} = I_R + I_z \\ &= 15 + 100 = 115 \text{ mA} \end{aligned}$$

$$\begin{aligned} \text{Minimum current} &= I_{\min} = I_R + (I_z)_{\min} \\ &= 15 \text{ mA} \end{aligned} \quad (I_z)_{\min} = 0$$

Hence, maximum voltage V_s is

$$\begin{aligned} &= I_{\max} \times R + V_z \\ &= 115 \times 40 + 10 \\ &= 115 \times 10^{-3} \times 40 + 110 \\ &= 4.6 + 110 = 114.6 \text{ V} \end{aligned}$$

Minimum voltage is

$$\begin{aligned} &= I_{\min} \times R + V_z \\ &= 15 \times 10^{-3} \times 40 + 110 \\ &= 0.6 + 110 \\ &= 110.6 \text{ V} \end{aligned}$$

Hence, the range of the voltage V is $110.6 \text{ V} - 114.6 \text{ V}$.

Q.6: A light-emitting diode (LED) has a wavelength of 800 nm. Obtain the energy gap.

Ans:

$$E_g = \frac{hc}{\lambda}$$

$$\lambda = 800 \text{ nm} = 8 \times 10^{-7} \text{ m}$$

$$\begin{aligned} E_g &= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{8 \times 10^{-7}} \\ &= 2.4 \times 10^{-34} \times 10^{15} \\ &= 2.4 \times 10^{-19} \text{ J} \end{aligned}$$

In eV,

$$\begin{aligned} E_g &= \frac{2.4 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 1.5 \text{ eV} \end{aligned}$$

Q.7: When the input characteristics of an $n-p-n$ transistor in CE configuration, obtain the resistance when $\Delta I_B = 3.5 \text{ mA}$ and $\Delta V_{EB} = 1.20 \text{ V}$.

Ans: The input resistance

$$R_{\text{input}} = \frac{\Delta V_{BE}}{\Delta I_B}$$

$$R_{\text{input}} = \frac{1.20}{3.5 \text{ mA}}$$

$$= 342.85 \Omega$$

Q.8: For a common-base configuration, $\alpha = 0.95$. For a base current of $30 \mu\text{A}$, obtain the emitter and collector currents.

Ans: We know that

Also

$$I_E = I_B + I_C$$

$$\alpha = \frac{I_C}{I_E} = 0.95$$

$$I_C = \alpha I_E = 0.95 I_E$$

$$I_E = I_B + 0.95 I_E$$

$$I_E = \frac{I_B}{(1 - 0.95)} = \frac{30 \mu\text{A}}{0.05} = 600 \mu\text{A}$$

$$I_E = 0.6 \text{ mA}$$

The collector current is $\alpha I_E = 0.95 \times 0.6$

$$I_C = 0.57 \text{ mA}$$

Q.9: For a common-base transistor, $\alpha = 0.98$. The voltage drop occurs across a resistance of $2.5 \text{ k}\Omega$. Find the base current if the collector voltage is 5 V .

Ans: The collector current is obtained by

$$I_C = \frac{\text{Collector voltage}}{\text{Resistance}}$$

$$I_C = \frac{5}{2.5} = 2 \text{ mA}$$

The current gain $\alpha = \frac{I_C}{I_E}$

$$I_E = \frac{I_C}{\alpha}$$

$$I_E = \frac{2 \text{ mA}}{0.98}$$

$$I_E = 2.04 \text{ mA}$$

The base current could be obtained using

$$\begin{aligned} I_E &= I_B + I_C \\ I_B &= I_E - I_C \\ &= 2.04 - 2 = 0.04 \text{ mA} \end{aligned}$$

Q.10: If $\alpha = 0.97$, obtain the parameter β .

Ans: Here, $\alpha = 0.97$

$$\begin{aligned} \text{As } \beta &= \frac{\alpha}{1 - \alpha} \\ \beta &= \frac{0.97}{1 - 0.97} \\ \beta &= \frac{0.97}{0.03} \\ \beta &= 32.33 \end{aligned}$$

OBJECTIVE QUESTIONS

- The resistance of mercury falls down sharply to zero at the temperature of
 - 4.15 K
 - 2.1 K
 - 6.08 K
 - 0 K
- Who discovered the phenomena of superconductivity?
 - Faraday
 - Maxwell
 - Kamerlingh Onnes
 - Ampere
- The temperature at which resistance abruptly falls to zero is called _____ temperature.
 - threshold
 - critical
 - both (a) and (b)
 - none of these
- The critical field H_c is given by
 - $H_c = H_o \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$
 - $H_c = H_o \left(\frac{T}{T_c} \right)$
 - $H_c = H_o \left(\frac{T_c}{T} \right)^2$
 - $H_c = H_o \left[1 - \left(\frac{T_c}{T} \right)^2 \right]$
- According to Silsbee effect, superconductivity gets destroyed by _____ associated with current.
 - voltage
 - current
 - resistance
 - magnetic field

6. For Meissner effect to occur, the sample should satisfy the following condition.

- (a) Free from strain
(b) Free from impurities
(c) None of the above
(d) Both (a) and (b)

7. Mathematically, for no field inside a superconductor, the following condition is given:

- (a) $H = -M$
(b) $H = M$
(c) $H = \frac{1}{M}$
(d) $H = \frac{-1}{M}$

8. For a perfect diamagnetic substance,

- (a) $\chi = 1$
(b) $\chi = 0$
(c) $\chi = -1$
(d) $\chi = 2$

9. For a perfect superconductor, which of the following is constant?

- (a) Magnetic field
(b) Electric field
(c) Current
(d) all of the above

10. Type-II superconductors have

- (a) superconducting state
(b) vortex state
(c) normal state
(d) all of the above

11. The variation of electronic specific heat varies with temperature as

- (a) $\exp(-k_B T)$
(b) $\exp\left(-\frac{\Delta}{k_B T}\right)$
(c) $k_B T$
(d) $\frac{1}{k_B T}$

12. When the specimen changes from normal to superconducting, then the thermal conductivity

- (a) decreases
(b) increases
(c) does not change
(d) increases exponentially

13. According to isotope effect,

- (a) $\frac{M^\alpha}{T_c} = \text{constant}$
(b) $\frac{T_c}{M} = \text{constant}$
(c) $M^\alpha T_c = \text{constant}$
(d) $T = \text{constant}$

14. The minimum value of a fluxoid is

- (a) 1×10^{-13} Wb
(b) 2.07×10^{-13} Wb
(c) 1 Wb
(d) 8.4×10^{-12} Wb

15. For normal state, the superconductivity is given by

- (a) $G_N(T, H) = G_N(0, H)$ (b) $G_N(T, H) = G_N(0, 0)$
 (c) $G_N(T, H) = G_N(T, 0)$ (d) $G_N(T, H) \neq G_N(T, 0)$

16. The Rutgers formula is given by

- (a) $G_N(T, H) = G_N(0, 0)$ (b) $G_N(T, 0) - G_S(T, 0) = \frac{H_c^2}{8\pi}$
 (c) $S_N = S_S - \frac{1}{8\pi} \left(\frac{dH_c}{dT} \right)^2$ (d) $C_S - C_N = \frac{T_c}{\pi} \left(\frac{dH_c}{dT} \right)^2$

17. Copper and silver are not good superconductors because

- (a) the amplitude of lattice vibrations is small
 (b) there are no free electrons
 (c) they have large amplitude of lattice vibrations
 (d) the bandgap is very large

18. Cooper pairs are formed via interactions of

- (a) photons (b) phonons
 (c) neutrons (d) electrons

19. Cooper pairs obey _____ statistics.

- (a) Maxwell–Boltzmann (b) Fermi–Dirac
 (c) Bose–Einstein (d) None of the above

20. The resistivity of metals is almost

- (a) $10^{-12} \Omega\text{m}$ (b) $10^{-6} \Omega\text{m}$
 (c) $10^{-8} \Omega\text{m}$ (d) $10^{-14} \Omega\text{m}$

21. For insulators, the bandgap between valence and conduction band is

- (a) $\approx 4 \text{ eV}$ (b) $\approx 2 \text{ eV}$
 (c) $\approx 10 \text{ eV}$ (d) $\approx 6 \text{ eV}$

22. The doping concentration should be

- (a) $1:10^8$ (b) $1:10^6$
 (c) $1:10^4$ (d) $1:10^{10}$

23. For a p-type semiconductor _____ impurity is added.

- (a) trivalent (b) tetravalent
 (c) pentavalent (d) hexavalent

24. For an n-type semiconductor _____ impurity is added.
 (a) trivalent (b) tetravalent
 (c) pentavalent (d) hexavalent
25. During forward biasing, the effective potential
 (a) remains same (b) decreases
 (c) increases (d) increases exponentially
26. For reverse biasing, the effective potential
 (a) remains the same (b) decreases
 (c) increases (d) decreases exponentially
27. For a half-wave rectifier, the output is
 (a) discontinuous (b) continuous
 (c) constant (d) very high
28. FWR has high efficiency than HWR. (Yes/No)
29. The drop resistance for a Zener diode is given by
 (a) $\frac{V_{\text{input}}}{I_z + I_R}$ (b) $\frac{V_{\text{input}} - V_z}{I_z + I_R}$
 (c) $\frac{V_{\text{input}} - V_z}{I_z}$ (d) $\frac{V_z}{I_z}$
30. The collector of a transistor is heavily doped. (True/False)
31. Following relations hold good for transistor currents.
 (a) $I_E = I_B - I_C$ (b) $I_B = \frac{I_C}{I_E}$
 (c) $I_E = I_B + I_C$ (d) $I_E = I_C - I_B$
32. For amplification, the transistor should be operated in
 (a) saturation region (b) cut-off region
 (c) active region (d) all of the above
33. β and α are related to each other as follows:
 (a) $\beta = \alpha(1 + \alpha)$ (b) $\alpha = \frac{\beta}{(1 - \alpha)}$
 (c) $\beta = 1 + \alpha$ (d) $\beta = \frac{\alpha}{1 - \alpha}$

Answers

- | | | | |
|--------|---------|---------|-------------|
| 1. (a) | 10. (d) | 19. (c) | 28. (Yes) |
| 2. (c) | 11. (b) | 20. (c) | 29. (b) |
| 3. (b) | 12. (a) | 21. (d) | 30. (False) |
| 4. (a) | 13. (c) | 22. (b) | 31. (c) |
| 5. (d) | 14. (b) | 23. (a) | 32. (c) |
| 6. (d) | 15. (c) | 24. (c) | 33. (d) |
| 7. (a) | 16. (d) | 25. (b) | |
| 8. (c) | 17. (a) | 26. (c) | |
| 9. (a) | 18. (b) | 27. (a) | |

Micro-assessment Questions

1. What do you understand by superconductivity?
2. How does magnetic field affect superconductivity?
3. What is critical field?
4. What are superconductors?
5. How does magnetic field vary with temperature?
6. List the finding of H. Kamerlingh Onnes.
7. What do you understand by flux exclusion?
8. What are hard superconductors?
9. What are soft superconductors?
10. How does electronic specific heat vary with temperature? Explain.
11. What is the value of energy gap parameter for superconductors?
12. Explain the flux quantization.
13. What is fluxoid?
14. What are Cooper pairs?
15. What are semiconductors?
16. List the differences between semiconductor and superconductor.
17. What are intrinsic semiconductors?
18. What are extrinsic semiconductors?
19. What is junction diode?
20. What is bipolar junction transistor?
21. Define the depletion region.
22. What is the principle of rectifiers?
23. What is Zener diode?
24. What is light-emitting diode?
25. Define forward current transfer ratio.
26. Define DC current gain (α) for common base transistor.
27. Define DC current gain (β) for common emitter transistor.
28. What is an amplifier?

Critical Thinking Questions

1. Show the variation of resistance with temperature.
2. Give the relation between magnetic field and critical field.
3. Explain and state Meissner effect in detail.
4. Show that a superconductor is a perfect diamagnetic substance.
5. How does the concept of diamagnetism in superconductors contradict Maxwell's equations?
6. Show that for a perfect superconductor, the magnetic field is constant even when it is cooled below critical temperature.
7. What is the difference between Meissner effect and Silsbee effect?
8. What is superconducting state? How does it differ from vortex state?
9. How do entropy and heat capacity vary with temperature for superconductors?
10. What is energy gap in superconductors? How does it differ from energy gap of semiconductors and insulators?

11. When a specimen changes its state from normal to superconducting, how will the thermal conductivity change?
12. How do electrons and photons interact with each other?
13. What is BCS ground state? Which statistics holds good in the ground state?
14. What are n-type and p-type semiconductors?
15. Show the bandgap diagram for intrinsic and extrinsic semiconductors.
16. Define the acceptor level for p-type semiconductor.
17. Define the donor level for n-type semiconductor.
18. Explain the biasing of junction diode. How does the voltage change on biasing?
19. What is rectifier? How does the p-n junction diode behave as rectifier?
20. What are emitter, collector, and base for a transistor?
21. Give the symbolic representation for n-p-n and p-n-p transistor.
22. Explain the active and saturation region for common emitter p-n-p transistor.
23. How does cut-off region differ from active region of transistor?
24. Give the relation between ac current gain in common emitter and common base gain.
25. Describe the power gain and voltage gain for common emitter amplifier.

Graded Question

1. What do you understand by superconductivity? How does Meissner effect takes place in superconductors?
2. Explain in detail the differences between type-I and type-II superconductors.
3. Give the properties of superconductors in detail.
4. What do you understand by isotope effect? Also explain the relation between superconducting state of specimen and phonon vibrations.
5. Give the thermodynamic changes, which take place during transition between superconducting and normal states.
6. Obtain the Rutgers formula for difference in heat capacity of normal and superconducting states.
7. Give the BCS theory of superconductivity. Explain the electron-phonon interaction and formation of Cooper pairs.
8. Give the classification of solids on the basis of energy bands and conductivity.
9. What are the two types of semiconductors? Explain in detail.
10. What is p-n junction diode? Also explain the forward biasing and reverse biasing of junction diode.
11. Explain the principle, construction, and working of half-wave rectifier.
12. Give the principle, construction, and working for the full-wave rectifier. In what way is a full-wave rectifier better than a half-wave rectifier?
13. What is zener diode? How does it act as voltage stabilizer? Obtain the drop resistance for zener diode.
14. Give the action and working of n-p-n transistor.
15. State and explain in detail the working of p-n-p transistor.
16. What are the characteristics for a transistor? Explain the common emitter input and output characteristics of n-p-n transistor.
17. Explain the common base input and output characteristics of n-p-n transistor.
18. How can transistor behave as an amplifier? Explain the working of p-n-p common base transistor as an amplifier.
19. Give in detail the working of p-n-p common emitter transistor as an amplifier.

Remember and Understand

1. The phenomena in which the resistivity of conductor approaches zero, even the temperature of conductor is reduced below critical temperature is called superconductivity.
2. Superconductivity is destroyed on application of strong magnetic field and the superconductor behaves as normal conductor.
3. According to the Silsbee, the superconductivity gets destroyed by the magnetic field associated with current rather than the current itself.
4. Meissner effect states that when superconductor is cooled below the critical temperature in magnetic field, then the magnetic field lines are pushed out of the superconductor.
5. There are two types of superconductors: type-I (soft) and type-II (hard) superconductors. Type-I superconductors follow Meissner effect strictly and type II do not follow Meissner effect strictly.
6. For superconductors, the entropy decreases as the temperature decreases below critical temperature. The heat capacity varies exponentially with temperature.
7. When the specimen changes from normal to superconducting state, then the thermal conductivity decreases.
8. According to isotope effect, the superconducting critical temperature is different for isotopes of materials.
9. Lattice vibrations play an imperative role in superconductivity. When the coulomb repulsive force between electrons gets overcome by attractive force between them via interaction of phonons, then the electron move together as pairs known as Cooper pairs.
10. The materials can be classified as metals, insulators and semiconductors. Semiconductors behave as insulators at 0 K.
11. The semiconductors are of two types: intrinsic and extrinsic semiconductors. Intrinsic semiconductors are pure and extrinsic semiconductors are made by doping.
12. Trivalent impurity is added to make p-type semiconductor and pentavalent impurity is added to make n-type semiconductor.
13. When a silicon or germanium material is doped in a way that one part contains trivalent impurity and second part contains pentavalent impurity, then it forms p–n junction diode.
14. During the forward biasing of p–n diode, the effective height of potential decreases; and in reverse biasing, it increases the barrier height.
15. The principle of rectifier states that the current will flow through p–n junction diode, if it is forward biased and very small or negligible current flows through it, when it is reverse biased.
16. Zener diode is specially designed diode with sharp breakdown voltage.
17. Transistor means “transfer resistor.” Transistor consists of two p–n junctions, that is, either p-type is sandwiched in two n-type semiconductors and vice versa.
18. The emitter region is heavily doped, the collector region is moderately doped and base region is lightly doped for semiconductors.
19. The CE amplifier produces output 180° out of phase w.r.t input waveform whereas CB amplifier produces in phase output.
20. α and β are transistor parameters which are related as follows

$$\beta = \frac{\alpha}{1 - \alpha}$$

21. The base current (I_B), collector current (I_C) and emitter current (I_E) are related as: $I_E = I_B + I_C$

Electronic Devices

Keywords: *h*-parameters, silicon-controlled rectifier, junction field effect transistors (JFET), FET biasing, MOSFET, feedback circuits, oscillators, RC oscillators, LC oscillators

Learning Objectives

- ◆ To know about hybrid parameters (*n*-parameters) as equivalent circuits
- ◆ To know about principle, construction, and working of silicon-controlled rectifier (SCR)
- ◆ To gain insight of field effect transistors and its classification and to differentiate from junction field effect transistors
- ◆ To learn about junction field effect transistors, their characteristic, and parameters.
- ◆ To understand biasing of JFET and amplification
- ◆ To know about metal oxide semiconductor, field effect transistors (MOSFET)
- ◆ To learn about enhancement and depletion MOSFET
- ◆ To understand about feedback circuits
- ◆ To know about oscillators and their principle
- ◆ To understand about classification of oscillators
- ◆ To learn about Barkhausen criteria
- ◆ To classify the oscillators into different categories
- ◆ To know about principle, construction, and working of Hartley oscillator
- ◆ To know about principle, construction, and working of tuned collector and Colpitt's oscillator
- ◆ To know about principle, construction, and working of phase-shift oscillator
- ◆ To know about principle, construction, and working of Wien bridge oscillator

In Chapter 12, we have studied about the transistors, p–n junction diode as half-wave rectifier and full-wave rectifier. We have seen the working of transistors as an amplifier. In this chapter, we will study about hybrid parameters and other electronic devices.

13.1 Hybrid Parameters as Equivalent Circuits

Transistors usually operate under small signals. Figure 13.1 shows transistor as four-port network. A and B are input ports and C/D are output ports. The amplified output is obtained at output ports. Three parameters, that is, z -parameters, h -parameter, and y -parameters, are used to describe the transistor characteristics. Input current i_i and output current i_o are taken to be positive, if they enter a port and are taken to be negative if they are coming out. In z -parameters i_i and i_o are independent variables, whereas y -parameters consider them to be dependent. In contrast, y -parameters consider input voltage V_i and output voltage V_o as independent variables and z -parameters consider them to be dependent variables. In z -parameters system, the parameters have dimension of ohm (impedance) and for y -parameter system, the parameters have dimension of ohm⁻¹ (admittance).

The hybrid parameters consider output voltage V_o and i_i as independent variables, whereas V_i and i_o are taken to be dependent variables. The dimensions of hybrid parameters depend on different ratios. Hybrid parameters are defined as the set of four parameters including impedance, admittance, and two dimensionless parameters for a linear circuit having fixed L, C, and R even if the voltage across them changes. We will obtain hybrid parameters now for transistors.

In hybrid parameters, i_o and V_i are taken to be function of i_i and V_o :

$$V_i = f(i_i, V_o) \quad (1a)$$

$$i_o = f(i_i, V_o) \quad (1b)$$

We can write Eqn. (1a) and (1b) in the form of partial derivatives as the network uses A.C. signals:

$$\partial V_i = \left(\frac{\partial V_i}{\partial i_i} \right)_{V_o} d i_i + \left(\frac{\partial V_i}{\partial V_o} \right)_{i_i} d V_o \quad (2a)$$

$$\partial i_o = \left(\frac{\partial i_o}{\partial i_i} \right)_{V_o} d i_i + \left(\frac{\partial i_o}{\partial V_o} \right)_{i_i} d V_o \quad (2b)$$

In Eqn. (2a) and (2b), we define the hybrid parameters as follows:

$$\left[\frac{\partial V_i}{\partial i_i} \right]_{V_o} = \left(\frac{V_i}{i_i} \right)_{V_o=0} = h_i = h_{ii} \quad (3a)$$

Equation (3a) is known as short-circuit input impedance.

Similarly,

$$\left[\frac{\partial V_i}{\partial V_o} \right]_{i_i} = \left(\frac{V_i}{V_o} \right)_{i_i=0} = h_r = h_{io} \quad (3b)$$

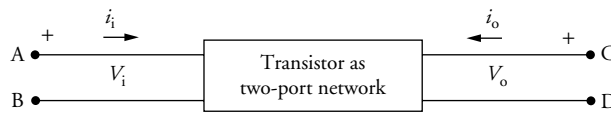


Figure 13.1 Two-port network.

Equation (3b) is known as open circuit reverse voltage ratio.

In Eqn. (2b), we obtain

$$\left[\frac{\partial i_o}{\partial i_i} \right]_{V_o} = \left(\frac{i_o}{i_i} \right)_{V_o=0} = h_f = h_{oi} \quad (3c)$$

Equation (3c) is known as the forward current ratio for short circuit.

From Eqn. (2b), we can write

$$\left[\frac{\partial i_o}{\partial V_o} \right]_{i_i} = \left(\frac{i_o}{V_o} \right)_{i_i=0} = h_o = h_{oo} \quad (3d)$$

Equation (3d) is known as output admittance for open circuit.

We can write Eqn. (2a) and (2b) using Eqn. 3(a)–(d) as follows:

$$V_i = h_i i_i + h_r V_o \quad (4a)$$

$$i_o = h_f i_i + h_o V_o \quad (4b)$$

h_f and h_r are dimensionless, whereas h_i has dimension of ohm and h_o has dimension of (ohm)⁻¹. We can write Eqn. (4a) and (4b) for different transistor configurations as follows:

(i) For common-emitter configuration,

input current = i_b , input voltage = V_b

output current = i_c , output voltage = V_c

$$\left. \begin{aligned} V_b &= h_{ie} i_b + h_{re} V_c \\ i_c &= h_{fe} i_b + h_{oe} V_c \end{aligned} \right\} \quad (5)$$

(suffix “e” indicates common-emitter configuration).

(ii) For common-base configuration,

input current = i_e , input voltage = V_e

output current = i_c , output voltage = V_c

The Eqn. (4a) and (4b) are given as Follows:

$$\left. \begin{aligned} V_e &= h_{ib} i_e + h_{rb} V_c \\ i_c &= h_{fb} i_e + h_{ob} V_c \end{aligned} \right\} \quad (6)$$

(suffix “b” indicates the common “base” mode).

(iii) For common-collectors configuration,

input current = i_b , input voltage = V_b

output current = i_e , output voltage = V_e

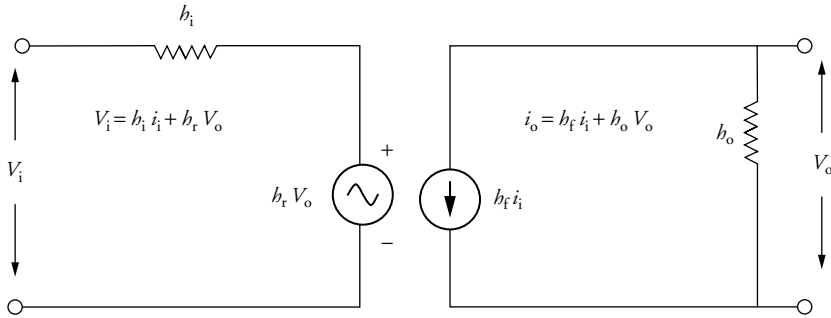


Figure 13.2 Hybrid equivalent circuit for a transistor.

The Eqn. (4a) and (4b) are given as follows:

$$\left. \begin{aligned} V_b &= h_{ic} i_b + h_{rc} V_e \\ i_e &= h_{fc} i_b + h_{oc} V_e \end{aligned} \right\} \quad (7)$$

The equivalent circuit for Eqn. (4a) and (4b) is given in Figure 13.2.

Hybrid circuits may replace the transistors during circuit analysis. For common-collector configuration, the hybrid equivalent circuit is shown in Figure 13.3.

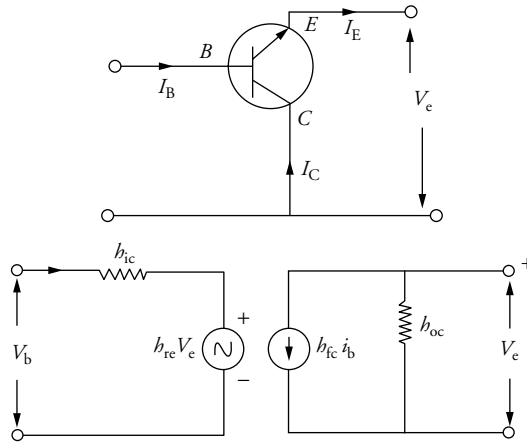


Figure 13.3 Equivalent circuit for common-collector amplifier.

13.2 Silicon-controlled Rectifier

Silicon-controlled rectifier (SCR) exhibits the features of transistor and rectifier. It acts as an electronic switch. It acts as a rectifier by changing alternating current (A.C.) to direct current (D.C.). SCR is a tri-junction device and its symbol are given in Figure 13.4. Another name for SCR is thyristor.

For making SCR, a parent wafer of *n*-type silicon material is taken. The two *p*-layers are formed by diffusion of acceptor atoms into the parent wafer. Three junctions J_1 , J_2 , and J_3 are formed (Figure 13.4).

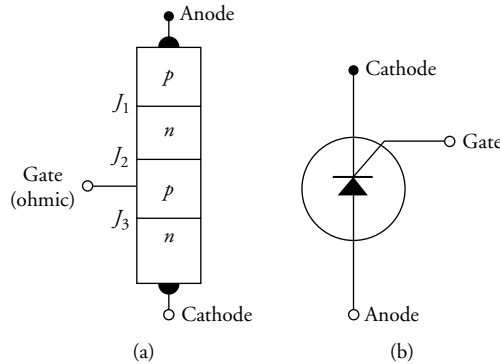


Figure 13.4 SCR and its symbol.

The n -type end forms the cathode and p -type end forms anode. An aluminum wire is used to form contact to the gate region with cathode. The gate layer is the first p layer from cathode side. If we look at Figure 13.4(a), then the SCR can be considered as a combination of two transistors: p - n - p and n - p - n . Moreover, SCR also exhibits rectifying properties. If anode is made negative and cathode is positive, then junctions J_1 and J_3 are reverse biased, whereas J_2 will be forward biased. On the other hand, if anode is positive and cathode is negative, then the junctions J_1 and J_3 are forward biased and J_2 gets reverse biased. Hence, SCR can control the power that is being fed to the load. SCR can exist only in two states, either it will conduct or will not conduct. That is why it behaves as a switch.

13.2.1 Working of SCR

SCR can be operated under two conditions, that is, gate positive w.r.t. cathode or open gate. When the gate is positive w.r.t. cathode, then SCR can conduct heavily (Figure 13.5).

When small positive potential is applied to gate, then the junction J_3 gets forward biased. In the region around junction J_3 , electrons from n -region will move toward p -region. Similarly, holes from p -region start diffusing toward n -region. Hence, electrons from junction J_3 are attracted toward J_2 and gate current starts flowing, which increases the anode current also. When the anode current flows,

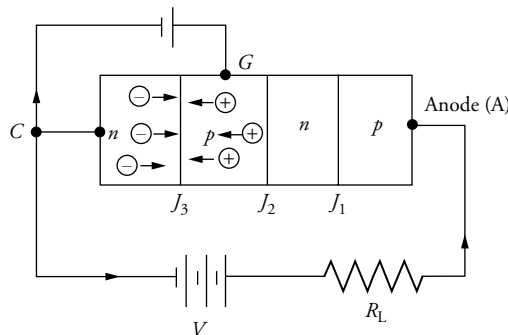


Figure 13.5 Gate positive with respect to cathode.

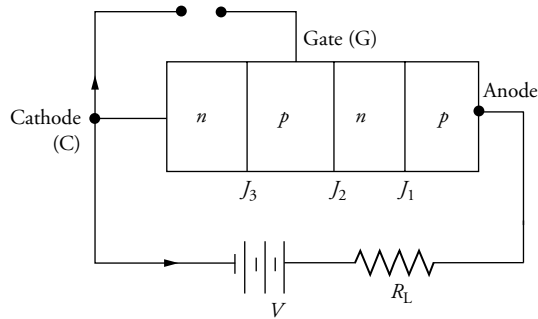


Figure 13.6 Gate open with respect to cathode for SCR.

then more electrons become available at J_2 . This process goes on, and finally junction J_2 breaks down making SCR to conduct heavily. Once, the breakdown condition for J_2 is achieved, the anode current no longer depends on the gate voltage. Only when the applied voltage V is reduced to zero, the SCR turns off.

Second condition of operation of SCR is by keeping gate open w.r.t. cathode (Figure 13.6). When gate (G) is open w.r.t. cathode, then junctions J_1 and J_3 are forward biased, whereas junction J_2 is reverse biased. The SCR is in cut-off stage and no current flows through the load R_L . When external voltage V is increased, then the reverse biased J_2 junction breaks down leading to heavy conduction of SCR. The SCR turns to on condition. The minimum forward voltage that is applied to make SCR to conduct heavily while the gate is open is said to be breakover voltage. Breakover voltages may vary from 50 V to 500 V. When gate is positive w.r.t. cathode, then the applied voltage has to be reduced to zero in order to make the SCR off. The maximum anode current that turns the SCR to off state while the gate is open is called holding current. Every SCR has ratings marked over it. Usually, in markets the commercial SCR has applied voltage slightly less than the breakover voltage. Every SCR has forward current rating that limits the maximum anode current to be passed through SCR to limit its destruction due to overheating.

13.2.2 Characteristics of SCR

The graphs between anode–cathode voltage and anode current keeping gate current at constant value is known to be V – I characteristics of SCR (Figure 13.7(a)). Like p–n junction diode, SCR has forward and reverse characteristics. During forward characteristics, the anode is made positive w.r.t. cathode. Then by keeping I_G constant, a graph is plotted between anode–cathode voltage and anode current. The voltage is varied from zero to breakover voltage ($I_G = 0$) and the SCR conducts heavily at breakover voltage. Most of the voltage appears across load as voltage across SCR drops suddenly (Figure 13.7(b)).

For forward characteristics, B_1 represents breakover voltage and C is the dropdown voltage. There is leakage current which is due to minority carrier. In reverse characteristics of SCR, anode is negative w.r.t. cathode, and the graph is plotted between anode–cathode voltage and current. Initially, the anode current will be small even after increasing the reverse anode–cathode voltage. This is due to

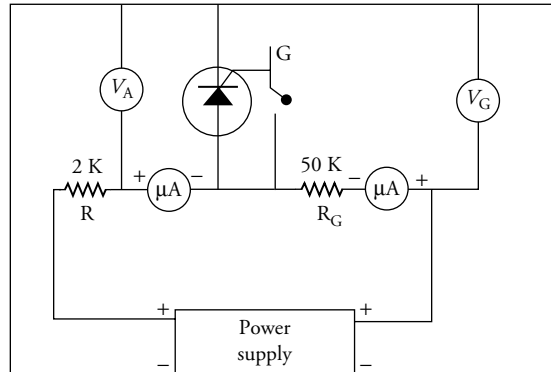


Figure 13.7(a) Circuit diagram for obtaining characteristics of SCR.

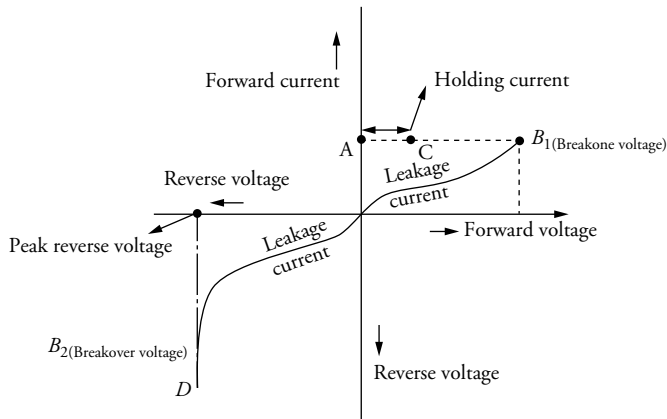


Figure 13.7(b) Characteristics of SCR.

small leakage current. When voltage is increased up to point B_2 , then the breakdown takes place and SCR conducts heavily shown by curve B_2D . B_2 is also breakover voltage for reverse characteristics.

13.3 Field Effect Transistors (FET) and their Classification

We have studied about transistor rectifiers and hybrid parameters. Transistors are also known as Bipolar junction transistors (BJTs) because they have two majority and minority carriers taking part in their operation. But for unipolar junction transistors (UJTs), only majority carriers contribute during the operation. FETs are field effect transistors that fall under the category of UJT as its operation depends on the flow of majority carriers only. It differs from transistor because it is not current controlled like transistor. FET is a voltage-controlled device and the classification of FET can be done as shown in Figure 13.8.

In the sections that follow, JFET and MOSFET are described in detail.

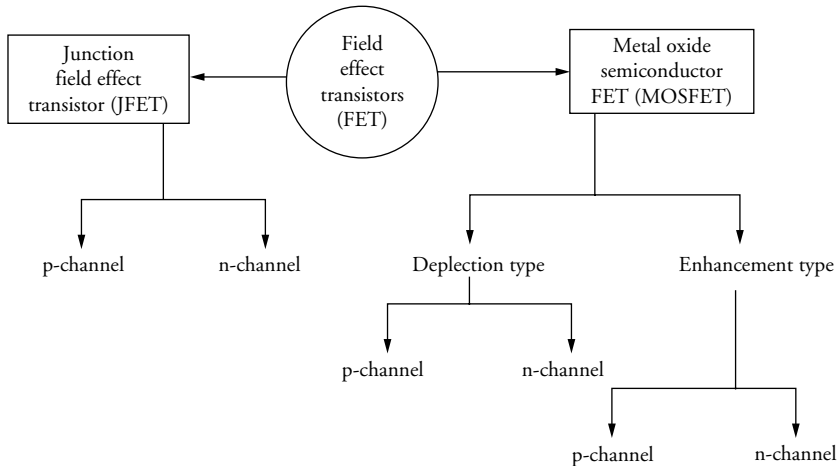


Figure 13.8 Classification of FET.

13.4 Junction Field Effect Transistors (JFET)

The junction field effect transistors (JFETs) are three-terminal devices, that is, source, drain, and gate, in which the current flow is only due to one type of charge, either electrons or holes. Two types of JFETs are shown in Figure 13.9(a) and (b).

JFET has ohmic contacts at both sides. JFET is a uniformly doped bar with trivalent or pentavalent impurities. When the semiconductor bar is of n -type, then the JFET is known as n -channel JFET. On the contrary, when the semiconductor bar is of p -type, then the JFET is known as p -channel JFET. The structure of p -channel JFET is shown in Figure 13.10. On either side of p -channel JFET, heavily doped n -regions are formed. These n -regions are connected to each other internally and form a common terminal known as gate (G). The p -channel bar has two terminals: source (S) and drain (D).

Within these two terminals, the bar behaves as a resistor. The voltage is applied between the end terminals of source (S) and drain (D), and the current starts flowing along the length of the channel. The current carriers are majority carriers, which are holes in this case. Source (S) is the terminal through which the majority charge carriers enter the bar and constitute current I_S (source current). The terminal through which the majority carriers leave the bar is known as drain and I_D is the drain current. The gate voltage is applied between the gate and the source such as to reverse the p - n junction, hence, source and gate are reverse biased. The gate-source voltage is denoted by V_{GS} , the gate current is denoted by I_G , and the drain-to-source voltage is denoted by V_{DS} [$V_{DS} = V_{DD} = \text{supply voltage}$]. The symbols for JFET are given in Figure 13.11(a) and (b). The source and drain terminals are interchangeable.

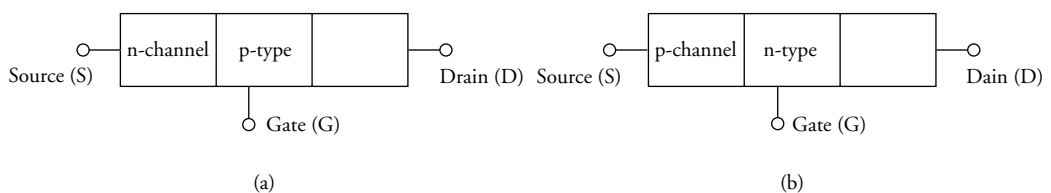


Figure 13.9(a) n -type channel **(b)** p -type channel.

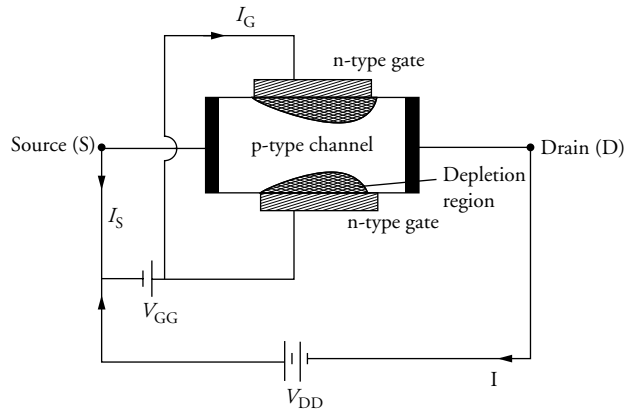


Figure 13.10 *p*-channel JFET.

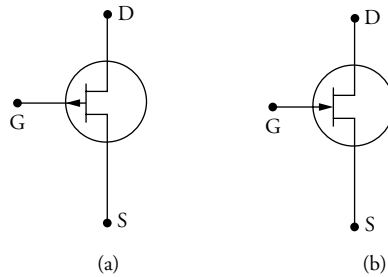


Figure 13.11 Symbols for (a) *p*-channel JFET (b) *n*-channel JFET.

13.4.1 Working of JFET

Let us consider *p*-channel JFET as shown in Figure 13.12(a) and (b). The major current carriers for *p*-channel JFET are holes, and they drift through the channel. The source is forward biased w.r.t. drain and the current starts flowing from source to drain that constitute drain current as shown in Figure 13.12(a). When the gate is reverse biased by apply gate voltage, then the depletion region increases and the width of channel gets narrow. The holes pass through the channel of reduced width

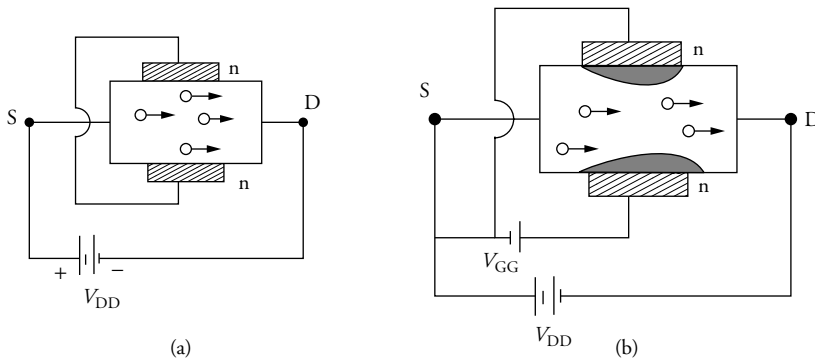


Figure 13.12 *p*-channel JFET: (a) without biasing and (b) under the effect of reverse biasing.

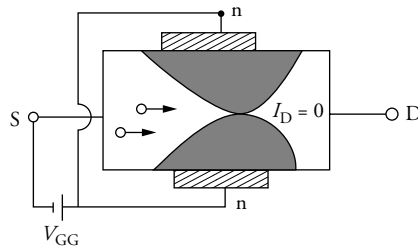


Figure 13.13 Pinch-off condition (at large reverse voltage).

that consequently decreases drain current. The reverse bias is not the same throughout the length of p–n junction; and, the drain end is narrower. The reverse bias is more between the gate and drain end than the gate and source end. The width of depletion region will increase more if the reverse bias is increased more. Hence, the increase in reverse bias of gate and source will decrease the drain current. If sufficient and large reverse bias is applied, then the depletion region will extend to channel region from both side, and hence the current flow will stop. In other words, the current is pinched off (Figure 13.13).

The gate–source voltage, at which the current is pinched off, is known pinch-off voltage, V_p . Hence, the extent of electric field decides the drain current and width of channel. Hence, the field has effect on its working and named as JFET.

13.4.2 Characteristics of JFET

JFETs have two types of characteristics. The schematic diagram of *p*-channel FET is given in Figure 13.14. The gate and source are forward biased by voltage V_{GS} . The gate is positive w.r.t. source whereas the drain is given negative potential w.r.t. source by V_{DS} (drain–source voltage). For *p*-channel JFET, the majority carriers through channel are holes. The two types of characteristics are output and transfer characteristics as demonstrated below.

1. Output Characteristics The output characteristics are also known as common source drain characteristics or static characteristics. The graph plotted between drain source voltage (V_{DS}) and drain current (I_D) keeping gate–source voltage (V_{GS}) at constant value are known as output characteristics (Figure 13.15(a)). The output characteristics curves a comprise of three regions: ohmic region (linear region), saturation region (pinch-off region), and breakdown region. In ohmic region, the *p*-bar

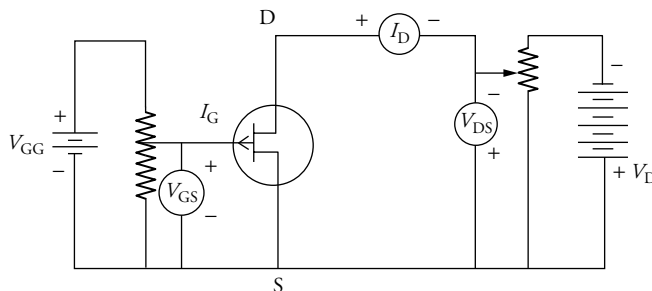


Figure 13.14 Schematic diagram of *p*-channel JFET.

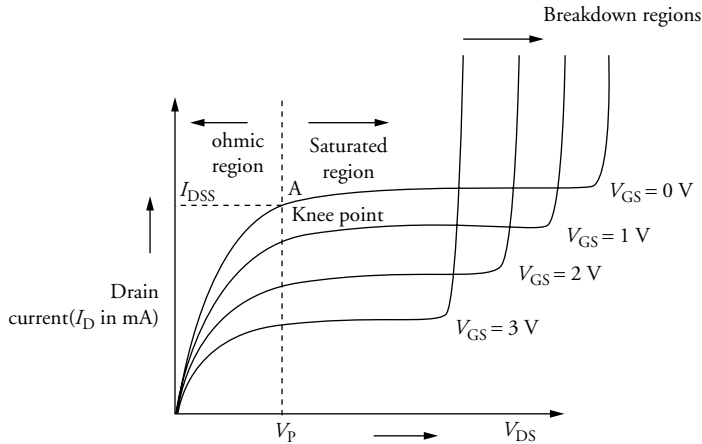


Figure 13.15(a) Output characteristics of JFET.

between the two terminal behaves as a resistor, and the resistance is given by $R = \frac{V_{DS} \text{ (in V)}}{I_D \text{ (in mA)}}$. This region is almost linear and exists for smaller values of V_{DS} . This region is useful for application of JFET as a voltage-dependent resistor (VDR).

The saturation region starts from pinch-off voltage (V_P). In saturation region, the drain current becomes constant of drain-to-source voltage (V_{DS}). This region is of practical importance for high-voltage amplifiers. In the breakdown region, the drain current rises abruptly with increase of drain-to-source (V_{DS}) voltage. When $V_{GS} = 0$ V, then the p–n junction is not reverse biased, Whereas for $V_{DS} = 0$ V, $I_D = 0$. As V_{DS} is increased, the drain current increases up to the knee point (A), which is also known as pinch-off voltage. The flow I_D contributes to voltage drop across the p -channel bar, and it contributes to reverse biasing of gate junction. With more and more increase of V_{DS} voltage, the channel starts narrowing at the drain region. The current I_D will not increase due to pinching off the channel and the current attain a saturated value in the saturated region. When V_{DS} is increased further such that it exceeds reverse-breakdown voltage, then large current I_D flows from drain to gate, and this condition is breakdown condition. As the gate–source voltage is increased, then the curve shifts down and breakdown as well as pinch off occurs for small values of drain–source (V_{DS}) voltage. In breakdown region, JFET is constant voltage source device whereas in saturation region, it is constant current source device.

2. Transfer Characteristics The graphs plotted between gate–source voltage (V_{GS}) and drain current (I_D) keeping the drain–source voltage (V_{DS}) constant are known as transfer characteristics (Figure 13.15(b)). From the output and transfer characteristics, we can obtain I_{DSS} (drain current at zero bias) and cut-off voltage (V_P) or $V_{GS} \text{ (off)}$. I_{DSS} is the drain current when $V_{GS} = 0$ V and $V_{DS} > V_P$. The voltage at which the channel is completely cut off making drain current zero is known as pinch-off voltage (V_P).

The pinch-off voltage is given by the following equation:

$$V_p = \frac{|q|N_a}{2\epsilon} a^2 \quad (8)$$

$|q| \rightarrow$ magnitude of charge

$N_a \rightarrow$ acceptor atom concentration

$\epsilon \rightarrow$ permittivity of channel material

$a \rightarrow$ half the channel width

The drain current (I_D) is related to I_{DSS} by the following expression:

$$I_D = I_{DSS} \left[1 - \frac{V_{GS}}{V_{GS(off)}} \right]^2$$

$$I_D = I_{DSS} \left[1 - \frac{V_{GS}}{V_p} \right]^2 \quad (9)$$

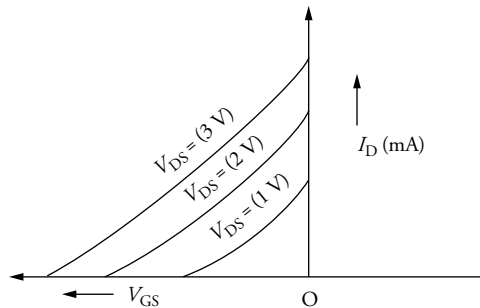


Figure 13.15(b) Transfer characteristics of JFET.

13.4.3 Parameters for JFET

The performance of JFET is defined by three important parameter as described below.

1. Transconductance (g_m) It can be obtained from the transfer characteristics of JFET. The ratio of small change in drain current to small change in gate–source voltage at constant drain–source voltage (V_{DS}) is said to be transconductance for an operating point.

i.e.

$$g_m = \left. \frac{\Delta I_D}{\Delta V_{GS}} \right|_{V_{DS} = \text{constant}} \quad (10a)$$

2. A.C. Drain Resistance (r_d) It can be derived from the output characteristics of JFET. The ratio of small change in drain–source voltage (V_{DS}) to small change in drain current (I_D), keeping constant V_{GS} is known as dynamic/A.C. drain resistance for an operating point.

$$r_d = \left. \frac{\Delta V_{DS}}{\Delta I_D} \right|_{V_{GS} = \text{constant}} \quad (10b)$$

3. Amplification Factor (μ) The ratio of small change in V_{DS} to the small change in V_{GS} keeping drain current constant is said to be amplification, that is,

$$\mu = \left. \frac{\Delta V_{DS}}{\Delta V_{GS}} \right|_{I_D = \text{constant}} \quad (10c)$$

$$\mu = \frac{\Delta V_{DS}}{\Delta V_{GS}} = \frac{\Delta V_{DS}}{\Delta I_D} \times \frac{\Delta I_D}{\Delta V_{GS}}$$

As

$$\mu = r_d g_m \quad (11)$$

Equation (11) gives the relationship between all the three parameters of JFET. JFET can act as buffer amplifier because it has high input impedance and low output impedance. Due to its high input impedance, it is also used as FET meters. In its linear region, it can be used for radio tuners.

13.4.4 Biasing of JFET

There are three ways of biasing JFET, that is, self-bias, voltage divider bias, and source biasing. Biasing means gate should be negative w.r.t. source. The biasing of FET is described as follows.

1. Voltage Divider Biasing As clear from Figure 13.16(a), the resistances R_1 and R_2 form voltage divider across the drain V_{DD} and voltage developed across R_2 is V_G , which is given by the following equation:

$$V_G = \frac{V_{DD} \cdot R_2}{R_1 + R_2} \quad (12)$$

Further,

$$V_{GS} = V_G - I_D R_S \quad (13a)$$

and

$$V_{DS} = V_{DD} - I_D (R_D + R_S) \quad (13b)$$

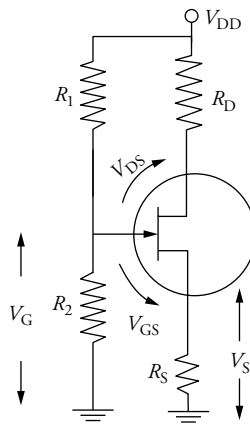


Figure 13.16(a) Voltage divider bias.

2. Self-Bias R_S is used as a bias resistor as shown in Figure 13.16(b) and

$$V_S = I_D R_S \quad (14a)$$

$V_G = 0$, therefore,

$$V_{GS} = -V_S = -I_D R_S \quad (14b)$$

where V_S is the desired bias voltage.

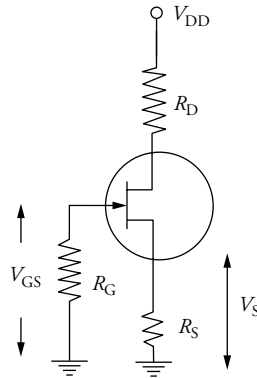


Figure 13.16(b) Self-bias.

3. Source Bias In source bias, the V_S appear across R_S and the condition for drain is

$$I_D \approx \frac{V_S}{R_S} \quad (15)$$

I_D is independent of JFET characteristics (Figure 13.16(c)).

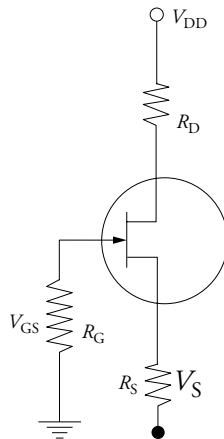


Figure 13.16(c) Source bias.

13.5 Metal-oxide Semiconductor FET

Metal-oxide semiconductor FETs (MOSFETs) are also known as insulated-gate field effect transistor (IGFET) or metal-oxide semiconductor transistor (MOTS). The MOSFET is also unipolar device

like FET because the current carriers are of one type, only that is, holes in p -channel and electrons in n -channel. MOSFETs are of practical importance for large integrated circuits and microprocessors.

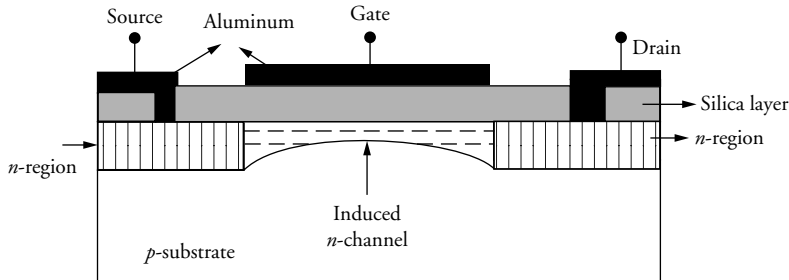


Figure 13.17 n -channel MOSFET.

The MOSFETs can be n -channel or p -channel. The n -channel MOSFET consists of slightly doped p -substrate. Two heavily doped n -regions are formed at the end by diffusion (Figure 13.17).

The heavily doped n -regions on both ends serve as source and drain. The distance of separation between these two layers is up to $10\ \mu\text{m}$. A layer of SiO_2 (insulating) is grown over the substrate. The whole channel is covered by a metallic (aluminum) region. This combination forms a parallel plate capacitor, that is, metallic gate and semiconductor substrate with dielectric medium inside it. The name IGFET is derived because the gate is insulated from the semiconductor channel due to SiO_2 (dielectric) layer. Hence, MOSFET possesses very high input resistance (up to $10^{15}\ \Omega$). For p -channel substrate, two heavily doped p -regions are formed at either ends of lightly doped n -substrate. The n -channel MOSFET are faster in their applications due to higher mobility of electrons. The symbolic representation of MOSFET is given in Figure 13.18(a) and (b).

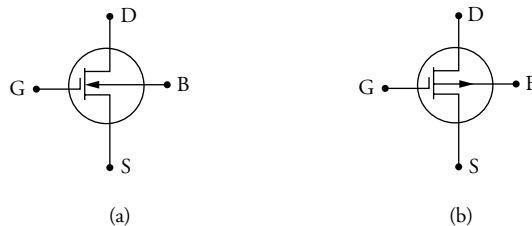


Figure 13.18 Symbolic representation of (a) n -channel and (b) p -channel MOSFET.

Martin M. "John" Atalla was one of the inventors of MOSFET who was born on August 4, 1924, in Port Said, Egypt. He was a graduate student at Purdue University, USA. He received his PhD in 1949. He investigated the surface properties of silicon semiconductors after joining Bell Laboratories. He also worked at Hewlett-Packard and Fairchild Semiconductor. He envisioned MOSFET in 1940, and he worked on it with Dawon Kahng ultimately creating MOSFET in 1960. He gifted the banks with his invention of data security system that is used in automated banking machines. He is also the founder of A4 Systems, TriStrata, and Atalla Corp.



M.M.J. ATALLA

13.5.1 Types of MOSFET

We have studied about the n -channel and p -channel MOSFET. Both of them either conduct due to holes or due to electrons. These n -channel or p -channel MOSFET can be categorized into enhancement MOSFET and depletion MOSFET. These MOSFETs are described in the following section.

1. Enhancement MOSFET

The enhancement MOSFET has been explained using n -channel (Figure 13.19). If we apply “positive” gate voltage, then negative charges will be set up under the oxide layer due to capacitor action. Under low-gate voltages, the negative charge is carried by acceptor ions in p -type substrate. This gives rise to a thin layer and the thickness of this layer will increase on further increase in gate voltage. When gate voltage becomes sufficiently large, then drain carries away negative charge supplied by source. Hence, a conducting channel is formed between drain (D) and source (S) due to negative charges n -type

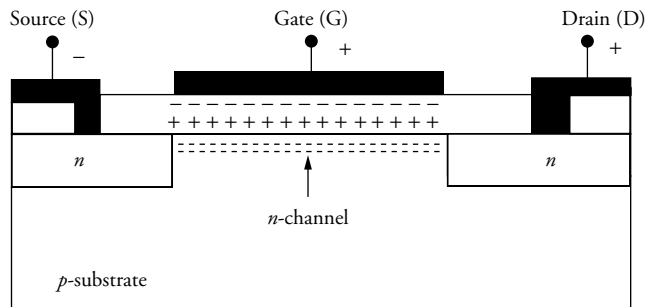


Figure 13.19 Enhancement n -channel MOSFET.

charge carriers are present under the oxide layer in p -type substrate and this is known as inversion. The threshold gate voltage (V_T) is defined as the minimum gate voltage required to produce the inversion. Conclusively, for n -channel MOSFET, the drain current gets enhanced due to induced n -channel produced by “positive” gate voltage. The characteristics of MOSFET are (i) drain characteristics and (ii) transfer characteristics. The drain characteristics represent the curves between drain current and drain-source voltage V_{DS} at constant gate source (V_{GS}) voltage (Figure 13.20a).

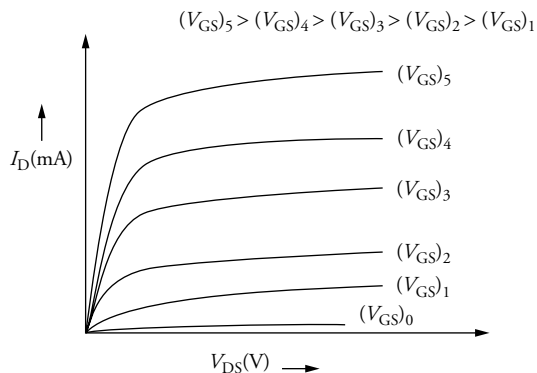


Figure 13.20(a) Drain characteristics for MOSFET.

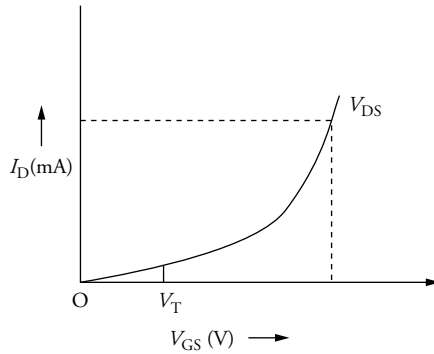


Figure 13.20(b) Transfer characteristics for MOSFET.

When V_{GS} is very small, then practically drain current is negligible. As the V_{GS} is increased and made more positive for n -channel MOSFET, and the drain current also increases.

The transfer characteristics represent the curves between drain-current and gate-source voltage (V_{GS}) at constant drain source (V_{DS}) voltage (Figure 13.20b). In transfer curve also the I_D is very small for small gate-source voltage (V_{GS}). It increases after a threshold voltage V_T (Figure 13.20(b)). The MOSFET usually have marking for threshold gate-source voltage.

2. Depletion MOSFET

For a MOSFET to operate in depletion mode, a “negative” gate voltage is applied for n -channel MOSFET and “positive” gate voltage for p -channel MOSFET (Fig. 13.21). A considerable amount of I_{DSS} will flow for $V_{GS} = 0$. As V_{GS} is made more negative for n -channel MOSFET, the positive charges are induced in channel and drain current drops. Hence, the channel region also gets depleted of majority charge carriers. The depletion region is more toward the drain side like JFET. Hence for characteristics curves also, for n -channel MOSFET, depletion region operates for “negative” gate voltage, whereas “positive” gate voltage is used for enhancement mode. The reverse happens for n -channel MOSFET, that is, the depletion region operates for “positive” gate voltage and enhancement for “negative” gate voltage.

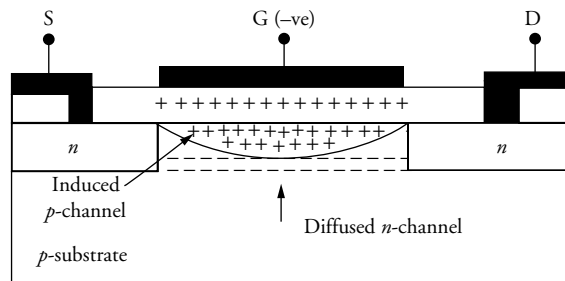


Figure 13.21 Depletion-type MOSFET.

Dawon Kahng was born on May 4, 1931, in Seoul, South Korea. In 1955, he completed his bachelor's degree from Seoul National University. He got his postgraduation as well as doctorate degree from the Ohio State University, USA. Kahng joined Bell Telephone Laboratories, in 1959, where he met Martin M. "John" Atalla. He was the coinventor of MOSFET along with John Atalla. At first, their discovery was not favored and admired by their coworkers at Bell Laboratories or the semiconductor industry; but today, the MOSFET are the most important components of microprocessors and integrated circuit.

Dawon Kahng was the founder of NEC Research Institute, which is very famous for conducting basic science research in communications and computing. He retired from the Bell Laboratories in 1988.



D. KAHNG

13.6 Introduction to Feedback

When we have to choose a device for working in particular range with desired values of input and output voltages, then it is important to choose an operating point of transistor (Q). Practically, the output is not an exact replica of the input waveform due to various types of distortions such as frequency distortion, phase distortion, or nonlinear distortion. Hence, the concept of feedback circuits is introduced which combines the output signal and external output signal. Hence, the feedback is the process in which a part of output signal is fed back to the input circuit (Figure 13.22).

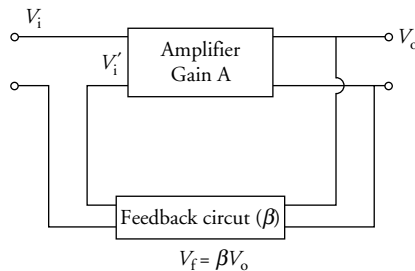


Figure 13.22 Block diagram of amplifier with feedback circuit.

Hence, the amplifier performance can be improved using feedback circuits. The feedback can be positive/regenerative or negative/degenerative. In positive feedback, the gain of amplifier is increased as the applied signal and feedback signal are in phase with each other. This type of feedback is very beneficial for oscillator circuits. The positive/direct/regenerative feedback leads to instability in gain of amplifiers. Hence, they do not find practical applications in amplifiers.

In negative feedback, the gain of amplifier is reduced because the applied signal and feedback signal are out of phase with each other. As clear from Figure 13.22, the feedback amplifier has amplifier circuit and feedback circuit. Feedback circuits are composed of resistors. The inputs of amplifier and feedback circuits are in series with each other, whereas the outputs are obtained in parallel. The feedback circuit feeds a part of its output back to input. The amplifier circuit has gain A , such that

$$A = \frac{V_o}{V_i'} \quad (16)$$

Let fraction β of output signal is fed to the input circuit, such that voltage feedback is given by the following equation:

$$A_f = \beta V_o \quad [\beta \text{ is feedback factor}] \quad (17)$$

β is usually less than 1. Hence, the feedback voltage will become

$$V_f = \beta V_o \quad (18)$$

V_i is the input signal for amplifier, which will modify the input voltage after the feedback voltage, that is,

$$V_i' = V_i \pm V_f \quad (19)$$

“+” symbol stands for positive feedback, whereas “-” symbol indicates negative feedback.

As A is the amplifier gain without feedback and from Eqn. (16),

$$A = \frac{V_o}{V_i'}$$

$$V_o = AV_i' \quad [\text{using Eqs (18) and (19)}]$$

$$V_o = A(V_i \pm V_f)$$

$$V_o = A(V_i \pm \beta V_o)$$

$$V_o(1 \pm A\beta) = AV_i$$

$$\Rightarrow \frac{V_o}{V_i} = \frac{A}{1 \pm A\beta} \quad (20)$$

$$\Rightarrow A_f = \frac{A}{1 \pm A\beta} \quad (21)$$

where

$$\Rightarrow A_f = \frac{V_o}{V_i} = \text{gain with feedback} \quad (22)$$

A_f is called gain of amplifier with feedback.

For positive feedback circuit,

$$A_f = \frac{A}{1 - A\beta} \quad (23a)$$

For negative feedback circuit,

$$A_f = \frac{A}{1 + A\beta} \quad (23b)$$

$A\beta$ is the loop gain/feedback factor. For negative feedback circuit, the following cases may arise:

- (i) When $|1 + A\beta| < 1$, then $A_f > A$. This type of condition is called regenerative/positive/ direct feedback. In this condition, the gain with feedback circuit is more than the normal gain.
- (ii) When $|1 + A\beta| > 1$, then $A_f < A$ which is the condition for negative feedback, that is, the gain using feedback circuit is less than the normal gain. Further, if $A\beta \gg 1$, then $A_f = \frac{1}{\beta}$, which indicates that gain depends only on feedback circuit and independent of A .
- (iii) When $|1 + A\beta| = 0$, then $A_f = \infty$. This condition represents the sinusoidal oscillator, that is, even when no input is fed, then also the output is obtained. To measure the feedback, following expression is used

$$\text{Feedback (in dB)} = 20 \log \left[\frac{1}{1 + A\beta} \right] \quad (24)$$

13.7 Feedback Circuits

Usually, for practical applications, negative feedback circuits are used because positive feedback introduces distortions in the circuit. Figure 13.23 demonstrates the types of negative feedback circuits.

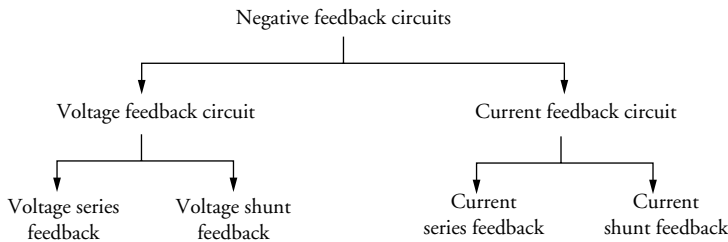


Figure 13.23 Schematic description of different types of feedback circuit.

In voltage feedback circuit, the voltage that is fed from amplifier output is proportional to load voltage. In contrast to this, for current feedback circuit, the voltage that is fed from amplifier output is proportional to load current. Other feedbacks can be explained as follows:

1. Voltage Series Feedback

In this circuit (Figure 13.24(a)), the input impedance is very high, whereas the output impedance is small. This is due to the fact that input possesses series connections, whereas the output has shunt connections. The part of output voltage is combined with input via feedback circuit in series.

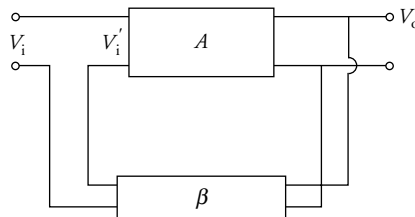


Figure 13.24(a) Voltage series feedback circuit.

2. Voltage Shunt Feedback

In this circuit (Figure 13.24(b)), the input and output possess shunt connection that reduces the input and output impedance. The fraction β of feedback is returned to amplifier circuit in parallel and output is also obtained in parallel.

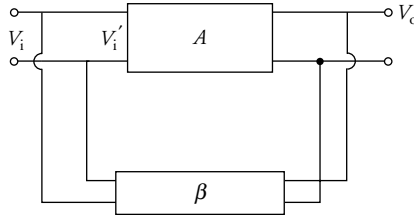


Figure 13.24(b) Voltage shunt feedback circuit.

3. Current Series Feedback

In this feedback circuit (Figure 13.24(c)), input and output circuit possesses series connections that lead to increase in the input and output impedance. The feedback factor (β) is returned the input voltage in series, the output is also obtained in series.

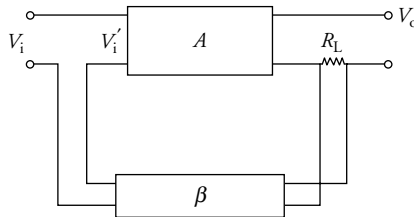


Figure 13.24(c) Current series feedback circuit.

4. Current Shunt Feedback

In this feedback circuit (Figure 13.24(d)), the input impedance decreases due to shunt connection and the output impedance increases due to series connection.

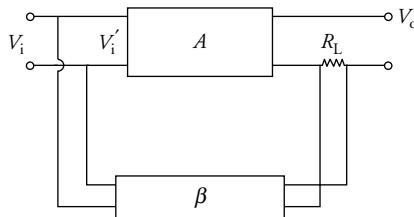


Figure 13.24(d) Current shunt feedback circuit.

The feedback factor (β) combines the part of output signal via feedback circuit to input signal in parallel. The feedback is transmitted to input through feedback circuit and input is transmitted to output through the amplifier circuit.

13.8 Oscillators and their Principle

For oscillators, we will use positive feedback circuit as they provide increased overall gain. An oscillator generates alternating voltage when the circuit is fed energy from D.C. source. Oscillators have wide range of applications such as audio signal generator that makes use of frequency from 20 Hz to 15 kHz. Oscillator circuit generates very high frequencies required for TV and radio receivers. Oscillators are also capable of supplying heat power. The oscillatory circuit consists of inductance L and capacitance C . L and C are connected in parallel constituting the tank circuit (Figure 13.25).

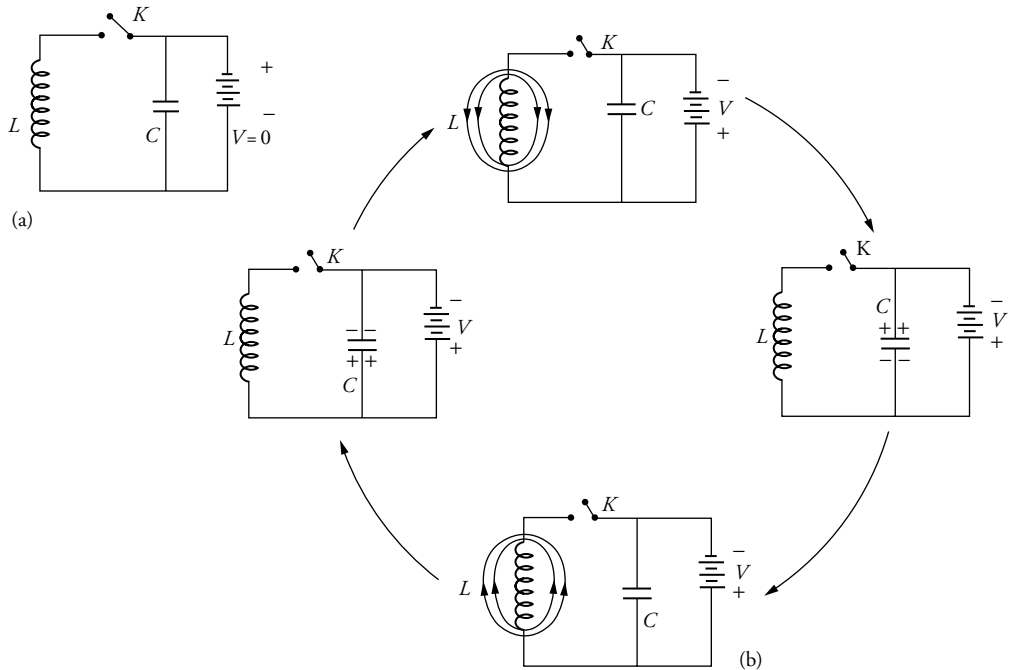


Figure 13.25 Tank circuit for oscillator: (a) at 0 voltage (b) at voltage V .

The tank circuit is connected to D.C. voltage source. The negative terminal of battery supplies energy, and hence the capacitor gets charged (Figure 13.25(b)). In capacitor, the energy is stored in the form of electrical energy. The inductor (L) is connected to the capacitor (C) which is charged. The capacitor discharges and sends current to inductor. This current is responsible for setting up magnetic field around the inductance coil. If the capacitor gets fully discharged, then the magnetic field around the coil is maximum. Hence, there is no electrical energy in capacitor when it is fully discharged. The electric energy of capacitor converts to the magnetic energy of coil. After the capacitor gets fully discharged, the magnetic field starts decreasing. The induced e.m.f. developed keeps the current flowing in the same direction. The charging of capacitor begins, but this time the polarity of plates is reversed. As the charge starts building up across the capacitor, the magnetic field starts decreasing. When the capacitor gets fully charged, then the magnetic field energy becomes zero. The magnetic energy of inductor gets converted to the electrical energy of capacitor. After the capacitor gets fully charged, it begins to discharge and the current flows in opposite direction (Figure 13.25(b)). Hence, the cycle

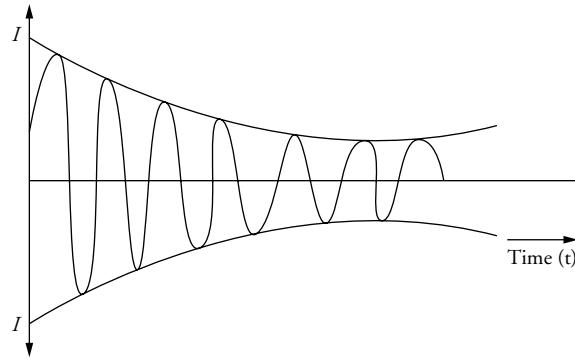


Figure 13.26 LC damped oscillations.

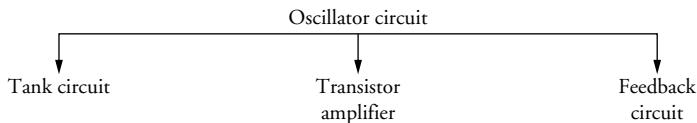


Figure 13.27 Components of oscillator.

repeats again and again, that is, electric energy gets converted to magnetic energy and vice versa. This means the energy is interchanged between L and C.

The oscillations are damped because the circuit usually has some resistance as shown in Fig. 13.26. For an ideal circuit, no loss of energy would occur and the oscillations are undamped. If energy is supplied continuously to the tank circuit, then undamped oscillations are obtained.

The oscillator circuit consists of three important components (Figure 13.27). The first component is tank circuit (LC circuit) which generates oscillations of frequency f given by the following equation:

$$f = \frac{1}{2\pi\sqrt{LC}} \quad (25)$$

These oscillations are generated due to exchange of energy between L and C.

The transistor amplifier changes the D.C. power of battery to the A.C. power by supplying it to the tank circuit. The oscillations of tank circuit are amplified, which reduce the losses in circuit. The feedback circuit provides positive feedback to obtain sustained oscillations of constant amplitude. The feedback circuit also helps in overcoming the losses of circuit. Hence, the fundamental principle of oscillators states that “The external positive feedback from the feedback circuit increases the overall gain by providing negative resistance to overcome the natural damping of oscillations.”

13.9 Classification of Oscillators

The oscillator can be classified as shown in Figure 13.28, that is, depending on the frequency of generated waveform, the nature of output waveform, and the way of producing oscillations.

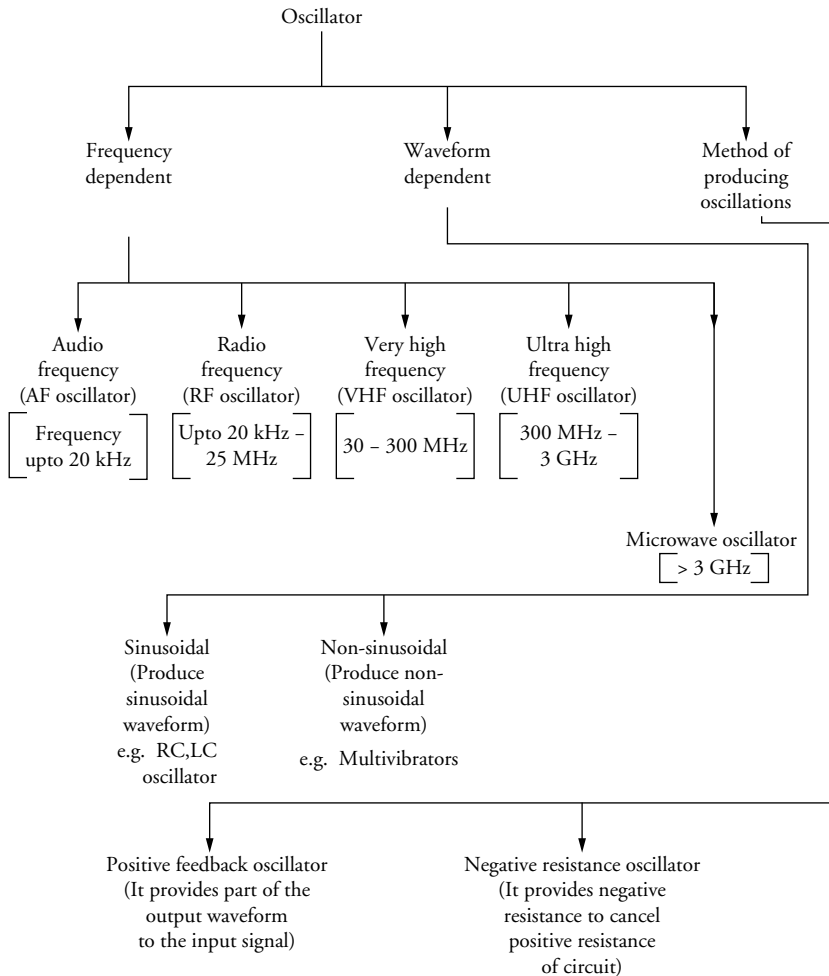


Figure 13.28 Classification of oscillators.

13.10 Barkhausen Criteria

We know that $A\beta$ is the loop gain. According to Barkhausen criteria, it states that the loop gain should be unity in order to produce sustained undamped oscillations. Hence, $|A\beta| = 1$ and $A\beta$ should have a phase of $2\pi n$, ($n = 0, 1, 2, \dots$). For an oscillator circuit, positive feedback should be given to the amplifier circuit. Let β is feedback fraction of feedback circuit and A be the voltage gain of amplifier (Figure 13.29). Then the feedback voltage for output V_o is given by the following equation:

$$V_f = \beta V_o \quad (26a)$$

Here,

$$V_i' = V_f = \beta V_o \quad (26b)$$

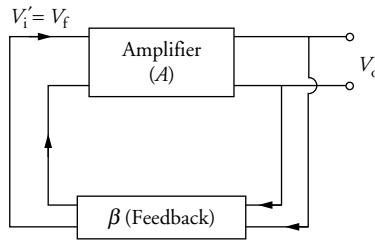


Figure 13.29 Oscillator with positive feedback.

$$V_i' - \beta V_o = 0 \quad (26c)$$

As $A = \frac{V_o}{V_i'}$ [Eqn. (16)], hence

$$V_i' - \beta A V_i' = 0$$

$$V_i' [1 - A\beta] = 0$$

As $V_i' \neq 0$, hence $[1 - A\beta] = 0$

$$A\beta = 1 \quad (27)$$

We can write down Eqn. (27) as follows:

$$A\beta = 1 + i(0) \quad (28)$$

Where i is complex function and $i = \sqrt{-1}$. Equation (28) gives the magnitude of $A\beta$ to be 1 and phase of $2n\pi$. Hence, no input signal V_i is applied for sustained oscillations. The oscillator will start producing undamped oscillations as soon as the loop gain becomes unity for a closed circuit.

As discussed in Section 13.6, the overall gain is $A_f = \frac{1}{1 - A\beta}$, when $|A\beta| = 1$, then $A_f = \infty$, which indicates that the output will be yielded even in the absence of external voltage.

13.11 Types of Oscillators

While designing an oscillator, the initial voltage is noise voltage produced by random motion of electrons in the resistors (used in feedback circuits). The magnitude of noise voltage is small, which subsequently gets amplified by feedback circuits. This noise voltage will drive the oscillator circuit. For sustained oscillation, the required condition of $|A\beta| = 1$ is satisfied by some particular frequency present in noise signal. Even the noise is combination of many sinusoidal frequencies, every frequency is not satisfying the phase condition of $2n\pi$. Hence, only one sinusoidal frequency is amplified. The loop gain should satisfy $|A\beta| > 1$, when the oscillator is switched on.

The oscillations are built up and the amplifier gain decreases to unity gradually. The following conditions must be satisfied for oscillator action:

- (i) When the oscillator is switched on, the gain (loop gain) should be greater than unity.
- (ii) The loop gain should gradually decrease to 1, once the desired level is attained.
- (iii) It works on positive feedback or negative resistor.
- (iv) D.C. supply is required as energy source.

The oscillators fall under two categories: LC and RC. Hartley, Colpitts, and tuned collector oscillators fall under LC oscillators; whereas, phase shift and Wien bridge oscillator fall under the category of RC circuits. We will discuss these oscillators in the following sections.

13.11.1 Hartley's Oscillator

Hartley's oscillators have two types of arrangement: series-fed oscillator and shunt-fed oscillator. Hartley oscillator is used in radio receivers due to its adaptability to wide frequency range and tuning capability. In shunt-fed Hartley oscillator, a transistor is used in CE configuration (Figure 13.30). The frequency f is determined by circuit made up of L_1 , L_2 , and C_1 . Coils L_1 and L_2 are coupled to each other, which in turn are connected to variable capacitance. Hence, this generates the tank circuit for LC oscillations.

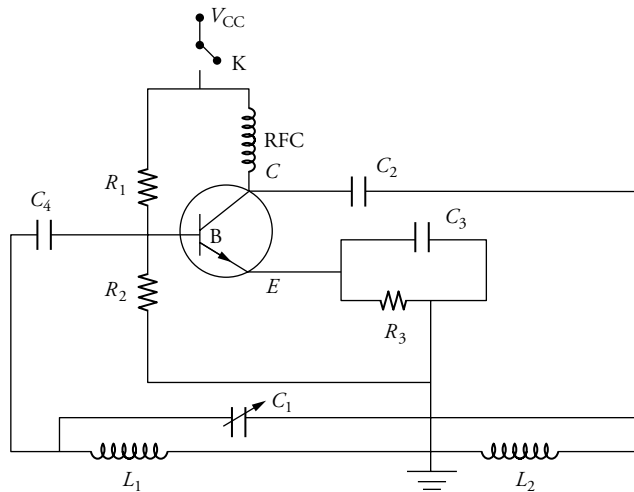


Figure 13.30 Shunt-fed Hartley oscillator.

The collector circuit has two bifurcations, collector is connected to radio frequency choke (RFC) coil and this RFC is further connected to voltage source V_{CC} . Hence, the RFC eliminates A.C. current out and provides path for the direct current. The collector is also connected to the LC tank circuit through capacitor C_2 . This capacitor C_2 provides path for the alternating current and eliminate D.C. The D.C. operating point of the transistor is maintained by the resistors R_1 , R_2 , R_3 , and voltage V_{CC} . The self-biasing is provided by C_4 and R_2 . Signal degeneration and A.C. ground is provided by capacitor C_3 which is connected to emitter. Variable capacitance (C_1) helps in adjusting frequencies so that the desired oscillations can be achieved through the tank circuit. The common emitter mode introduces a phase shift of 180° between input and output voltages.

As auto transformer in the circuit (L_1 , L_2 , and C_1 circuit) also introduces another phase shift of 180° . Conclusively, input and output are in phase with each other.

In series-fed Hartley oscillator, again the common emitter mode is used (Figure 13.31). R_1 , R_2 , and R_3 are bias resistances whose magnitude is large. C_3 blocks the D.C. and allows A.C. to pass through it. C_2 acts as a bypass capacitor. The voltages V_{CC} is directly connected to the LC tank circuit. L_1 and L_2 are two induction coils coupled together. L_1 , L_2 , and C_1 constitute the tank circuit. (This combination is also known as auto transformer.) Collector of transistor is also connected to the auto transformer circuit.

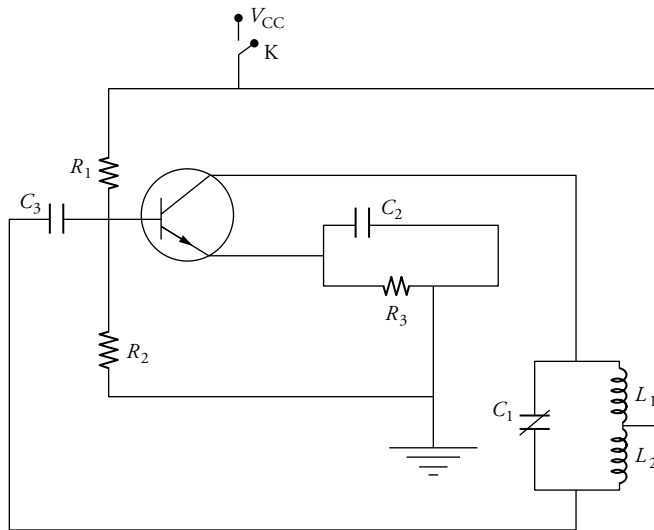


Figure 13.31 Series-fed Hartley oscillator.

Working

When key K is closed, then current flows through the circuit that charges the capacitor C_1 until it is fully charged. Then the capacitor is discharged through induction coils L_1 and L_2 . Hence, LC oscillations are set up in the tank circuit during which electric field energy and magnetic field energy are interchanged. The varying voltage due to these LC oscillations is applied between emitter and base. The base current is varying (different frequencies of LC oscillations). The β is current gain for common emitter transistor, that is, $\beta = I_C / I_B$. Hence for different I_B , different β amplification is obtained, which appears in collector circuit. Mutual inductances L_1 and L_2 help in providing feedback from collector–emitter circuit to base–emitter circuit. Hence, sustained or undamped oscillations are obtained due to continuous source voltage.

13.11.2 Tuned-Collector Oscillator

This oscillator is known as tuned-collector oscillator because the collector is connected to the tuned circuit (Figure 13.32). The tuned circuit is the same as tank circuit. The capacitor C_1 is connected to the primary coil of transformer. The frequency of oscillations depends on the tank circuit. The secondary coil of the transformer is connected to base of common emitter transistor.

The CE transistor introduces phase difference of 180° . The transformer also introduces a phase change of 180° . Hence, the total phase change of 360° keeps the input and output signals in phase, which makes the feedback positive. Resistance R_1 , R_2 , and R_3 provide bias to the transistor. R_2 and R_3 do not effect A.C. operation of circuit. C_2 and C_3 act as bypass capacitors. R_1 and R_2 make potential divider arrangement. The potential divider arrangement is connected to the base of transistor through the secondary coil of the transformer. C_3 plays an important role in preventing voltage drop. If capacitor C_3 would not have been connected across the resistor R_2 , then the voltage drop would have occurred across resistor R_2 . The feedback voltage developed across secondary of transformer bypasses through C_3 .

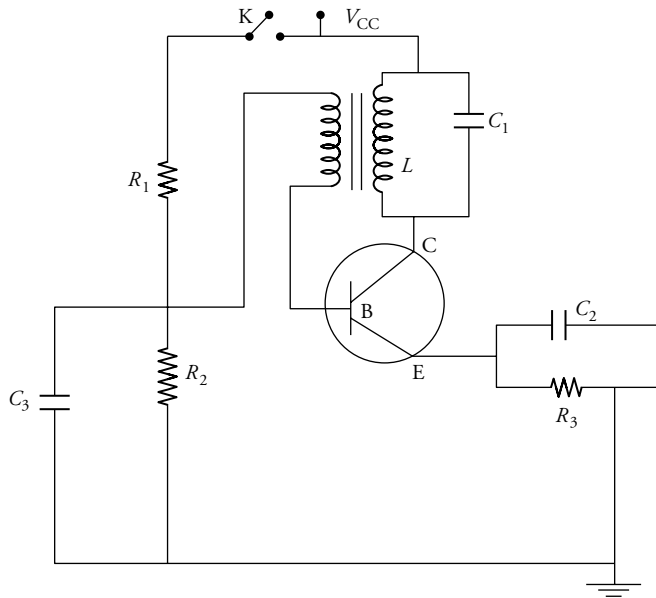


Figure 13.32 Tuned-collector oscillator circuit.

Working

When key K is closed, then the current charges the capacitor. When the capacitor gets fully charged, then it starts discharging through inductance L, giving rise to oscillations in tank circuit. These LC oscillations induce varying voltage. The magnitude of varying voltage depends on the number of turns in inductor and coupling between primary and secondary windings of the transformer. This induced voltage is applied to base. The base current I_B varies and is amplified by common-emitter circuit. This amplified current appears across collector. Hence, the energy is also used to overcome the losses in tank circuit.

13.11.3 Colpitt's Oscillator

The Colpitt oscillator is shown in Figure 13.33. The Colpitt oscillator has transistor in common-emitter (CE) mode. The tank circuit is made up of L , C_1 , and C_2 . The capacitors C_1 and C_2 are tapped at the center. The D.C. operating point is defined by R_1 , R_2 , R_3 , and supply voltage V_{CC} . The collector is connected to RFC and LC tank circuit. RFC allows path for direct current. The collector is connected to tank circuit via capacitor C_5 . C_5 gives path for the alternating current. The feedback is returned from LC circuit to base through capacitor C_3 . R_2 and C_3 form self-bias circuit. C_4 prevents signal degeneration and provide A.C. ground. C_1 and C_2 form voltage divider arrangement that introduces phase change of 180° . CE transistor also introduces phase change of 180° . Hence, total phase change of 360° keeps the input and output in phase.

Working

In Colpitt oscillator, the values of C_1 and C_2 decide the feedback. The frequency f is given by the following equation:

$$f = \frac{1}{2\pi\sqrt{LC}}$$

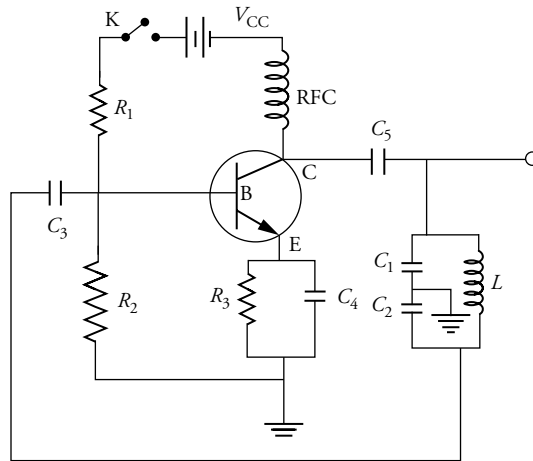


Figure 13.33 Colpitt's oscillator circuit.

Whereas

$$C = \frac{C_1 C_2}{C_1 + C_2} \quad [C_1 \text{ and } C_2 \text{ are in series}]$$

When key K is closed, then the current flows through the circuit and charges the capacitor C_1 and C_2 . After the capacitors are fully charged, then they discharge through inductor L setting up undamped LC oscillation. These oscillations will provide varying voltage that is fed to the base. I_B gets amplified by a factor β , which is obtained at collector. Some part of amplified output is used to avoid any kind of damping.

13.11.4 Phase-Shift Oscillator

We have discussed LC oscillator that has the advantage of producing high-frequency oscillations. If the output is required at low frequencies, then RC circuits are used. Phase shift is an RC oscillator. The RC oscillators also give good frequency stability. Figure 13.34 gives schematic circuit diagram of phase-shift oscillator.

The transistor is used in common-emitter mode. R_4 is the load resistor that is connected to the collector. The A.C. operating point is defined by collector power supply V_{CC} , R_2 , R_3 , and R_5 . The common-emitter transistor introduces a phase change of 180° between the input and output voltages. For positive feedback, the phase change should be 0° or 360° . Hence, additional 180° are required to produce "positive" feedback. The phase change of 180° is obtained by three cascade sections of CR. In these three-cascade sections, the series capacitor is connected to the shunt resistor. Each cascade circuit introduces a phase change of 60° and three-cascade CR will introduce phase change of 180° , provided R and C are chosen accurately. Hence, the total phase change of 360° is obtained, which fulfills the condition of positive feedback.

Working

Some voltage variations are done in V_{CC} , which introduce random oscillations in the circuit. Sometimes, the noise in the transistor can also be used to induce oscillations. The varying voltage will cause variation in the base current. The amplified current is obtained at collector with phase change of 180° . This current is fed to the three-cascade CR circuits. This cascade circuit introduces a phase change of 180° in the input and output signals. Hence, a total phase change of 360° is obtained, which fulfills the condition of in-phase of input and output signals.

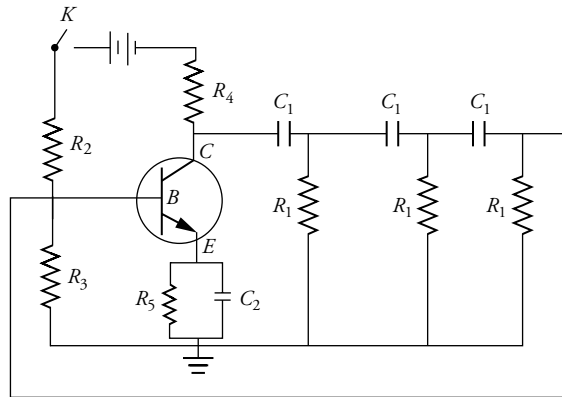


Figure 13.34 Phase-shift oscillator circuit.

13.11.5 Wien Bridge Oscillator

The Wien bridge oscillator is a two-stage RC amplifier. The first stage consists of common-emitter amplifier and the second stage consists of common collector amplifier (Fig. 13.35). The output of common-collector goes to the feedback network. The feedback network consists of R_1 , C_1 in parallel and R_2 , C_2 in series. The coupling network is of bridge nature; hence, it is named as Wien bridge oscillator.

Working

The input is applied to the base of common-emitter amplifier. The output is amplified with a phase change of 180° across R_6 . The transistor CC introduces an additional phase change of 180° . Hence, the total feedback is of 360° , which satisfies the condition of positive feedback.

The condition for the phase shift to be zero occurs at frequency,

$$f = \frac{1}{2\pi\sqrt{R_1 C_1 R_2 C_2}} \tag{29}$$

RC provides negative feedback that precludes oscillations for every frequency. In Wien bridge oscillators, the frequency can be varied; whereas in phase-shift oscillators, the frequency of oscillator is fixed.

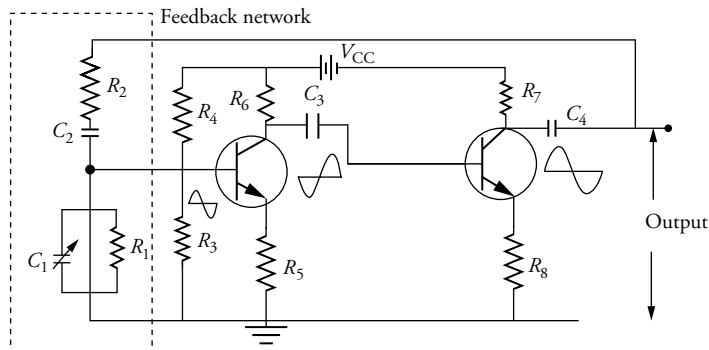


Figure 13.35 Wien-Bridge oscillator circuit.

SUMMARY

In this chapter, we studied about hybrid parameters that are used to replace the transistors in the circuits. In hybrid parameters, output current and input voltage are functions of input current and output voltage. Silicon-controlled rectifier (SCR) exhibits the combined features of transistor and rectifier and is a trifunction device. SCR can be operated under gate open or gate “positive” w.r.t. cathode condition. Unlike transistors, JFET and MOSFET fall under the category of unipolar devices, where only one type of charges are involved in current conduction process, that is, majority carriers. JFET is a voltage-controlled device. Both MOSFET and JFET have source and drain on either ends. Source and drain are connected to each other through gate terminal. MOSFET have practical applications in large integrated circuits such as microprocessors. MOSFET can be n-channel or p-channel, which can further be classified as depletion or enhancement type. When a fraction of output signal is combined with the input signal, it gives rise to feedback circuits. The feedback can be positive or negative and usually obtained by current/voltage in series/shunt mode. Positive feedback is used for the oscillators. Oscillators convert dc to ac without external energy. Oscillators produce LC oscillations using tank circuit in which electric energy is converted to magnetic energy and vice versa. For sustained oscillations, $|A\beta|=1$ and phase of $A\beta$ should be $2n\pi$. There are RC oscillators also that are used for low-frequency generation and have cascade RC circuits.

SOLVED PROBLEMS

Q.1: For a JFET, the μ and r_d are given to be 100 and $5\text{ k}\Omega$. Obtain the trans conductance:

Ans:

$$\begin{aligned}\mu &= r_d g_m \\ g_m &= \frac{\mu}{r_d} = \frac{100}{5 \times 10^{-3} \Omega} \\ &= 20 \times 10^{-3} \Omega^{-1} \\ &= 20 \text{ m}\Omega^{-1}\end{aligned}$$

Q.2: A change in V_{DS} of 5 V produces a change in I_D of $50\text{ }\mu\text{A}$ at constant V_{GS} . Obtain the dynamic resistance.

Ans:

$$\Delta V_{DS} = 5\text{ V},$$

$$\Delta I_D = 50\text{ }\mu\text{A}, \quad V_{GS} = \text{constant}$$

$$r_d = \left. \frac{\Delta V_{DS}}{\Delta I_D} \right|_{V_{GS} = \text{constant}}$$

$$r_d = \frac{5}{50 \times 10^{-6} \text{ A}} = 100 \text{ k}\Omega$$

Q.3: For a JFET, $V_p = -6$ V, $I_{DSS} = 30$ mA, and $V_{GS} = -3$ V, obtain drain current

Ans:

$$I_D = I_{DSS} \left[1 - \frac{V_{GS}}{V_p} \right]^2$$

$$I_D = 30 \left[1 - \left(\frac{-3}{-6} \right) \right]^2$$

$$I_D = 30 \left[1 - \frac{1}{2} \right]^2 = \frac{30}{4} = 7.25 \text{ mA}$$

Q.4: A JFET has drain current of 5 mA, $I_{DSS} = 10$ mA, $V_p = -6$ V. Obtain V_{GS} .

Ans:

$$I_D = I_{DSS} \left[1 - \frac{V_{GS}}{V_p} \right]^2 = 10 \left[1 - \frac{V_{GS}}{-6} \right]^2$$

$$5 \text{ mA} = 10 \left[1 + \frac{V_{GS}}{6} \right]^2$$

$$\sqrt{\left(\frac{1}{2} \right)} = 1 + \frac{V_{GS}}{6}$$

$$V_{GS} = -1.757 \text{ V}$$

Q.5: Negative feedback is applied to a circuit that reduces the gains from 40 to 20. Obtain the feedback fraction.

Ans:

$$A_f = \frac{A}{1 + A\beta}$$

$$A_f (1 + A\beta) = A$$

$$A_f + A_f A\beta = A$$

$$\beta = \frac{A - A_f}{A A_f}$$

$$A_f = 20 \quad \text{and} \quad A = 40$$

$$\beta = \frac{40 - 20}{40 \times 20} = \frac{20}{800} = \frac{1}{40}$$

$$\Rightarrow \beta = 7.5\%$$

Q.6: The voltage gain of amplifier without feedback is 800. If the feedback fraction is 0.04 for a negative feedback circuit. Obtain the voltage gain with feedback.

Ans: For “positive” feedback,

$$A_f = \frac{A}{1 + A\beta}$$

$$\beta = 0.04 \quad \text{and} \quad A = 800$$

$$A_f = \frac{800}{1 + 800(0.04)}$$

$$A_f = \frac{800}{1 + 32} = \frac{800}{33} = 24.24$$

OBJECTIVE QUESTIONS

1. The short-circuit input impedance is given by

(a) $\frac{V_i}{i_i}$

(b) $\frac{V_o}{i_i}$

(c) $\frac{V_i}{i_o}$

(d) $\frac{V_o}{i_o}$

2. For h -parameters, the dependent parameters are

(a) V_o

(b) i_i

(c) V_i and i_o

(d) V_o and i_i

3. At breakover voltage, SCR conducts _____

(a) lightly

(b) heavily

(c) moderately

(d) does not conduct

4. The forward characteristics of SCR are between

(a) current and voltage at $I_G = (I_a)_{\max}$

(b) gate current and voltage

(c) gate current and voltage at $I = 0$

(d) current and voltage at $I_G = 0$

5. FET is a

(a) bipolar transistor

(b) unipolar transistor

(c) junction rectifier

(d) junction diode

6. The drain and source of FET are interchangeable (Yes/No)

7. FET has _____ off-set voltage at 0 drain current

(a) infinite

(b) 5 V

(c) 0 V

(d) 10 V

8. In JFET, the flow of current is due to
- (a) majority carriers (b) minority carriers
(c) both majority and minority (d) leakage carriers
9. In JFET, the potential drop is more toward _____ region.
- (a) source (b) channel
(c) gate (d) drain
10. The pinch-off voltage is given by
- (a) $\frac{|q|a^2}{2\epsilon}$ (b) $\frac{|q|Na^2}{2\epsilon}$
(c) $\frac{|q|2\epsilon}{Na^2}$ (d) $\frac{Na^2}{2\epsilon}$
11. The pinch off voltage is equal to the gate source cut-off voltage. (Yes/No)
12. The drain current is given by
- (a) $I_D = I_{DSS} \left[1 - \frac{V_{GS}}{V_P} \right]^2$ (b) $I_{DSS} = I_D \left[1 - \frac{V_{GS}}{V_P} \right]^2$
(c) $I_D = I_{DSS} \left[1 - \frac{V_P}{V_{GS}} \right]^2$ (d) $I_D = I_{DSS} \left[1 - \frac{V_P}{V_{GS}} \right]^2$
13. The A.C drain resistance for JFET is
- (a) $\left(\frac{\Delta I_D}{\Delta V_{GS}} \right)_{V_{DS}=\text{constant}}$ (b) $\left(\frac{\Delta V_{DS}}{\Delta V_{GS}} \right)_{I_D=\text{constant}}$
(c) $\left(\frac{\Delta V_{DS}}{\Delta I_D} \right)_{V_{GS}=\text{constant}}$ (d) $\Delta V_{DS} \cdot \Delta I_D$
14. The parameters of JFET are related as
- (a) $\mu = \frac{r_d}{g_m}$ (b) $r_d = \mu g_m$
(c) $\mu_r g_m r_d = 1$ (d) $\mu = r_d g_m$
15. The threshold gate voltage V_T is the
- (a) voltage to produce breakdown
(b) minimum gate voltage to produce inversion
(c) maximum source voltage to produce breakdown
(d) minimum drain voltage to produce pinch-off

16. The input resistance of MOSFET is
(a) $\sim 10^{15} \Omega$ (b) $10^3 \Omega$
(c) $10^1 \Omega$ (d) $10^5 \Omega$
17. The negative feedback in amplifier
(a) increases voltage gain (b) does not affect voltage gain
(c) decreases voltage gain (d) increases the look factor
18. When $|A\beta + 1| > 1$, then the feedback
(a) is positive (b) is zero
(c) is negative (d) does not change
19. Positive feedback is used for
(a) low-gain amplifiers (b) oscillators
(c) integrated circuits (d) high-gain amplifiers
20. For LC tank circuit, the exchange occurs for
(a) mechanical and electrical energy (b) electrical and thermal energy
(c) magnetic and mechanical energy (d) electric and magnetic energy
21. The phase shift oscillators use _____ cascades.
(a) 3 (b) 5
(c) 1 (d) 4

ANSWERS

- | | | |
|----------|-----------|---------|
| 1. (a) | 8. (a) | 15. (b) |
| 2. (c) | 9. (d) | 16. (a) |
| 3. (b) | 10. (b) | 17. (c) |
| 4. (d) | 11. (yes) | 18. (c) |
| 5. (b) | 12. (a) | 19. (b) |
| 6. (yes) | 13. (c) | 20. (d) |
| 7. (c) | 14. (d) | 21. (a) |

Micro-assessment Questions

1. What are z -parameters?
2. Define y -parameters. How do they differ from z -parameters?
3. Define h -parameters.
4. What is output admittance?
5. What is silicon-controlled rectifier?
6. Define the breakover voltage for SCR.
7. What are field effect transistors (FETs)?
8. What are unipolar devices?
9. Define the bipolar devices with examples.
10. Give the symbols for p -channel and n -channel JFET.
11. What is the gate voltage for FET?
12. Define the pinch-off voltage for JFET.
13. How is drain current related to drain current at zero bias?
14. Give the magnitude of pinch-off voltage.
15. What is amplification factor for JFET?
16. Define transconductance for JFET.
17. Give the relation between all the three parameters for JFET.
18. Give the symbols for n - and p -channel MOSFET.
19. Explain the threshold voltage for MOSFET.
20. What do you understand by feedback circuits?
21. Give the block diagram for feedback circuits.
22. Explain negative and positive feedback for amplifiers.
23. How is the feedback measured?
24. Define voltage shunt feedback.
25. Explain current series feedback.
26. Define oscillators.
27. Define the resonance frequency for LC oscillators.
28. Define RC oscillators.

Critical Thinking Questions

1. What is short-circuit input impedance and forward current ratio?
2. Give the h -parameters for common-base configuration.
3. Draw the equivalent circuit for a common-collector amplifier.
4. Write the hybrid equations for transistor.
5. Define the characteristics of SCR with help of circuit diagram.
6. How do field effect transistors differ from transistors?
7. What are source and drain for JFET? Are they interchangeable?
8. Define all the parameters for JFET.
9. How does transconductance differ from ac drain resistance?
10. Give the principle for n -channel metal oxide semiconductor field effect transistors.
11. What is the difference between n - and p -channel MOSFET?
12. Describe the depletion MOSFET in detail.
13. Obtain the gain of amplifier with feedback.

14. How does current shunt feedback differ from voltage shunt feedback?
15. Explain how magnetic energy is converted to magnetic energy in tank circuit.
16. Give the components for oscillator circuit.
17. Derive the Barkhausen criteria for oscillators.
18. How do RC oscillators differ from LC oscillators?
19. Write down the conditions necessary for oscillator action.
20. Give the working action of phase shift oscillators with a circuit diagram.
21. Describe the principle and working action of Wien bridge oscillator with the help of a circuit diagram.

Graded Questions

1. What are h -parameters? Explain in detail all the four parameters. Draw the equivalent circuit for CE configuration.
2. Give the working of SCR in gate open and gate positive w.r.t. cathode.
3. Explain in detail the construction and principle of n -channel JFET.
4. Give the working of p -channel FET without biasing and under the effect of reverse biasing.
5. Describe the output and transfer characteristics of p -channel JFET.
6. Explain the working of p -channel FET without biasing and under the effect of reverse biasing.
7. Explain in detail the self-bias and source bias for JFET.
8. What are MOSFETs? Give their types and working in detail.
9. Explain in detail the working and characteristics for n -channel MOSFET.
10. Explain in detail the working and characteristics for p -channel MOSFET.
11. What are feedback circuits? Explain in detail with their types.
12. What are oscillators? Give their principles. Why is the tank circuit used in oscillators?
13. Give in detail the classification of oscillators based on frequency dependence, waveform dependence, and method of production of oscillations.
14. Describe any one LC type of oscillator with the help of a circuit diagram.
15. Explain in detail the construction and working of Hartley's oscillator in shunt-fed and series-fed mode.
16. Give the construction and working of tuned-collector oscillator.
17. Describe in detail the principle, construction, and working of the Colpitt's oscillator.
18. What are phase-shift oscillators? How do they differ from Wien bridge oscillators?

Remember and Understand

1. y , z , and h -parameters describe the transistor characteristics. In y -parameters, input and output voltage are independent variables; whereas in z -parameters, input and output current are considered to be independent.
2. The hybrid parameters consider output voltage and input current as independent variables. The dimensions of hybrid parameter depend on different ratio. The hybrid equations are given by the following equation:

$$\partial V_i = \left(\frac{\partial V_i}{\partial i_i} \right)_{V_o} di_i + \left(\frac{\partial V_i}{\partial V_o} \right)_{i_i} dV_o$$

$$\partial i_o = \left(\frac{\partial i_o}{\partial i_i} \right)_{V_o} d i_i + \left(\frac{\partial i_o}{\partial V_o} \right)_{i_i} d V_o$$

3. The various hybrid parameters ratio are given by the following equation:

$$\left[\frac{\partial V_i}{\partial i_i} \right]_{V_o} = \left(\frac{V_i}{i_i} \right)_{V_o=0} = h_i = h_{ii}$$

$$\left[\frac{\partial V_i}{\partial V_o} \right]_{i_i} = \left(\frac{V_i}{V_o} \right)_{i_i=0} = h_r = h_{ro}$$

$$\left[\frac{\partial i_o}{\partial i_i} \right]_{V_o} = \left(\frac{i_o}{i_i} \right)_{V_o=0} = h_f = h_{oi}$$

$$\left[\frac{\partial i_o}{\partial V_o} \right]_{i_i} = \left(\frac{i_o}{V_o} \right)_{i_i=0} = h_o = h_{oo}$$

4. The silicon-controlled rectifier (SCR) is an electronic switch that is a trijunction device. It can act as a rectifier by changing ac to dc. SCR can operate under two operations, that is gate positive w.r.t. cathode and open gate. The SCR conducts heavily when gate is positive w.r.t. cathode.
5. Field effect transistors (FET) are unijunction transistors as their operation depends only on the flow of majority carriers. FET is a voltage-controlled device, and is classified as junction FET and metal oxide semiconductor FET (MOSFET).
6. JFET has three terminals, that is, gate, source, and drain. JFET is uniformly doped bar with trivalent or pentavalent impurities. When the bar is of n -type carriers, then the JFET is n -channel. When the bar is of p -type carriers, then the JFET is p -channel type.
7. Source is the terminal through which the majority carriers enter the bar and constitute source current, whereas the terminal through which the majority carriers exit is known as drain. Gate is the common terminal and the gate voltage e is applied between gate and source.
8. The gate–source voltage at which the current is pinched off is known as pinch-off voltage. Its magnitude is given by the following equation:

$$V_p = \frac{|q| N_a}{2\epsilon} a^2$$

9. There are three parameters for JFET: transconductance, ac drain resistance, and amplification factor. Amplification factor is the product of transconductance and ac drain resistance.
10. There are three ways to bias JFET, that is, keeping the gate negative w.r.t. source. JFET can be biased using self-bias, voltage divider bias, and source bias.
11. MOSFET are also unipolar devices, which are of practical importance for large integrated circuits and microprocessors. MOSFET are of two types: n -channel and p -channel. n -channel has

slightly doped p -substrate and p -channel has slightly doped n -substrate. MOSFET have silicon dioxide layer that keeps the gate insulated from the semiconductor.

12. Both the n -channel and p -channel MOFETs are further classified as enhancement and depletion types.
13. In feedback circuits, a part of output signal is fed back to the input circuit. Feedback can be of two types: negative and positive. In negative feedback, the gain of the amplifier is reduced as the applied signal and feedback signal are out of phase with each other. In positive feedback, the gain of amplifier is increased as the applied signal and feedback signal are in phase with each other.
14. The gain A and A_f for amplifier is given by the following equation:

$$A = \frac{V_o}{V_i}$$

$$A_f = \frac{V_o}{V_i} = \text{gain with feedback}$$

15. The negative feedback circuits are of four types: voltage series/shunt feedback and current series/shunt feedback.
16. Oscillators use positive feedback circuits. An oscillator generates alternating voltage when the circuit is fed energy from a dc source. Oscillator circuit consists of tank circuit, amplifier, and feedback circuit. Tank circuit consists of capacitor and inductor. Hence, in tank circuit, the electric energy is converted to magnetic energy and vice versa, which gives rise to LC oscillations.
17. For the oscillator action to occur, the gain should be > 1 , when the oscillator is switched on. The loop gain should gradually decrease to unity.
18. Hartley, Colpitt, and tuned collector oscillators fall under the category of LC oscillators, whereas phase shift and Wien bridge oscillators are RC oscillators.

Lasers

Keywords: spontaneous emission, stimulated emission, ruby laser, He–Ne laser, coherence, monochromaticity, population inversion, optical pumping

Learning Objectives

- ◆ To know about the fundamental principle of lasers
- ◆ To get an understanding of Einstein coefficients
- ◆ To learn about the ground, excited, and metastable states
- ◆ To get insight about spontaneous and stimulated emission/absorption
- ◆ To learn about population inversion and optical pumping
- ◆ To know about He–Ne laser
- ◆ To understand the principle and working of ruby lasers
- ◆ To get insight about principle and working of CO₂ laser
- ◆ To learn about the working and principle of Nd: YAG laser
- ◆ To get insight of the principle of holography
- ◆ To learn about the properties of lasers such as directionality, monochromaticity, coherence, etc.

Quantum mechanics defines the discrete energy states and also states that emission/absorption of energy takes place in discrete packets of energy known as photons. In 1917, Einstein predicted about spontaneous and simultaneous emissions; with the help of quantum theory, he was able to explain them. In 1954, Townes used simulated emission to construct microwave amplifier, that is, microwave amplification by stimulated emission of radiation (MASER). Further, Townes and Schawlow extended the principle of MASER to optical region and LASER was developed, that is, light amplification by stimulated emission of radiations. Therefore, this chapter deals with LASER and phenomena associated with it.

14.1 Preliminary Idea about Transitions

Basically, three types of transitions occur in an atomic system with discrete energy states. Consider two allowed energy states for an atomic system. The lower energy level is denoted by E_1 and the higher energy level is denoted by E_2 as shown in Figure 14.1.

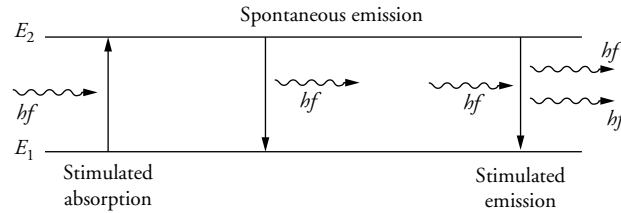


Figure 14.1 The three transitions between energy emission levels.

The three processes are summed up as follows:

- 1. Stimulated absorption:** The atom in its lower energy state is also known as ground state. By absorbing radiation of photon energy hf , it raises to higher energy level E_2 . The energy difference between two energy levels is $E_2 - E_1$. This process is known as induced absorption. B_{12} is the probability coefficient atom to go from ground state to excited state.
- 2. Spontaneous emission:** An atom in higher excited state can de-excite by emitting a photon with energy hf , which equal to energy difference between E_2 and E_1 . This process in called spontaneous emission. A_{21} is the probability coefficient for spontaneous emission from excited state to ground state.
- 3. Stimulated emission:** When a photon of energy hf causes transition of atom from excited state to ground state, then it is called stimulated emission. We get a coherent beam light in this case because the emitted photon is in coherence with the incident photon. The coefficient for stimulated emission in B_{21} .

14.1.1 Mathematical Analysis

Usually, the probability that the atom will undergo a transition depends on the rate at which photons interact with atom.

Let us suppose $U(f)$ is the energy density of atom in its ground state. Then, the probabilities are given as follows:

- (i) Probability to go in higher state:

$$P_{1 \rightarrow 2} = B_{12} U(f) \quad (1)$$

- (ii) Probability to go in ground state (via spontaneous and stimulated emission):

$$P_{2 \rightarrow 1} = A_{21} + B_{21} U(f) \quad (2)$$

At thermal equilibrium, the transitions from ground level to higher level is same as that from excited state to lower ground level, that is,

$$B_{12} U(f) = A_{21} + B_{21} U(f) \quad (3)$$

Let $N_1 \rightarrow$ number of atoms in ground level

$N_2 \rightarrow$ number of atoms in excited level

Then Eqn. (3) becomes

$$N_1 B_{12} U(f) = N_2 A_{21} + N_2 B_{21} U(f)$$

$$U(f) = \frac{N_2 A_{21}}{N_1 B_{12} - N_2 B_{21}}$$

$$U(f) = \frac{A_{21}}{(N_1/N_2)B_{12} - B_{21}} \quad (4)$$

According to Boltzmann's law the ratio of atoms in ground state to the atoms in excited state is given by

$$N_1/N_2 = e^{(hf/k_B T)} \quad (5)$$

where k_B is Boltzmann's constant and T is absolute temperature.

Substitute Eqn. (5) in Eqn. (4),

$$U(f) = \frac{A_{21}}{e^{(hf/k_B T)} B_{12} - B_{21}} \quad (6)$$

According to Planck's theory of black body radiation, the energy density is given by

$$U(f) = \frac{8\pi hf^3}{c^3 (e^{hf/k_B T} - 1)} \quad (7)$$

Comparing Eqs (6) and (7)

$$B_{12} = B_{21} = B \quad (8a)$$

and

$$\frac{A_{21}}{B} = \frac{A}{B} = \frac{8\pi hf^3}{c^3} \quad (8b)$$

From Eqn. (8a), it can be concluded that the probability for stimulated absorption and stimulated emission are the same. Eqs (8a) and (8b) are known as Einstein's relations. A and B are known as Einstein's coefficients.

By looking at Eqs (6)–(8), it can be noted that the stimulated emission and spontaneous emission compete with each other. The process of amplification takes place only when the stimulated emission is more. The principle of stimulated emission is used for the amplification in lasers, and this is discussed in the following section.

14.2 Lasers and their Principle

The principle of LASERS is based on stimulated emission of light radiations as shown in Figure 14.2.

Let us assume that a photon of frequency f passes through a medium consisting of large number of atoms. The incident photon may stimulate some atom to go to higher energy state. Then, the atom may return to its ground state by emitting a photon along with the incident photon. Hence, one photon produces two photon, two photons will produce four photons, and so on. Therefore, only

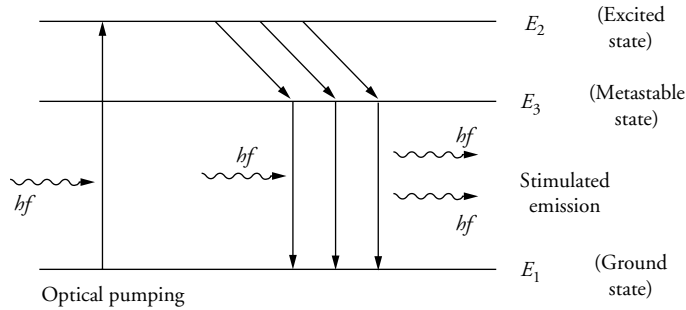


Figure 14.2 Schematic showing LASER action.

a single incident photon can produce a chain of photons. This chain of photons make very intense beam; hence, the beam is amplified. Conclusively, the following two conditions for laser action need to be followed:

- 1. Optical pumping:** This is the process by which the number of atoms in excited state is more than the number of atoms in ground state.
- 2. Population inversion:** Usually, three levels are required for laser action. Ground level, excited level, and metastable level (in between ground and excited level). Population inversion is the accumulation of more atoms in excited state than in ground state. Metastable state has an average lifetime of 10^{-3} sec.

The transition from $E_2 \rightarrow E_3$ is allowed, but $E_2 \rightarrow E_1$ is forbidden. Through the optical pumping, the atoms from ground state are excited to higher energy level E_2 . The atoms undergo spontaneous emission and come to level E_3 from E_2 . The average lifetime of E_2 is only 10^{-8} sec. Hence, the spontaneous emission is fast and atoms come to E_3 level, where it can stay for 10^{-3} sec. Hence, at the E_3 level, the atoms get accumulated. Or, in other words, the phenomenon of population inversion has taken place. When the atom returns to ground level E_1 from metastable E_3 level, it emits a photon of frequency $f = \left(\frac{E_3 - E_1}{h} \right)$. This photon further stimulates some atom to release photon. This process continues, and hence intense and amplified photon beam is obtained. This beam is also known as laser beam.

14.3 Properties of Lasers

Laser beam is intense, coherent, and monochromatic. Moreover, it is an electromagnetic beam, which means it has electric and magnetic components perpendicular to each other as well as in the direction of propagation of light. The properties of lasers are discussed below.

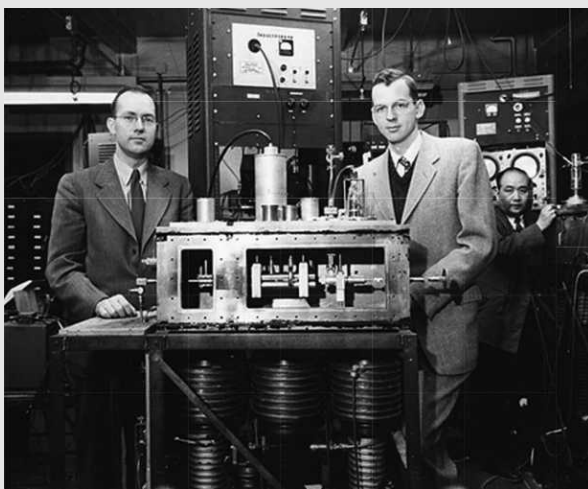
14.3.1 Monochromaticity

In laser light, all the photons are of the same frequency and hence energy hf . Therefore, it produces monochromatic light beam with single spectral color. Hence, laser transitions involve well-defined energy levels. Laser is generated inside a laser cavity. The laser oscillations sustain on resonant frequencies inside the cavity, and hence laser line gets narrowed down. Hence, the narrower the linewidth, the higher the monochromaticity of laser light.

Charles Hard Townes was born in Greenville, South Carolina, on July 28, 1915, to Henry Keith Townes, an attorney, and Ellen (Hard) Townes. He completed his BSc in Physics and BA in Modern Languages from Furman University. Townes did MA Physics at Duke University in 1936. After that, he graduated from California Institute of Technology, where he obtained his PhD in 1939. Dr Townes worked extensively in designing radar-bombing systems during World War II. Then, he turned his focus toward microwave technique for radar research to spectroscopy. He was appointed at Columbia University in 1948, and he continued his research in microwave physics. He studied the interactions between microwaves and molecules.

Dr Townes conceived the idea of the

maser in 1951, and furthermore his group began working on a device using ammonia gas as the active medium. In 1954, the first amplified electromagnetic waves by stimulated emission were obtained. Dr Townes and his students coined the word "maser" for this device, which means for microwave amplification by stimulated emission of radiation. In 1958, Dr Townes and his brother-in-law, Dr A.L. Schawlow, a professor at Stanford University worked on optical and infrared masers, or lasers (light amplification by stimulated emission of radiation).



**CHARLES TOWNES AND JAMES GORDON
WITH THEIR SECOND MASER DEVICE, 1955**

14.3.2 Coherence

An excited atom comes to ground state by emitting photon of energy corresponding to the difference in two states, that is,

$$f = \left(\frac{E_2 - E_1}{h} \right) \quad \left[\begin{array}{l} E_2 \rightarrow \text{energy of excited level} \\ E_1 \rightarrow \text{energy of ground level} \end{array} \right]$$

This type of emission is called spontaneous emission, which is usually characterized by the lifetime of excited state. As explained earlier, when another photon of the same frequency induces the emission of an atom, then two photons are emitted. Hence, this phenomenon of stimulated emission leads to the overall gain of output of light. In this process, a group of photons is created, and they have fixed phase relationships with each other. Before proceeding, we should understand the coherence of light. Two sources of light are coherent, when there is a fixed or constant phase relationships between their wave trains. Similarly, two photons are said to be phase or coherence when the crest of wave emitted by one photon falls on the crest of wave emitted by second photon. Hence, the laser beam is having

property of coherence due to fixed phase relationships between photons in the active medium. In the case of spontaneous emission, no relationship is found between the photons, and hence no net amplification is obtained. Moreover, under normal conditions, the atoms are more in ground state, whereas stimulated emission demands population inversion. Laser light is coherent due to additive phase relationship between photons that usually contribute to its high brightness. Ordinary light source is incoherent in nature as shown in Figure 14.3. Laser light has in-phase wave trains, whereas ordinary light has out-of-phase wave trains.

There are two types of coherence: (i) spatial and (ii) temporal.

Spatial coherence represents the correlation between waves at different places at same time, whereas temporal coherence represents the correlation between waves at different time but at same place. For example, we take two points on wave front [for time = 0]. The phase difference between these two points remains the same even after some lapsed time interval, then this wave exhibits perfect coherence between these points. Hence, the wave is said to possess spatial coherence between these two points. Spatial coherence represents uniphase wave fronts as well as directionality. In contrast to this, consider a point on wave front. Let $d\phi$ be the phase difference for same point at time t_1 and t_2 , respectively, that is, $t_1 - t_2 = dt$ represent phase difference $d\phi$. If the phase difference corresponding to all is always the same, then it is known as temporal coherence. But it is important to note that partial and spatial coherence are independent of each other.

We can also analyze temporal coherence as explained to combine the wave at time t_1 with its delayed wave at t_2 . Then Δt is the duration over which the two waves will produce interference pattern, Δt represents coherence time. Corresponding, the coherence length may be estimated as follows:

$$l_c = c \Delta t \quad (9)$$

The coherence length is inversely proportional to the band width (Δf):

$$\Delta t \propto \frac{1}{\Delta f} \quad (10)$$

Hence, the narrower the frequency band width, the higher the temporal coherence. If multiple longitudinal modes are supported by lasers, then the laser output exhibits perfect spatial coherence. But the temporal coherence may be partial. The longitudinal modes are spaced at a distance of $(c/2L)$. L is the effective length of resonator and c is the velocity. The following relations give the relation between number of modes (N), coherence length (l_c), and resonator length (L) as follows:

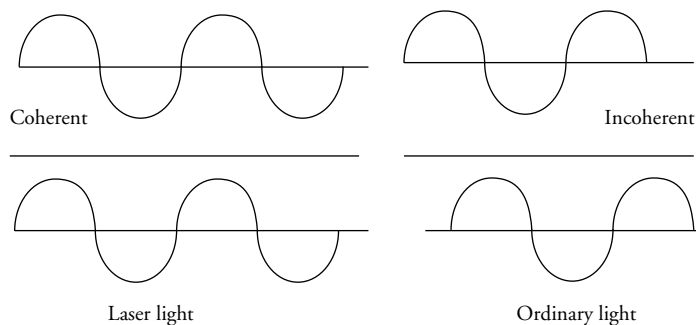


Figure 14.3 (a) Laser light and (b) ordinary light.

$$N = \frac{L}{l_c} \quad (11)$$

The coherence length is the length over which the energy in two waves remains constant. Also for spatial coherence, the sphere and plane waves give better output. By using spatial filters, the spatial coherence can be increased for example, putting a small pinhole in condenser lens. When light comes out of the pinhole, then with increase in distance, the wave front becomes plane. Ordinary light produces light on time scale of about 10^{-8} sec. Hence, the coherency cannot be easily obtained.

14.3.3 Directionality

Ordinary source of light gives energy and radiation in all the directions. Hence, by placing an aperture in front of ordinary light beam, a directional beam is obtained. But lasers give directional output of energy. Laser cavity has mirrors at both the ends; hence, the beam travels back and forth, which increases its beam intensity due to stimulated emission of photons. Only the photons that travel along the cavity are reflected back. The off-axis photons do not contribute to the total intensity of beams. Hence, the laser beam is highly collimated. Collimation refers to the degree up to which the beam remains parallel to cavity axis, or in other words the divergence is zero. Hence, the directionality is expressed in terms of “full-angle beam divergence.” It is defined as twice the angle which the outer edge of beam makes with the axis of beam. As the divergence of beam is related to diffraction effects, the angular spread is given by

$$\theta = \frac{\beta\lambda}{D} \quad (12)$$

where β is coefficient depending on amplitude distribution diverge and diameter of beam. D is the aperture diameter, and λ is the wavelength of light used. Usually, the lasers exhibit 2θ (beam divergence) less than 10^{-3} radian. For an ordinary light, 2θ can be more than 10^{-3} radian for every kilometer it traverses.

Equation (12) also demonstrates that divergence increases with wavelength and decreases with beam diameter. Hence, a large diameter beam has small divergence. For a Gaussian beam, the half-angle divergence is given by the following relation:

$$\theta_h = \frac{w_0}{\pi\lambda} \quad (13)$$

where w_0 represents beam waist radius. Hence, due to small divergence of laser beams, the planetary distances could be measured with great accuracy.

14.3.4 Intensity and Beam Quality

The output of laser can go up to 10^9 W for solid-state laser. It is defined as power that is emitted per unit solid angle (Ω). The relation between solid and planar angle is given by the following equation:

$$\Omega = \frac{\pi\theta^2}{4} \quad (14)$$

For 1 milli-radian, the solid angle is given by

$$\Omega = \left(\frac{\pi}{4} \right) (1 \text{ mrad})^2 = 0.8 \times 10^{-6} \text{ sterad}$$

For a laser with 1 mm output diameter and 1 mW output, the radiance can be calculated as

$$\text{Radiance} = \frac{\text{Power}}{\text{Area of beam} \times \text{area of solid angle}}$$

$$\text{Radiance} = \frac{10^{-3} \text{ W}}{(0.785 \times 10^{-6}) \times (0.8 \times 10^{-6})} = 1.6 \times 10^9 \text{ W/m}^2 \text{sr}$$

The radiance of sun is $10^6 \text{ W/m}^2 \text{ steradian (sr)}$. Hence, laser emits more focused and bright light as compared to the radiations of sun. As far as the quality of beam is concerned, the following properties of laser come into action:

- (i) Laser can be focused more tightly due to less diffraction.
- (ii) Figure of merit is necessary to determine the characteristics of beam. Hence, beam propagation constant M^2 was developed in 1970. According to ISO (11146), M^2 is defined as beam parameter product (BPP) divided by λ/π .

$$M^2 = \frac{\theta w_o}{(\lambda / \pi)} \quad (15)$$

θw_o is called beam parameter product, and it is the product of laser beam divergence angle and beam waist w_o (diameter of beam at its narrowest point). M^2 can also be defined as the ratio of BPP of original beam to that of Gaussian beam $M^2 \geq 1$ for TEM_{00} laser beam. But for poor-quality beam, it can go up to several hundreds. For single-mode TEM_{00} beam, M^2 is always 1.

The strength of early lasers was measured in Gillette's, which was the number of blue razor blades a beam could puncture. In 1960, the first working laser was actually demonstrated by Theodore Maiman at the Hughes Research Laboratories.

14.4 Types of Lasers

The following section explains the various kinds of lasers depending upon their active medium pumping mechanism and levels.

14.4.1 Ruby Laser

This was the first laser that was successfully fabricated by T.H. Maiman in 1960. Basically, it is a solid-state laser. To understand this laser, the meaning of "ruby" must be understood. Ruby is a crystal of aluminum oxide (Al_2O_3) in which some aluminum ions (Al^{3+}) are replaced by chromium (Cr^{3+}) ions. Usually, 0.05 percent Cr_2O_3 is the threshold value of doping. The red color of ruby laser is due to chromium ions. Usually, Al_2O_3 atoms do not participate in lasing action. It only acts as host for

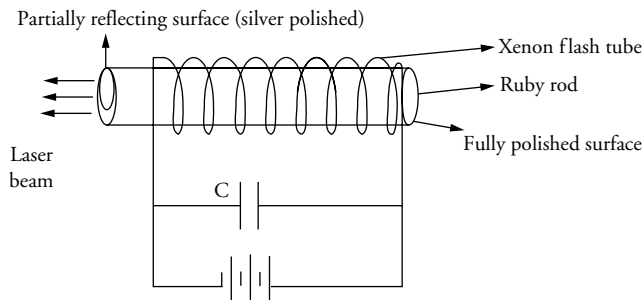


Figure 14.4 Schematic of ruby laser.

chromium ions. The ruby crystals are grown in rods of length 2–30 cm and diameter between 0.5 and 2 cm. The end faces of this laser are made parallel for coherent output. One face is fully reflecting, whereas the second face is partially reflecting. Hence, the faces are polished with Ag as per the desired surface. These faces form the end of resonant cavity. During the operation of this laser, very high temperature is produced. Hence, the ruby rod is placed inside liquid nitrogen ($T = 77$ K) in order to keep the rod cool.

Active medium is chromium ions and optical resonator cavity system is formed with the help of completely and partially silvered faces at the end. For pumping, helical xenon flash lamp is used. Ruby rod is placed inside the xenon lamp, so that population inversion can be obtained using optical pumping. Furthermore, the xenon lamp is connected to capacitor through which it can discharge energy frequently. Almost a few thousand joules of energy is released in few milliseconds, which results in Megawatt power output for the laser. The schematic of ruby laser is shown in Figure 14.4.

Ruby laser is basically a three-level laser system. E_1 is the ground level, E_2 and E_3 are the excited levels, and E_4 is the metastable level. The optical pumping raises the chromium ions to E_2/E_3 level from ground level through stimulated absorption. Basically, E_2 and E_3 are very close to each other, and therefore considered as a single band. These levels are also known as pumping levels, as they are responsible for the lasing action. Figure 14.5 illustrates the lasing action.

When atom absorbs 6600\AA and 4000\AA wavelength radiation, then it excites to level E_2 and E_3 respectively. During interaction with crystal lattice, the Cr^{3+} ions lose some energy and decay to metastable state E_4 through non-radiative transitions (or no photons). The lifetime of Cr^{3+} in metastable state is 0.003 sec; hence, they can stay in metastable state for longer time periods. After the population inversion is achieved, some of the chromium may come back to ground level via spontaneous

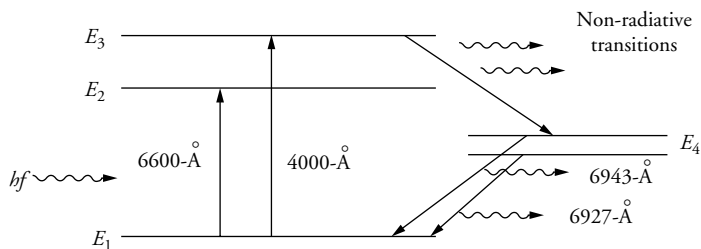


Figure 14.5 Lasing action and energy-level diagram.

emission by emitting photon of wavelength 6943\AA . This photon will travel through the ruby rod and gets reflected between the end reflecting plates. It will get reflected until it stimulates some excited atom, thereby stimulating it to emit a coherent photon. Hence, the reflections result in stimulated emission resulting in net amplification of laser light. These emitted photons will stimulate more and more chromium ions, and hence series of photons are produced. Until the flash lamp is active, it will keep on maintaining population inversion, and therefore lasing action. Therefore, output is pulsed in ruby laser.

Ruby laser produces very high output of radiations (10^4 – 10^6 W) with wavelength 6943\AA . 6927\AA photons do not contribute to lasing action. The ruby laser requires high power pumping source and the output is not continuous. Further, these lasers find potential applications in holography, welding as well as cutting.

Lasers we come across today operate at a low level of power. Lasers in DVD players will be around 5–10 mW, CD-ROMs drives will be around 5 mW, and recordable CD drives will be around 100 mW. The most powerful laser is in California and recorded at 1.25 PW.

14.4.2 He–Ne Laser

It was the first gas laser consisting of 90 percent helium and 10 percent neon gas. This gas mixture is the active medium. Figure 14.6 shows the schematic of He–Ne laser. The tube is made up of glass consisting of narrow capillary tube at the center. The electrical discharge is directed through this capillary tube. The cross-section of bore is small in order to produce high current densities. The high reflecting mirror and less reflecting mirror are placed opposite to each other, and they form resonant cavity. The tube consists of small metallic cathode and anode. The direction of current is through cathode to anode. The gas reservoir provides the gas that maintains the tube pressure as well as the leakage losses inside the tube. The He:Ne ratio can vary from 5:1 to 20:1.

For optical pumping, electrical discharge is used. A high-power incandescent lamp or flash lamp is used for population inversion. Upon passing discharge through gaseous mixture, electrons are accelerated, which collide with helium atoms and raise them to higher energy levels as shown in Figure 14.7.

When helium atoms move through the lasing medium, then they collide with neon atoms. Upon collision with neon atoms, the helium atoms transfer some of their energy to neon atoms. Hence, the neon atoms get raised to excited state/metastable state, and furthermore the population inversion is achieved. Therefore, pumping source excites helium atom that transfers its energy to neon, and neon is involved in lasing action.

The transition occurring from $E_4 \rightarrow E_7$ produces infrared photon with wavelength $3.39\ \mu\text{m}$. The transition from $E_4 \rightarrow E_8$ produces more energetic photon corresponding to wavelength $632.8\ \text{nm}$. This transition corresponds to red-light of He–Ne laser. $E_5 \rightarrow E_8$ transition also produces as photon of

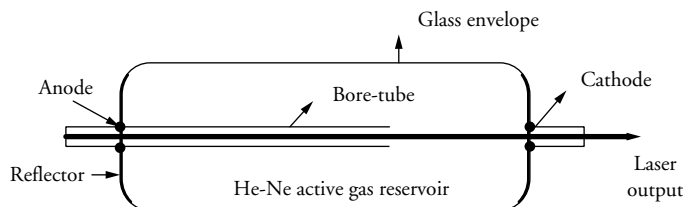


Figure 14.6 He–Ne laser tube.

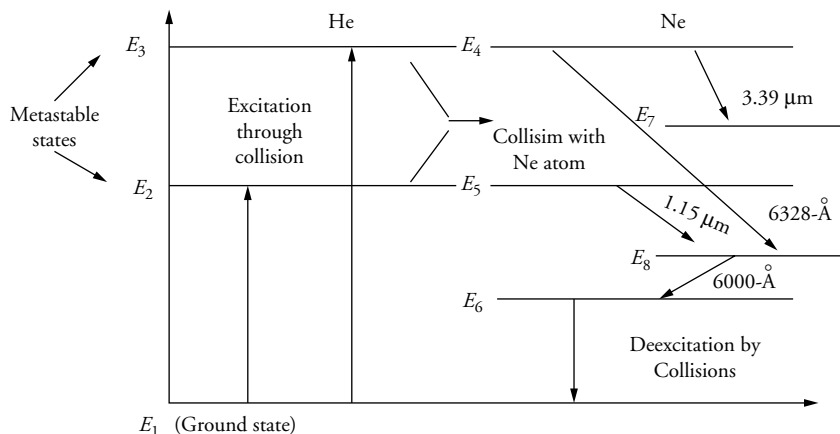


Figure 14.7 Energy-level diagram for He–Ne laser.

wavelength $1.15 \mu\text{m}$ is infrared region of spectrum. When the neon atom drops from $E_8 \rightarrow E_6$, then photon is emitted corresponding to wavelength 6000\AA . Hence, the wavelength 632.8 nm is the main output of He–Ne laser, but the photons of 1.15 and $3.39 \mu\text{m}$ can also be obtained if desired He–Ne laser is a low-gain system, but good coherence is obtained in it. The tube length is $10\text{--}100 \text{ cm}$ and lifetime can go up to 2000 h , He–Ne laser require high power in but and leakage losses are also predominant. In order to avoid the unwanted photons of undesired wavelengths ($1.15 \mu\text{m}$, $3.39 \mu\text{m}$), the mirrors are coated with high reflectance of 632.8 nm . A magnet may also be placed near the laser tube that can provide suppression of infrared wavelength. This makes, the structure of He–Ne lasers complex sometimes.

Lasers are grouped into classes Class of 1–5 that indicate level of dangers. Reaching level 5 means permanent blindness as well as burning skin. Sometimes, the laser light seems to be harmless, but the continuous contact can cause skin injuries.

14.4.3 CO_2 Laser

CO_2 lasers were invented by Kumar Patel of Bell Labs in 1964. These CO_2 lasers produce continuous output and produce infrared light. The active medium is inside a tube, whose end mirrors are silvered. One mirror is fully silvered for high reflectivity and other is partially silvered for obtaining power output. The windows of lasers are made of either germanium or zinc selenide. Diamond windows can also be used for these lasers. The active laser medium consists of CO_2 (10–20 percent), nitrogen (10–20 percent), hydrogen (H_2), and xenon (Xe). Remaining component is helium (He_2).

In CO_2 laser, the transitions occur between a rotational sublevel of vibrational level and rotational level of lower vibration state. By passing a gas discharge through the medium, and outputs are produced at 10.6 and $9.6 \mu\text{m}$. N_2 gas increases the efficiency of CO_2 laser. In this laser also N_2 gets excited which excites CO_2 molecules. Hence, CO_2 are lasing atoms. Nitrogen is excited first, and it holds its excited state for a long time. When they collide with CO_2 molecule, they are raised to higher excited levels and population inversion is achieved. Figure 14.8 shows the energy-level diagram for CO_2 laser.

N_2 is an excellent partner for CO_2 as the energy difference between ground level of nitrogen and excited state of nitrogen is almost equal to that required for exciting CO_2 molecule. The laser light is so powerful as the gas is surrounded by mirrors, which reflects a part of light passing through the tube. This reflection causes more nitrogen molecules excited, which ultimately excites more CO_2 molecule, thereby

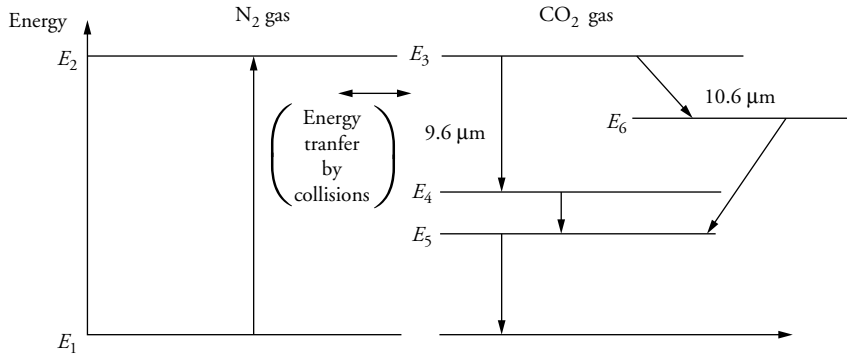


Figure 14.8 Energy-level diagram for CO₂ laser.

leading to population inversion. Hence after a certain intensity, when it comes out of laser, the output is quite high. This gives continuous power output, which is most powerful among gas lasers. This laser can be used for cutting, drilling, and welding applications. Due to its low attenuation in atmosphere, it can be used in optical radar systems, etc. These lasers may also be used for engraving and surgical procedures.

Cold lasers are used for acupuncture, engraving, detect and killing tumors. There is a new laser that can detect cancer and diabetes called the “breathalyzer.” Lasers are used for hair removal, eye surgeries, and tattoo removal. Clear scan laser technology can rid you of vascular lesions, spider veins, and skin discolorations.

14.4.4 Nd: YAG Lasers

It is a solid-state laser with four levels. The active medium is neodymium (Nd) and Yttrium aluminum garnet (Y₃Al₅O₁₂). It was developed by J.E. Geusic, L.G. Van Viter and H.M. Marces in 1964. Nd³⁺ ions are present as substitutional impurities on lattice sites being occupied by yttrium ions and YAG acts as host. The optical pumping is done by krypton arc lamp and sometimes by xenon lamp also.

YAG does not directly participate in lasing action. When Nd³⁺ is present inside the YAG lattice, then it is under the effect of crystal field exhibited by surrounding atoms. The crystal field interacts with impurity Nd³⁺ atom in various ways depending on structure, strength, and symmetry. For free Nd³⁺, some transitions are forbidden; but when they are under the influence of field, those transitions become allowed. Figure 14.9 represents the schematic of Nd: YAG laser. Figure 14.10 represents the energy-level diagram for Nd: YAG laser.

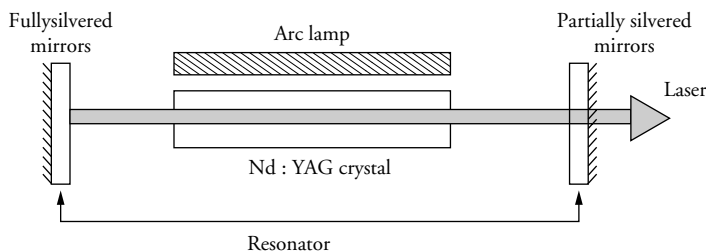


Figure 14.9 Nd: YAG laser.

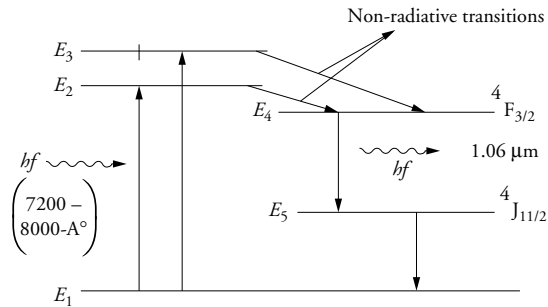


Figure 14.10 Energy-level diagram for Nd:YAG lasers.

The wavelength of $7200\text{--}8000\text{\AA}$ excites the atoms from ground state to higher state. From E_3 and E_2 states, they come back to E_4 level via nonradiative transitions. But E_4 state is metastable state. Hence for E_4 level, the population inversion is achieved. When the Nd comes from upper metastable level (E_4) to lower metastable level (E_5), then photon of wavelength $1.06\ \mu\text{m}$ is emitted, which is the laser output.

14.5 Application of Lasers

1. It can be used in metallurgical applications because lasers produce localized heating that helps in welding and cutting proposes.
2. Laser beams are used in under water communication due to high coherent nature of optical photons.
3. It is also helpful in finding distance between stars and planets.
4. Lasers are used for skin and body resurfacing, cancer diagnosis, and dental surgeries.
5. Cooling of atoms to externally low temperatures by slowing down atoms is also done by lasers. "Optical molasses" is the term used for cooled atoms.

14.6 Holography

Holography is a technique for the re-construction of 3-D image for an object. Holography involves the following stages:

1. Recording the image of object using interference of light waves from the source and that reflected from object.
2. Using the diffraction of waves, the image of object is to be reconstructed.

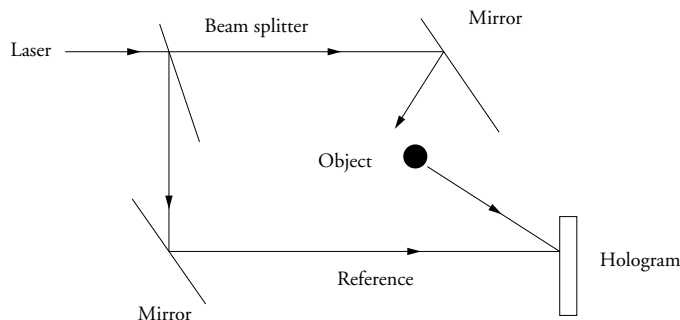


Figure 14.11 Principle of holography.

Figure 14.11 shows the principle of holography. Light waves scattered from the object and from the beam derived from laser source expose the photographic plate. These two beams are highly coherent, and they produce interference pattern. This pattern is recorded in the photographic emulsion and forms a hologram. The reference beam light diffracts through the hologram, but most of it passes straight. Hologram is window for object scene. After illuminating it with laser light, it can be viewed with different angles.

SUMMARY

The chapter deals with lasers, that is, light amplification by stimulated emission of radiations. Stimulated emission, optical pumping, and population inversion are prerequisites for lasers. A_{21} , B_{21} and B_{12} are the Einstein's coefficients. By optical pumping, the atoms from ground state are excited to excited state. This further yields population inversion, that is, accumulation of more atoms in excited state than ground state. There is a metastable state between ground and excited state, having an average lifetime of 10^{-3} sec. Lasers are monochromatic and coherent monochromaticity means the photons are of same frequency. Two types of coherence are there for lasers, that is, spatial and temporal. Spatial coherence represents the correlation between waves at different places at same time, whereas temporal coherence represents the correlation between waves at different time but same place. Lasers are also very intense and directional in nature. Various kinds of lasers have been studied depending on the type of active medium used. For ruby lasers, aluminum (Al^{3+}) and chromium (Cr^{3+}) are used as active medium, and Cr^{3+} ions give red color to lasers. The output is produced at 6943 \AA . For He-Ne laser, 90 percent helium and 10 percent neon are used as active medium, although neon is involved in lasing action. The output occurs at 632.8 nm for He-Ne laser. CO_2 lasers have CO_2 , N_2 , H_2 , Xe , and He as active medium, and the outputs are produced at 10.6 and $9.6 \mu\text{m}$. For Nd:YAG lasers, active medium is neodymium and yttrium aluminum garnet. Output is produced at $1.06 \mu\text{m}$. Holography technique is used to construct 3-D image for any object.

SOLVED PROBLEMS

Q.1: Sodium D_2 line has coherence length of 2.5 cm . Obtain the coherence time.

Ans: Coherence time $(\Delta t) = \frac{l_c}{c}$

Here, $l_c = 2.5 \text{ cm}$ and $c = 3 \times 10^8 \text{ m/s}$

$$\Delta t = \frac{2.5 \times 10^{-2}}{3 \times 10^8} \text{ sec}$$

$$\Delta t = 0.833 \times 10^{-10} \text{ sec}$$

$$\Delta t = 8.33 \times 10^{-11} \text{ sec}$$

Q.2: The aperture of laser light is 1 cm and wavelength 5890 \AA . This laser light is sent to moon having a distance of $4 \times 10^8 \text{ m}$ from earth. Obtain the (i) angular spread and (ii) areal spread upon reaching the moon's surface.

Ans: (i) Angular spread is given by

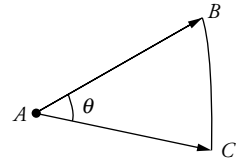
$$\theta = \frac{\lambda}{d}$$

Here, $d = 1 \text{ cm}$ and $\lambda = 5890 \text{ \AA}$

$$\theta = \frac{5890 \times 10^{-10}}{10^{-2}}$$

$$\theta = 5890 \times 10^{-8} \text{ rad}$$

$$\left[\begin{array}{l} \lambda = d \sin \theta \\ \text{For small } \theta \\ \sin \theta \approx \theta \end{array} \right]$$



(ii) Areal spread = πr^2

$$= \pi \left(\frac{BC}{2} \right)^2$$

We will calculate BC first:

We know

$$\text{angle} = \frac{\text{arc}}{\text{radius}}$$

$$\theta = \frac{BC}{\text{radius}}$$

Here, $\theta = 5890 \times 10^{-8} \text{ rad}$ and $\text{radius} = 4 \times 10^8 \text{ m}$

$$BC = 5890 \times 10^{-8} \times 4 \times 10^8$$

$$BC = 23560 \text{ m}$$

Hence, areal spread

$$= \frac{\pi}{4} \times (23560)^2$$

$$\text{Areal spread} = 4.35 \times 10^8 \text{ m}^2$$

Q.3: Obtain the intensity of laser beam with 20 mW power and diameter of 1.2 mm. (Assume the intensity to be uniform across the beam.)

Ans:

$$\text{Power } P = 20 \text{ mW} = 20 \times 10^{-3} \text{ W}$$

$$\text{diameter } d = 1.2 \text{ mm} = 1.2 \times 10^{-3} \text{ m}$$

$$\text{Intensity} = \frac{\text{Power}}{\text{Area}} = \frac{20 \times 10^{-3}}{\pi \left(\frac{d}{2}\right)^2}$$

$$\text{Intensity} = \frac{20 \times 10^{-3} \times 4}{3.14 \times (1.2 \times 10^{-3})^2}$$

$$\begin{aligned} \text{Intensity} &= 17.692 \times 10^{-3} \times 10^6 \\ &= 17692 \text{ W/m}^2 \end{aligned}$$

$$\text{Intensity} = 17.692 \text{ kW/m}^2$$

Q.4: Calculate the intensity for laser beam if it focuses on an area equal to λ^2 for ruby laser ($\lambda = 6940 \text{ \AA}$), given the laser radiates energy at a rate of 2 mW.

Ans: $P = 2 \text{ mW} = 2 \times 10^{-3} \text{ W}$

and $\lambda = 6940 \text{ \AA} = 6940 \times 10^{-10} \text{ m}$

Hence,

$$\begin{aligned} \text{Area} &= \lambda^2 \\ &= (6940 \times 10^{-10})^2 \\ &= 48163600 \times 10^{-20} \text{ m}^2 \end{aligned}$$

$$\begin{aligned} \text{Intensity } (I) &= \frac{\text{Power}}{\text{Area}} \\ &= \frac{2 \times 10^{-3} \text{ W}}{48163600 \times 10^{-20} \text{ m}^2} \end{aligned}$$

$$\begin{aligned}
 &= \frac{2 \times 10^{17}}{48163600} \\
 &= \frac{20000000 \times 10^{10}}{48163600} \\
 &= 0.4152 \times 10^{10} \text{ W/m}^2 \\
 &= 4.152 \times 10^9 \text{ W/m}^2
 \end{aligned}$$

Q.5: A ruby laser emits pulse of 2 J and wavelength 6940 \AA . Obtain the minimum number of chromium Cr^{3+} ions in ruby.

Ans: $E = 2 \text{ J}$

and $\lambda = 6940 \text{ \AA}$

We know

$$E = nhf$$

$$E = \frac{nhc}{\lambda}$$

$$E = \frac{nhc}{\lambda}$$

$$n = \frac{E\lambda}{hc}$$

$$n = \frac{2 \times 6940 \times 10^{-10}}{6.63 \times 10^{-34} \times 3 \times 10^8}$$

$$n = 697.838 \times 10^{-10} \times 10^{34} \times 10^{-8}$$

$$n = 697.838 \times 10^{16}$$

$$n = 6.978 \times 10^{18}$$

Q.6: The power of a laser beam is 30 mW. It has an aperture of 3×10^{-3} m emitting wavelength of 7200 \AA . The beam is focused with lens of focal length 0.3 m. Obtain the areal spread of image and line spread.

Ans:

$$P = 30 \times 10^{-3} \text{ W}$$

$$d = 3 \times 10^{-3} \text{ m}$$

$$\lambda = 7200 \text{ \AA}$$

$$f = 0.3 \text{ m}$$

$$\text{Angular spread } \theta = \frac{\lambda}{d}$$

$$\theta = \frac{7200 \times 10^{-10}}{3 \times 10^{-3}}$$

$$= 2400 \times 10^{-7}$$

$$= 2.4 \times 10^{-4} \text{ rad}$$

The line spread is given by the product of angular spread and focal length:

$$\text{Line spread} = 2.4 \times 10^{-4} \times 0.3$$

$$= 0.72 \times 10^{-4} \text{ m}$$

OBJECTIVE QUESTIONS

1. Lasers was discovered by

- | | |
|-------------------------|-----------------------|
| (a) Einstein | (b) Newton |
| (c) Townes and Schawlow | (d) None of the above |

2. B_{12} represents the probability of transition for

- | | |
|-----------------------------------|---------------------------------------|
| (a) ground state to excited state | (b) ground state to metastable state |
| (c) excited state to ground state | (d) excited state to metastable state |

3. A_{21} represents the probability coefficient for transition from

- | | |
|---------------------------------------|--------------------------------------|
| (a) ground state to excited state | (b) excited state to ground state |
| (c) excited state to metastable state | (d) ground state to metastable state |

4. Probability to go in higher state is given by

- (a) $B_{21} U(f)$ (b) $B_{12} U(f)$
 (c) $A_{21} U(f)$ (d) None of the above

5. Probability to go in ground state is given by

- (a) $B_{12} U(f)$ (b) $B_{21} U(f)$
 (c) $A_{21} + B_{12} U(f)$ (d) $A_{21} + B_{21} U(f)$

6. The condition at thermal equilibrium.

- (a) $B_{12} U(f) = A_{21} + U(f)$ (b) $A_{21} = B_{12} U(f) + B_{21} U(f)$
 (c) $B_{12} U(f) = A_{21} + B_{21} U(f)$ (d) $B_{21} = A_{21}$

7. The Boltzmann's law states that

- (a) $\frac{N_1}{N_2} = e^{(hf/k_B T)}$ (b) $\frac{N_2}{N_1} = e^{hf/k_B T}$
 (c) $N_1 N_2 = e^{hf/k_B T}$ (d) $N_1 = \frac{N_2}{e^{hf/k_B T}}$

8. The ratio of constant A and B is

- (a) $\frac{A}{B} = \frac{c^3}{8\pi h f^3}$ (b) $\frac{A}{B} = \frac{c^3 f^3}{8\pi h}$
 (c) $\frac{A}{B} = \frac{4\pi c^3}{f^3}$ (d) $\frac{A}{B} = \frac{8\pi h f^3}{c^3}$

9. During optical pumping, the number of atoms in excited state is _____ than the number of atoms in ground state.

- (a) less (b) equal
 (c) more (d) none of the above.

10. Metastable state lies

- (a) in between ground and excited level (b) below ground state
 (c) above excited state. (d) exists as a separate entity.

11. The average lifetime of metastable state is

- (a) 10^{-15} sec (b) 10^{-10} sec
 (c) 10^{-8} sec (d) 10^{-3} sec

12. The average lifetime of excited state is

- (a) 10^{-10} sec (b) 10^{-8} sec
 (c) 10^{-13} sec (d) 10^{-3} sec

13. If metastable level is E_3 and ground state is E_1 , then the atom on returning from E_0 to E_1 will emit a photon of frequency (f):

$$(a) f = \left(\frac{E_1 - E_3}{h} \right)$$

$$(b) f = \frac{h}{(E_1 - E_3)}$$

$$(c) f = \left(\frac{E_3 - E_1}{h} \right)$$

$$(d) f = \frac{E_3}{h}$$

14. The photons in laser light have

(a) same frequency and energy

(b) different frequency and energy

(c) same frequency and different energy.

(d) different frequency and same energy

15. Higher monochromaticity of laser light is determined by

(a) broad line width

(b) energy barrier

(c) narrow line width

(d) ground state

16. Laser beam is coherent due to

(a) high amplification

(b) high monochromaticity

(c) narrow line width

(d) fixed phase relationships among the photons

17. The condition for stimulated emission is

(a) amplification

(b) optical pumping

(c) population inversion

(d) none of the above

18. Spatial coherence represents the relation between waves

(a) at same time only

(b) at same place only

(c) at different places and same time

(d) at same place and different time

19. Temporal coherence represents the relation between waves

(a) at different time but at same place

(b) at same time but different place

(c) at same time and same place

(d) at different time and different place

20. Spatial and temporal coherence are independent of each other. (Yes/No)

21. The coherence length is given by

$$(a) l_c = c / \Delta t$$

$$(b) l_c = c \Delta t$$

$$(c) D = v / \Delta t$$

$$(d) D = v \Delta t$$

22. The resonator length is given by

$$(a) N = Ll_c$$

$$(b) N = \frac{l_c}{L}$$

$$(c) N = \frac{L^2}{l_c}$$

$$(d) N = \frac{L}{l_c}$$

23. The off-axis photons also contribute to the intensity of laser beam. (Yes/No)

24. The half-angle divergence for a Gaussian beam is given by

- (a) $\theta_n = \pi\lambda w_o$ (b) $\frac{\pi\lambda}{w_o} = \theta_n$
 (c) $\theta_n = \frac{w_o}{\pi\lambda} = \theta_n$ (d) $\pi\lambda = \theta_n$

25. For 1 milli-radian angular spread of laser, then the solid angle is given by

- (a) 0.8×10^{-6} sterad (b) 1×10^{-5} sterad
 (c) 0.8×10^{-8} sterad (d) 0.9×10^{-7} sterad

26. The beam parameter is given by

- (a) $\frac{\theta}{w_o}$ (b) θw_o
 (c) $\frac{w_o}{\theta}$ (d) none of the above

27. Ruby laser contains _____ doping of Cr_2O_3 .

- (a) 0.01% (b) 0.02%
 (c) 0.05% (d) 0.5%

28. Al_2O_3 atoms do not participate in lasing action. (Yes/No)

29. To keep the ruby laser cool, the ruby rod is place inside

- (a) liquid N_2 (b) liquid H_2
 (c) liquid (He) (d) O_2

30. Ruby laser uses _____ for optical pumping.

- (a) CO_2 (b) electric discharge
 (c) plasma (d) xenon flash lamp

31. The photons contributing to lasing action of ruby laser are

- (a) 6943 Å (b) 6927 Å
 (c) both (a) and (b) (d) None of these

32. Ruby laser gives continuous output. (Yes/No)

33. He-Ne laser have composition

- (a) 10% helium and 90% neon (b) 50% helium and 50% neon
 (c) 20% helium and 80% neon (d) 90% helium and 10% neon

34. Which atom is involved in lasing action of He–Ne laser?
(a) Helium (b) Neon
(c) Both helium and neon (d) Neither helium nor neon
35. Which photons can be obtained during lasing action of He–Ne laser
(a) 632.8 nm (b) 1.15 μm
(c) 3.39 μm (d) All of these
36. The active medium of CO_2 laser consist of
(a) CO_2 (b) N_2
(c) H_2 and xenon (d) All of these
37. For CO_2 laser, the outputs are produced at
(a) 10.6 μm (b) 9.6 μm
(c) Both (a) and (b) (d) 12.8 μm
38. Yttrium aluminum garnet ($\text{Y}_3\text{Al}_2\text{O}_{12}$) is active medium for Nd: YAG laser. (Yes/No)
39. What range of wavelength is used to excite the atoms from ground to excited state in Nd: YAG laser?
(a) 7200 – 8000 Å (b) 6000 – 7000 Å
(c) 9000 – 9500 Å (d) 5500 – 6500 Å
40. Holography is technique used to construct
(a) 2-D image (b) 3-D image
(c) 1-D image (d) All of these

ANSWERS

- | | | | |
|---------|-----------|-----------|-----------|
| 1. (c) | 11. (d) | 21. (b) | 31. (a) |
| 2. (a) | 12. (b) | 22. (d) | 32. (No) |
| 3. (b) | 13. (c) | 23. (No) | 33. (d) |
| 4. (b) | 14. (a) | 24. (c) | 34. (b) |
| 5. (d) | 15. (c) | 25. (a) | 35. (d) |
| 6. (c) | 16. (d) | 26. (b) | 36. (d) |
| 7. (a) | 17. (c) | 27. (c) | 37. (c) |
| 8. (d) | 18. (c) | 28. (Yes) | 38. (Yes) |
| 9. (c) | 19. (a) | 29. (a) | 39. (a) |
| 10. (a) | 20. (Yes) | 30. (d) | 40. (b) |

Micro-Assessment Questions

1. What is stimulated emission?
2. What are lasers?
3. Give the applications of lasers. What is the basic principle of lasers?
4. What is the difference between masers and lasers?
5. List the properties of lasers.
6. What is population inversion in lasers?
7. Define optical pumping. How can it be done in ruby lasers?
8. What is coherence?
9. Differentiate between spatial and temporal coherence.
10. What is coherence time and length?
11. Which process is the backbone of lasing action of lasers?
12. Is ruby laser a three- or four-level laser?
13. Differentiate between three- and four-level laser.
14. Give the angular spread of lasers.
15. What do you understand by figure of merit?
16. Explain the beam parameters.
17. Give the source of pumping in Nd-YAG laser.
18. Which pumping is used for carbon dioxide lasers.

Critical Thinking Questions

1. What is spontaneous emission? How does it differ from stimulated emission?
2. Why lasing medium must have at least three energy levels?
3. Explain the role of neon in He-Ne lasers.
4. Give the energy-level diagram for He-Ne lasers.
5. Give the energy-level diagram for carbon dioxide lasers.
6. Differentiate between optical and electrical pumping.
7. Give the basic principle of holography.
8. How is metastable state different from excited state?
9. List the medical uses of lasers.
10. Calculate the Einstein's coefficients using probability function.
11. What is the coherence length for laser beam having frequency bandwidth of 2 kHz?

Graded Questions

1. What is the monochromaticity for light of wavelength 5,475 angstrom emitted by source having temporal coherence of 10^{-9} sec?
2. Find out the temperature at which the stimulated and spontaneous emissions for 800 nm light are equal.
3. Find out the coherence length corresponding to bandwidth of 10^7 Hz.
4. Give the energy-level diagram for Nd-YAG laser.
5. The coherence length for Na light of wavelength 5,890 angstrom is 2.94×10^{-2} m. Calculate the number of oscillations corresponding to coherence length and time.

6. With a neat labeled diagram, give the construction and working of a ruby laser.
7. Give the construction and working of He–Ne laser.
8. Give the construction and working of Nd–YAG laser. Is it three- or four-level laser?
9. Give the energy-level diagram for carbon dioxide laser.
10. Why are laser beams considered to be intense beams?
11. Describe holography.

Remember and Understand

1. Laser works on the principle of stimulated emission of radiations.
2. Population inversion is necessary for lasing action. For inducing population inversion, optical or electric pumping is carried out.
3. For a light source, the coherence length is defined as the length over which phase relationship holds good.
4. The frequency spread is inversely proportional to coherence length. This spread is attributed to Doppler broadening, natural damping, and collision broadening.
5. In ruby lasers, the lasing action is produced by chromium ions; whereas in He–Ne laser, neon atoms are responsible for lasing action.
6. Laser light is highly directional and monochromatic in nature.
7. The helium neon lasers have 90 percent helium and 10 percent neon as active medium helium atoms transfer their energy to neon atoms, and neon atoms contribute to lasing action.
8. For CO₂ laser, the active medium consist of CO₂, N₁, H₂, Xe, and He.
9. In Nd:YAG lasers, YAG does not directly participate in lasing action. Nd³⁺ ions are present as substituted impurities on lattice sites are being occupied by yttrium ions.
10. Holography is reconstruction of 3-D image for an object that records the image of objects using inter-ference of light waves.

Optoelectronics

Keywords: fiber optics, numerical aperture, step index, multimode index, semiconductor diodes, Fermi energy, quasi Fermi levels

Learning Objectives

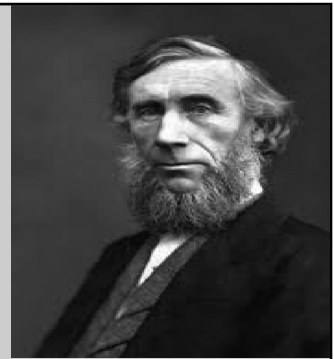
- ◆ To understand the relation of light and electricity
- ◆ To learn about optical fibers as an important part in long distance communication
- ◆ To know about the components of optical fiber, that is, core, cladding, and sheath
- ◆ To get insight of single-mode and multimode fibers
- ◆ To know about acceptance angle, acceptance cone, and numerical aperture
- ◆ To understand about various power loss in optical fibers such as Rayleigh scattering loss, microbend and macrobend losses, material loss, temperature losses, mode leaking, and mode coupling losses
- ◆ To distinguish between fiber attenuation and the attenuation coefficient
- ◆ To understand semiconductor diode lasers and its voltage compatibility with the integrated circuit
- ◆ To know about band structure and density of states
- ◆ To understand the concept of effective mass of electron as a function of wave vector k
- ◆ To get insight of Fermi–Dirac distribution.
- ◆ To understand Schawlow–Townes condition for lasers and threshold condition for sustained oscillations
- ◆ To understand the quasi-Fermi levels for semiconductors, in terms of equilibrium time between bands and the carrier scattering time
- ◆ To know about lasing action of semiconductor laser (GaAs)
- ◆ To learn about direct and indirect semiconductor

Optoelectronics combine light and electricity together in one regime. Optoelectronic include devices operating in electrical to optical regime or vice versa. The fiber optics, remote-sensing systems, and laser systems fall under the category of optoelectronics. In this chapter, we will discuss optical fibers and semiconductor diode lasers.

15.1 Introduction to Fiber Optics

Usually, the communication is through electromagnetic radiations. The electromagnetic radiations are modulated using suitable carrier waves. This communication is termed as optical communication. But optical communication has many disadvantages including small bandwidth and attenuation losses. Optical fibers have resolved this problem. The branch of physics which deals with the phenomena related to transmission of light through transparent fiber or glass is optoelectronics (John Tyndall invented optical fibers in 1870). The optical fiber has very small loss of signal, hence they are very suitable for long-distance transmission. They have more efficiency than the coaxial cable. The optical fibers are made up of polymeric plastic which are quite resistant to external disturbances. These fibers contain information that can be transmitted at microwave frequencies.

John Tyndall was born and brought up in Ireland. His father was a local constable. In 1839, Tyndall joined the Irish Ordnance Survey. He also did some survey work in England. In 1840, he worked in railway construction department. He started teaching at Queenwood College Hampshire in 1847. Tyndall obtained his PhD in 1848 from Germany, and most of his scientific work was in the field of atmospheric gases. Tyndall became a lecturer in physics Royal Institution in London in 1850.



JOHN TYNDALL

15.2 Optical Fibers

Optical fiber is used in optical communication as a waveguide. It is cylindrical in shape and is made from transparent dielectric material. It consists of core, clad, and sheath. These components can be described as follows:

- (i) **Core:** It is the innermost part of optical fiber. This is made of transparent dielectric material such as plastic or glass. This core is responsible for signal propagation.
- (ii) **Cladding:** Core is surrounded by cladding of almost $125\ \mu\text{m}$ such that $\mu_{\text{clad}} < \mu_{\text{core}}$. The cladding keeps the light confined to core. This is also made of plastic or glass.
- (iii) **Sheath:** Sheath is a polyethylene jacket that surrounds cladding. It provides safety to core as well as cladding from environmental conditions. The cross-section of optical fiber is shown in Figure 15.1.

The principle of communication in optical fibers is based on the principle of total internal reflection (TIR) as shown in Figure 15.2.

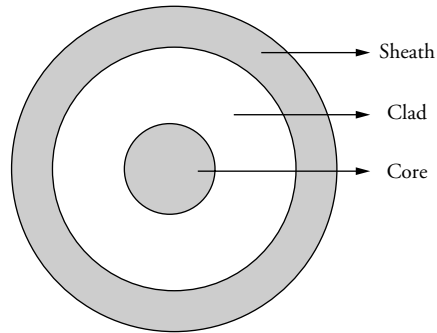


Figure 15.1 Optical fiber's cross-section.

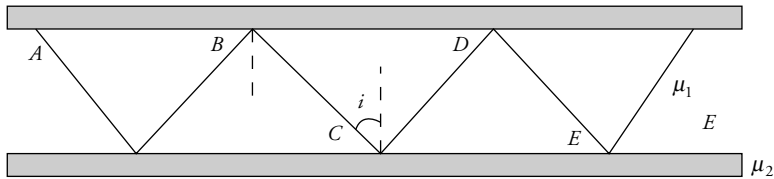


Figure 15.2 Total internal reflection.

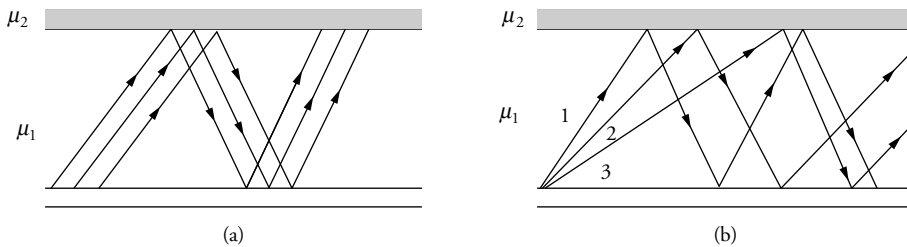


Figure 15.3 (a) Single mode and (b) multimode fiber.

The core has refractive index μ_1 and cladding μ_2 such that $\mu_2 < \mu_1$. According to the principle of TIR, whenever light ray travels from denser to rarer medium then at a certain angle known as critical angle, the light ray is only reflected in the same medium. From Figure 15.1, it is clear that when light ray strikes the core at angle greater than critical angle (critical angle is the angle of incidence at which the refracted ray grazes along the interface), then the ray is totally reflected. This process repeats, and hence the ray is transmitted along the fiber.

Mode: When many parallel light rays are totally internally reflected through a single-fiber, such that all the rays suffer from equal reflections and hence take same time to travel, these rays are said to constitute a mode. Parallel light rays constitute single mode and nonparallel rays make multimode as demonstrated in Figure 15.3(a)–(b).

For multimode fibers, different rays take different time to travel, which is known as time dispersion. Sometimes, due to time dispersion, the information gets distorted due to overlapping of pulses. This distortion can be reduced by taking the diameter of core and wavelength of light of same order. The propagation of light ray inside an optical fiber continues until and unless the fiber is having some shape distortion, especially any sharp bend in fiber.

15.3 Acceptance Angle and Cone

In Figure 15.4, the rays enter at the launching end, μ_o is the refractive index of air, μ_1 is refractive index of core, and μ_2 is refractive index of cladding ($\mu_2 < \mu_1$).

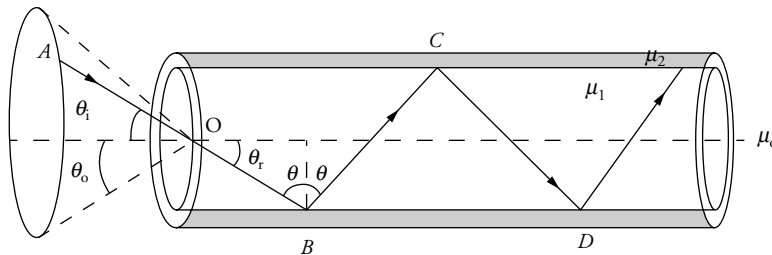


Figure 15.4 Light path in fiber.

θ_i is the incident angle and θ_r is refracted angle. When light AO is refracted at an angle θ_r , then it strikes core – cladding interface (OB) at an angle θ . Here θ is greater than the critical angle (θ_c) such that ray undergoes TIR and propagates through fiber.

Applying Snell's law at point O .

$$\mu_o \sin \theta_i = \mu_1 \sin \theta_r$$

$$\mu_o \sin \theta_i = \mu_1 \sin (90 - \theta)$$

$$\mu_o \sin \theta_i = \mu_1 \cos \theta$$

$$\sin \theta_i = \frac{\mu_1}{\mu_o} \cos \theta \quad (1)$$

At critical angle, $\theta = \theta_c$ [At critical angle, incidence is maximum]

$$(\sin \theta_i)_{\max} = \frac{\mu_1}{\mu_o} \cos \theta_c \quad (2)$$

Critical angle can also be obtained from Snell's law:

$$\mu_1 \sin \theta_c = \mu_2 \sin 90^\circ \quad [\text{at point } B]$$

$$\sin \theta_c = \frac{\mu_2}{\mu_1}$$

$$\cos \theta_c = \sqrt{1 - \left(\frac{\mu_2}{\mu_1}\right)^2} \quad (3)$$

Substituting Eqn. (3) in Eqn. (2),

$$(\sin_i)_{\max} = \frac{\mu_1}{\mu_o} \sqrt{1 - \frac{\mu_2^2}{\mu_1^2}} = \frac{\sqrt{\mu_1^2 - \mu_2^2}}{\mu_o} \quad (4)$$

Usually, $\mu_o = 1$ as the surrounding medium is air and $(\theta_i)_{\max}$ can be regarded as θ_o .

$$\sin \theta_o = \frac{\sqrt{\mu_1^2 - \mu_2^2}}{\mu_o} \quad (5)$$

Maximum angle of incidence θ_o is known as acceptance angle of the fiber. Following are two important terms associated with the propagation of waves inside the optical fiber:

- Acceptance angle:** The maximum value of angle of incidence at the launching end (entrance of optical fiber) so that the ray just propagated through the core of optical fiber is known as acceptance angle.
- Acceptance cone:** The acceptance cone is $2\theta_o$, that is, only the rays that are contained within cone of full angle $2\theta_o$ can propagate and transmit to the other end.

In addition to this, the fractional difference between of refractive index is given by following expression:

$$\Delta = \frac{\mu_1 - \mu_2}{\mu_1} \quad (6)$$

Hence, the ratio of difference between refractive index of core and cladding to refractive index of core is known as fractional refractive index change. As $\mu_1 > \mu_2$, therefore Δ is always positive and is of the order of 0.01. Further, we can describe numerical aperture of fiber. Numerical aperture is defined as the sine of angle of acceptance for optical fiber.

$$NA = \sin \theta_o$$

$$NA = \frac{1}{\mu_o} \sqrt{\mu_1^2 - \mu_2^2} \quad [\text{from Eqn. (5)}]$$

$$NA = \frac{1}{\mu_o} \sqrt{(\mu_1 - \mu_2)(\mu_1 + \mu_2)} \quad (7)$$

Usually $\mu_o \approx 1$, hence

$$NA = \sqrt{(\mu_1 - \mu_2)(\mu_1 + \mu_2)}$$

$$NA = \sqrt{(\mu_1 + \mu_2)\Delta\mu_1} \quad [\text{from Eqn. (6)}]$$

$\mu_1 \approx \mu_2$, hence, we can take

$$NA = \mu_1 \sqrt{2\Delta} \quad (8)$$

Numerical aperture is also known as figure of merit for optical fiber. Basically, it measures how much light can be accepted by the fiber. Its value is usually between 0.13 and 0.3 for long-distance transmission and 0.3–0.5 for short-distance communications. NA depends only on fractional refractive index change and refractive index of core and cladding. It is independent of incident and refractive angles. Small numerical aperture means fiber will accept small light and vice versa.

15.4 Types of Optical Fibers

The optical fibers can be classified on the basis of mode operation, that is, whether the fiber can provide path to a single ray of many rays. Hence, optical fibers can be classified as single mode and multimode fibers. There is another parameter that should be taken into account, that is, V parameter. The V parameter is given by

$$V = \mu_1 \sqrt{2\Delta} kr \quad (9)$$

Where r is radius of core and $k = 2\pi/\lambda$

V is normalized frequency parameter and determines the number of modes that could be supported by the optical fibers. 2.405 is V parameter for most of single-mode operation. When, we plot refractive index versus the distance from core axis, we get index profile. The index profile can be step index type and graded index type. Usually, the single-mode fiber exhibits step index type. But multimode fiber can have step index as well as graded index profile, and it is discussed below.

15.4.1 Single-Mode Step Index Fiber (SMSIF)

For the step index fibers, refractive index of core are μ_1 is constant ($\mu_1 > \mu_2$). The refractive index decreases abruptly at the interface of core and cladding, that is, from $\mu_1 \rightarrow \mu_2$. Clad also has uniform value of refractive index. The refractive index profile is shown in Figure 15.5.

The profile is same as that of step; hence, its name is step index fiber. Usually, the core of SMSIF is made up of germanium (Ge)-doped silicon. The fraction refractive index difference is almost 0.2 percent. The cladding that surrounds core is made up of phosphorous oxide-doped silica and the Δ is almost 0.02 percent. The V parameter for step index fiber is less than 2.405 laser is the light source for them. Single-mode step index fiber (SMSIF) can transmit the information to a longer distance. and, the dispersion factor is very small. SMSIF has very thin core so that only one mode can propagate. These smaller cores may make the coupling of light difficult.

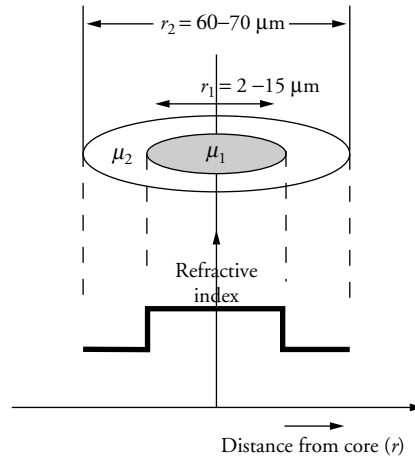


Figure 15.5 Index profile for SMSIF.

15.4.2 Multimode Step Index Fiber (MMSIF)

The diameter for multimode step index fiber is large so that multiple modes can propagate through the core (fig 15.6). Different modes take different time to travel as they travel different distances (Figure 15.3(b)). Hence, different modes reach at different time and this effect is known as modal dispersion. For MMSIF, V parameter is greater than 2.405.

Maximum number of modes that are supported by MMSIF is

$$N = \frac{V^2}{2} \quad (10)$$

The cut-off wavelength is given by the following equation:

$$\lambda_{\text{cut}} = \frac{\lambda V}{2.405} \quad (11)$$

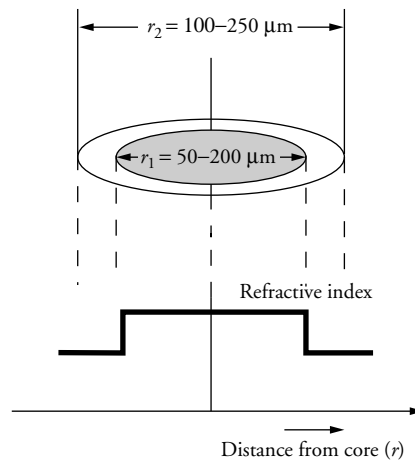


Figure 15.6 Index profile for MMSIF.

15.4.3 Multimode Graded Index Fiber (MMGIF)

The refractive index of core is not constant for graded index fiber (fig 15.7). Refractive index is a function of radial distances and the relation between NA and radial function as well as Δ is given by

$$NA = \mu_1 \sqrt{2\Delta \left[1 - \left(\frac{r}{r_1} \right)^2 \right]} \quad (12)$$

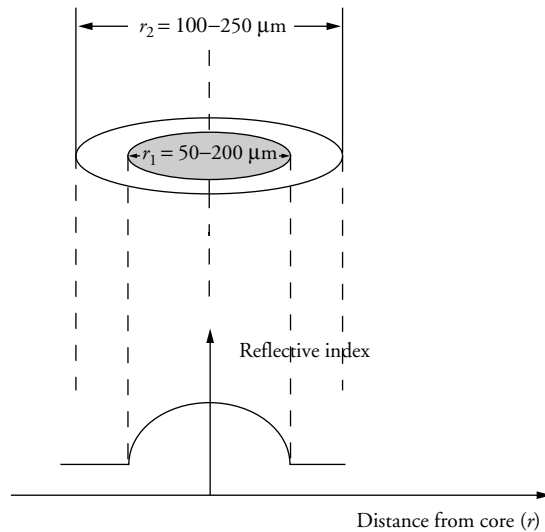


Figure 15.7 Multimode graded index fiber.

where r_1 is the core radius and r is the distance of variation of core. The refractive index variation is given by the following equation:

$$\mu_1(r) = \mu_1 \left[1 - 2\Delta \left(\frac{r}{r_1} \right)^\alpha \right]^{1/2} \quad (13)$$

Here α is the profile function that determines the shape of core profile. When α increases, the shape of profile changes from triangular to step. Usually $\alpha = 2$ exhibits parabolic profile, which is known to exhibit best performance.

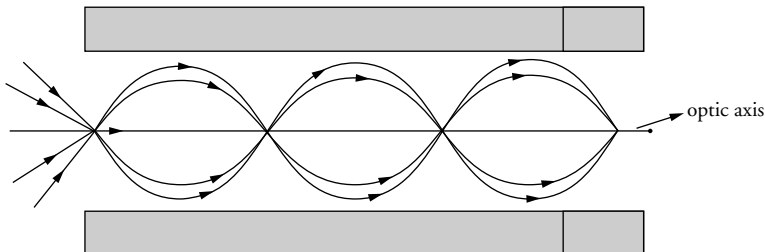


Figure 15.8 Typical propagation of light through MMGIF.

Figure 15.8 shows the variation of light rays in multimode graded index fiber (MMGIF). Those light rays that travel far from optic axis traverse long distance. But these light rays travel in lower refractive index part; hence, they travel with high velocity as compared to the rays that travel close to optic axis. Hence, all the rays take more or less the same time to reach at the end. The bandwidth of MMGIF fibers is high. Multimode fibers have large radii; hence, light rays can be launched easily into fiber. These are used for short transmission distances and LAN systems.

15.5 Power Loss in Optical Fibers

While the light is propagating through the fiber, there are many losses, which are listed as follows:

- (i) **Rayleigh scattering loss:** Optical material may contain large inhomogeneities. These inhomogeneities may be due to some impurities or variation in density. Usually, inhomogeneities act as scattering centers. For example, there is loss of 2.5 dB/km and 0.012 dB/km at 0.82 and 1.55 μm , respectively. The variation of loss with wavelength for silica fiber is given in Figure 15.9.
- (ii) **Microbend and macrobend losses:** Sometimes, the core is of nonuniform diameter as it is very difficult to fabricate the core of optical fiber with uniform diameter throughout. The place of small irregularities in the cladding or core causes the reflection of light at such angles that it hinders total internal reflection is known as microbends. At microbends, the leakage of light may occur; and hence, such losses are known as microbending losses. Macrobend causes certain modes not to be reflected because it is a bend of entire cable and hence again the loss may occur known as macrobending losses. Both the losses are shown in Figure 15.10.

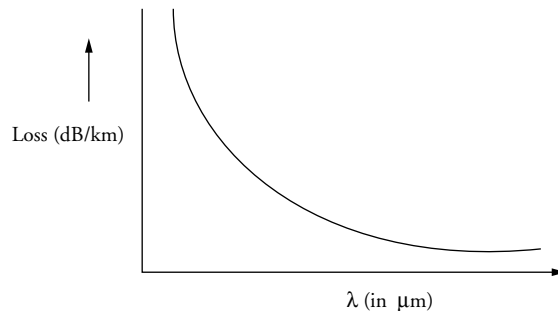


Figure 15.9 Rayleigh scattering loss in silica fibers.

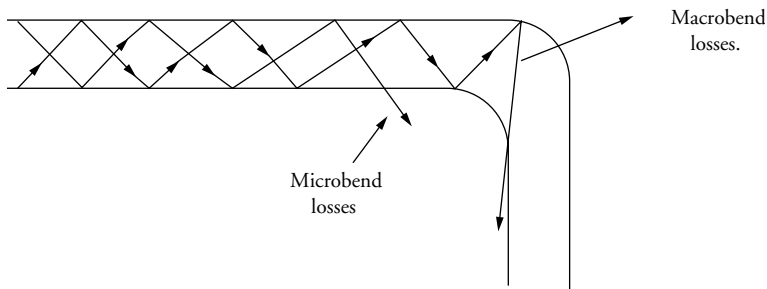


Figure 15.10 Microbend and macrobend losses in optical fiber.

- (iii) **Material loss:** Certain types of materials such as P_2O_5 and B_2O_3 have got high absorption for the wavelength range of 800–1300 nm. These dopants are used to modify the refractive index of fiber. Hence, these dopants may cause loss in the output by absorbing a portion of incident optical light. The hydroxyl ions (OH^-) also contribute to losses.
- (iv) **Induced loss by radiation:** The structure of glass gets altered when it comes in contact with electrons, neutrons, X-rays or gamma rays. Hence, optical power gets reduced.
- (v) **Temperature-dependent losses:** Due to temperature difference between the polymer coating and glass materials, there exists a considerable difference in coefficient of thermal expansion, especially below temperature of $-10^\circ C$. These can cause microbends and hence power losses.
- (vi) **Mode leaking:** Usually, the rays travelling through optical fibers can be classified as meridional and skew rays. Meridional rays propagate in single plane, but skew rays change their plane of propagation on reflections. Meridional rays are guided, whereas skew rays can suffer from reflecting. Skew rays may propagate in leaky modes causing losses.
- (vii) **Mode-coupling loss:** There is a limitation on fiber length, that is, fiber with infinite length cannot be manufactured. Hence, connectors are used to connect the fibers. If the improper matching of fibers occurs, then the signal cannot be transferred. Therefore, these losses contribute to coupling losses and are known as mode-coupling losses.

15.6 Total Attenuation in Optical Fibers

Figure 15.11 represents the losses corresponding to all the wavelengths. Corresponding to wavelengths of 800–900, 1200–1300, and 1500–1600 nm, the optical losses are low. These three regions are known as optical windows.

Now, we will find out the total attenuation in the ray of initial power P_0 . Attenuation is decrease in intensity of light with distance traversed by light. Let P is the power at distance r from the launching end of fiber such that power gradient is proportional to optical power at that point.

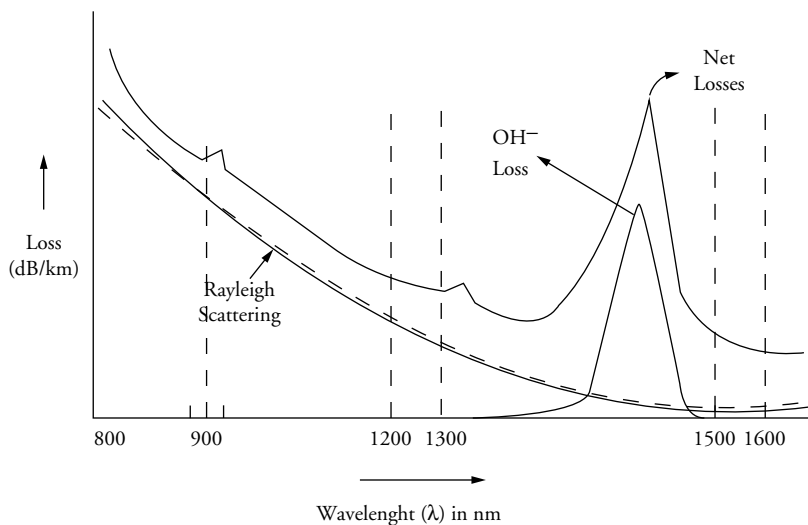


Figure 15.11 Losses in optical fibers vs wavelength.

such that
$$-\frac{dP}{dr} \propto P \quad (14)$$

$$-\frac{dP}{dr} = K_p P \quad (15)$$

$$\frac{dP}{dr} = -K_p P$$

$$\int_{P_o}^P \frac{dP}{P} = -\int_0^r K_p dr$$

$$\frac{P}{P_o} = e^{-K_p r}$$

$$P = P_o e^{-K_p r} \quad (16)$$

Hence, the optical power decreases exponentially w.r.t. distance r . K_p is attenuation coefficient (in km^{-1}). The attenuation can be converted to decibels/km as follows:

$$K = \frac{10}{r} \log_{10} \left(\frac{P_o}{P} \right) \quad (17)$$

Where “ K ” is “fiber attenuation” and its units dB/km.

Further from Eqn. (17),

$$K = \frac{10}{2.303r} \ln \left(\frac{P_o}{P} \right)$$

$$K = \frac{4.343}{r} \ln \left(\frac{P_o}{P} \right) \quad (18)$$

$$Kr = 4.343 \ln \left(\frac{P_o}{P} \right)$$

$$P = P_o e^{-\left(\frac{Kr}{4.343}\right)} \quad (19)$$

From Eqs (19) and (16), the relation between K_p and K can be found as follows:

$$K_p = \frac{K}{4.343} \quad (20)$$

Substituting $K_p = \frac{1}{r}$ in Eqn. (16),

$$P = \frac{P_o}{e} \quad (21)$$

Hence, the attenuation coefficient is defined as the reciprocal of distance, at which the power is reduced to $1/e$ times as that of initial power.

15.7 Semiconductor Diode Lasers

This field of optoelectronics has been of technological importance especially for optical data storage and fiber communication. Losses and electronics when integrated together have given rise to the field of optoelectronics. Semiconductor diode lasers can be pumped to the desired optical level so that the voltage becomes compatible with the integrated circuit. Before proceeding further for the field of semiconductor diode lasers, we should know about Schawlow-Townes condition and band structure, etc., which is discussed in following sections.

15.7.1 Band Structure and Density of States

For a solid-structure, the Fermi energy represents the energy corresponding to a Fermi level such that all the levels above Fermi levels are empty at 0 K and the levels below Fermi level are filled. The Fermi level is given by n_F (fig 15.12). It is well known that every level contains two electrons: one having spin-up and the other having spin-down. We have derived equation for energy in Chapter 4. i.e

$$E = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \quad (22)$$

For Fermi level, this energy can be interpreted as follows:

$$E_F = \frac{n_F^2 \pi^2 \hbar^2}{2ma^2} \quad (23)$$

The volume occupied by space represented by n_F is $\frac{4}{3}\pi n_F^3$. Each point occupies on an average volume of $\frac{1}{8}\left(\frac{4}{3}\pi n_F^3\right)$. Hence, $\frac{1}{8}\left(\frac{4}{3}\pi n_F^3\right)$ represents the total number of points also. But the spins of electrons also have to be taken into consideration, hence total number of electron becomes:

$$\text{Total number of electrons} = 2\left(\frac{1}{6}\pi n_F^3\right) \quad (24)$$

If N is total density, then, $N = \frac{\text{Total number of electron}}{\text{Volume of box of dimension } a}$

$$N = \frac{\text{Total number of electrons}}{a^3}$$

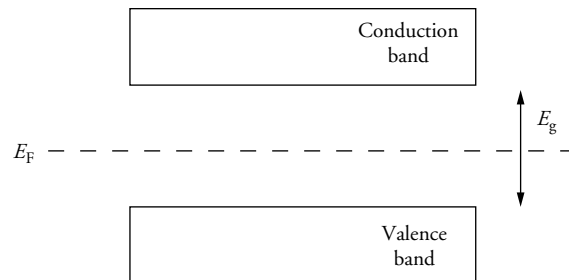


Figure 15.12 Fermi level and forbidden energy gap for semiconductor.

$$Na^3 = \text{Total number of electrons} \quad (25)$$

Using Eqs (25) and (24),

$$Na^3 = \frac{1}{3} \pi n_F^3$$

$$\frac{n_F}{a} = \left(\frac{3N}{\pi} \right)^{1/3} \quad (26)$$

Substituting Eqn. (26) in Eqn. (23), we obtain

$$E_F = \frac{\pi^2 \hbar^2}{2m} \left(\frac{3N}{\pi} \right)^{2/3}$$

$$E_F = \frac{\hbar^2}{2m} (3\pi^2 N)^{2/3} \quad (27)$$

For a continuous energy range between E and $E + dE$, we have to figure out the total allowed states per unit volume. Hence, the density of states can be given by

$$\int_0^{E_F} \rho(E) dE = N \quad (28)$$

Only the limit from 0 to Fermi energy (E_F) will contribute because the levels above Fermi level are empty. From Eqs (27) and (28),

$$\int_0^{E_F} \rho(E) dE = \frac{1}{3\pi^2} \left[\frac{2mE_F}{\hbar^2} \right]^{3/2} \quad (29)$$

from Eqn. (27) and Comparing (28) and (29), we obtain.

$$N = \frac{1}{3\pi^2} \left(\frac{2mE_F}{\hbar^2} \right)^{3/2} \quad (30)$$

Taking natural log on both sides,

$$\ln N = \frac{3}{2} \ln E_F + \text{constant}$$

Differentiating w.r.t. E_F

$$\frac{1}{N} \frac{dN}{dE_F} = \frac{3}{2} \frac{1}{E_F}$$

$$\frac{dN}{dE_F} = \frac{3}{2} \frac{N}{E_F}$$

$$\frac{dN}{dE_F} = \frac{3}{2} \frac{1}{3\pi^2} \left[\frac{2mE_F}{\hbar^2} \right]^{3/2} \frac{1}{E_F}$$

[from Eqn. (30)]

$$\frac{dN}{dE_F} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E_F^{1/2} \quad (31)$$

↓

Density $\rho(E_F)$

Therefore, the density of states depends on Fermi energy. The Eqn. (31) is not as simple as it looks, that is, the major concern is mass of electron. When the electron is in crystal, then its mass is usually different from 9.1×10^{-31} kg and is given by the following formula:

$$m_{\text{eff}} = \hbar^2 \left[\frac{d^2 E}{dk^2} \right]^{-1} \quad (32)$$

Which implies that effective mass is a function of wave vector k . Usually, m_{eff} is positive for valence band and negative for conduction band, which implies that electron behaves as a hole or positively charged particle. For conductors, $m_{\text{eff}} = 9 \times 10^{-31}$ kg due to the partial filling of band.

But the valence band for semiconductors and insulators is almost filled, and hence the effective mass of electron is not the same as that of free electron and is given by Eqn. (32). Therefore, Eqn. (31) can be written as follows:

$$\frac{dN}{dE} = \frac{1}{2\pi^2} \left[\frac{2m_v}{\hbar^2} \right]^{3/2} E^{1/2} \quad (33)$$

(for valence band m_v is mass of electron)

Similarly,
$$\frac{dN}{dE} = \frac{1}{2\pi^2} \left[\frac{2m_c}{\hbar^2} \right]^{3/2} E^{1/2} \quad (34)$$

(for conduction band m_c is mass of electron).

15.7.2 Fermi–Dirac Distribution

The probability of occupation of an energy state E by an electron is given according to Fermi–Dirac distribution as follows:

$$f(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1} \quad (35)$$

T is the temperature and E_F is the Fermi energy. The Fermi factor is temperature dependent, and Where describes the behavior of material.

At $T = 0$ K, three cases may arise as follows:

(i) When $E < E_F$

Then Eqn. (35) becomes

$$f(E) = \frac{1}{e^{-(E_F-E)/k_B T} + 1}$$

$$f(E) = \frac{1}{e^{-(E_F - E)/0} + 1} = \frac{1}{e^{-\infty} + 1} = \frac{1}{(1/e^\infty) + 1}$$

$$f(E) = \frac{1}{(1/\infty) + 1} = \frac{1}{0 + 1} = 1$$

$$f(E) = 1 \quad \text{for } E < E_F \text{ at } T = 0 \quad (36)$$

Hence, all the quantum states are occupied for which the energy is less than the Fermi energy at temperature $T = 0$ K.

(ii) When $E > E_F$

Then Eqn. (35) becomes

$$f(E) = \frac{1}{e^{(E - E_F)/k_B T} + 1}$$

$$f(E) = \frac{1}{e^\infty + 1} = \frac{1}{\infty + 1} = 0$$

$$f(E) = 0 \quad \text{for } E > E_F \text{ at } T = 0 \quad (37)$$

Hence, all the quantum states are empty for which the energy is greater than Fermi energy at temperature $T = 0$ K.

(iii) When $k_B T \ll E_F$ (especially for metals for which the value is almost 0.03 eV], we get $E = E_F$

Hence,

$$f(E) = \frac{1}{e^{(E - E_F)/k_B T} + 1}$$

$$f(E) = \frac{1}{e^0 + 1} = \frac{1}{1 + 1} = \frac{1}{2}$$

$$f(E) = \frac{1}{2} \quad \text{for } E = E_F \text{ at small temperature.} \quad (38)$$

From Eqn. (38), it is clear that when $E = E_F$, then the Fermi levels lie exactly in the middle of conduction and valence band where the probability of occupation is 50 percent.

When $k_B T$ approaches Fermi energy, then the distribution is no longer Fermi–Dirac. In other words the distribution becomes Maxwell–Boltzmann as shown in Figure 15.13.

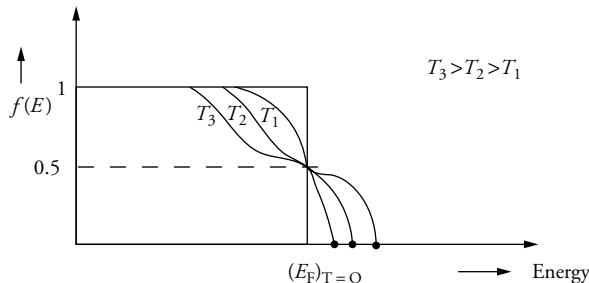


Figure 15.13 Deviation from Fermi–Dirac distribution.

15.7.3 Schawlow–Townes Condition for Lasers

We know from Chapter 14, that the principle of lasers is based on the principle of stimulated emission, that is, one photon can produce 2 photons, 2 photons can produce 4; and hence, the multiplication of photons goes on as more and more photons strike the lasing media.

In most of cases, the excited atoms may decay via spontaneous decay. But, for laser action, a condition is required which is derived as follows: The most important part for lasers is the optical resonator. The optical resonator consists of parallel plane reflecting mirrors that enclose active lasing medium. The mirrors are provided at both ends so that the light photons can be reflected back and forth as shown in the fig 15.14.

Let L be the original length of optical cavity and μ be the refractive index of medium. Hence, the optical length (L') becomes $\mu L = L'$

For reinforcement, the optical length should be some integral multiple of $\lambda/2$, where λ is wavelength of light used i.e.

$$\begin{aligned} L' &= n \lambda / 2 \\ \mu L &= n \lambda / 2 \\ \mu L &= \frac{nc}{2f} \\ f &= \frac{nc}{2L\mu} \end{aligned} \quad (39)$$

If the reinforcement condition is set up, then stationary waves set up in the resonant cavity. Let I_o be the intensity of light falling on mirror and I_r be the reflected light intensity. Then the reflection coefficient of mirror is given by

$$R = \frac{I_r}{I_o} \Rightarrow I_r = RI_o \quad (40)$$

For partially silvered mirror, $R < 1$,

The intensity decreases exponentially with distance as given below:

$$I(x) = I(0) e^{(-\alpha_f x)} \quad (41)$$

where α_f is absorption coefficient and is function of frequency.

Let $K = -\alpha_f$ at $x = L$, then Eqn. (41) becomes

$$I(L) = I(0) e^{(KL)} \quad (42)$$

Let R_1 and R_2 be the reflectivity's of two mirrors, such that light intensity reduces by factor $e^{-2\gamma}$ i.e.

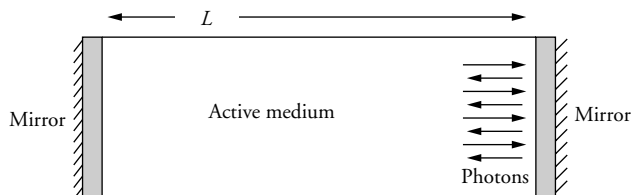


Figure 15.14 Active medium between the mirrors.

$$R_1 R_2 = e^{-2\gamma} \quad (43)$$

γ measures intensity loss/pass, Eqn. (42) can be written as follows:

$$I(L) = I(0) \exp(KL - \gamma) \quad (44)$$

For sustained oscillations, the following conditions should be satisfied:

$$\exp(KL - \gamma) \geq 1$$

$$KL \geq \gamma \quad (45)$$

The threshold condition for sustained oscillations is

$$K = \frac{\gamma}{L} \quad (46)$$

The value of absorption coefficient is given by

$$\alpha_f = \frac{\pi^2 c^2 \mu g_2 A_{21}}{g_1 w_o^2} \left(N_1 - \frac{g_1}{g_2} N_2 \right) g(w, w_o) \quad (47)$$

g_1 and g_2 are degeneracies of ground and excited states. A_{21} is spontaneous emission from excited state to ground state.

$g(w, w_o)$ is line shape function dependent on central angular resonant frequency w_o and w which is angular frequency spread of atomic line

$$K = -\alpha_f = \frac{\pi^2 c^2 \mu g_2 A_{21}}{g_1 w_o^2} \left[\frac{g_1}{g_2} N_2 - N_1 \right] g(w, w_o) \quad (48)$$

As $K \geq \frac{\gamma}{L}$ (from Eqn. (45)), hence

$$\frac{\pi^2 c^2 \mu g_2 A_{21}}{g_1 w_o^2} \left[\frac{g_1}{g_2} N_2 - N_1 \right] g(w, w_o) \geq \frac{\gamma}{L}$$

For threshold condition, only equality holds good, and it can be written as follows:

$$\frac{g_1}{g_2} N_2 - N_1 = \frac{\gamma g_1 w_o^2}{\pi^2 c^2 L \mu g_2 A_{21} g(w, w_o)} \quad (49)$$

This is the case for degenerate level. But for nondegenerate levels, $g_1 = g_2 = 1$, and Eqn. (49) can be written as follows:

$$N_2 - N_1 = \frac{\gamma w_o^2}{\pi^2 c^2 L \mu A_{21} g(w, w_o)} \quad (50)$$

Equation (50) represents critical inversion for nondegenerate states. The average lifetime of photons (t_c) is defined as the time during which the number of photons gets reduced by $1/e$ times. The expression of t_c is given by

$$t_c = \frac{L}{c\gamma} \quad (51)$$

Hence, using Eqn. (51) in Eqn. (50),

$$N_2 - N_1 = \frac{w_o^2}{\pi^2 \mu c^3 A_{21} g(w_1, w_o) t_c} \quad (52)$$

Let $A_{21} = \frac{1}{t_s}$ (reciprocal of spontaneous lifetime), then

$$N_2 - N_1 = \frac{w_o^2}{\pi^2 \mu c^3 g(w, w_o) t_c} t_s \quad (53)$$

This Eqn. (53) is known as Schawlow–Townes condition. When t_c is large, then the losses in resonant cavity are small. When t_c is large and t_s is small, then low value of threshold for population inversion is obtained. The population inversion depends upon angular frequency; hence, laser action can be obtained easily for UV rays rather than visible radiations (Ultraviolet radiations have high frequency value than the visible radiations). Therefore the Schawlow–Townes condition can be regarded as very important condition for population inversion.

15.7.4 Quasi-Fermi Levels for Semiconductors

In p–n junction, there is hole-rich region and electron-rich region separated by a depletion region. Depletion region is regarded as the recombination region and the thickness of depletion region depends on biasing. For forward biasing, the depletion region is thin; whereas for reverse biasing, the depletion region gets thicker. In other words, it can be said that when current passes through junction diode, there is no more thermal equilibrium in the p–n junction diode. The Fermi levels get separated for p–n diode, that is, E_{FC} and E_{FV} are quasi Fermi levels for conduction and valence band, respectively. For Fermi quasi levels to exist, the equilibrium time between bands should be smaller than the carrier scattering time. Hence, Eqn. (27) can be separated for conduction and valence band as follows:

$$E_{FC} = \frac{\hbar^2}{2m_c} (3\pi^2 N)^{2/3} \quad (54a)$$

$$E_{FV} = \frac{\hbar^2}{2m_v} (3\pi^2 N)^{2/3} \quad (54b)$$

where m_c and m_v are effective mass of electron in conduction and valence band, respectively. For degenerate p-type semiconductor the Fermi level lies in conduction band and for degenerate n-type semiconductor, the Fermi level lies in valence band.

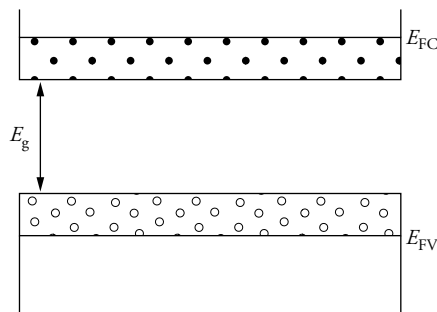


Figure 15.15 Quasi-Fermi levels for degenerate p-type semiconductor.

Figure 15.15 shows a non-thermal equilibrium state where electrons are excited to conduction band of degenerate p-type semiconductor. This can be attained by two processes, that is, via subjecting the semiconductor to intense laser beam or injecting electrons into p-regions across p–n junction. When we say intense laser beam, it means the energy hf of laser photon should satisfy the following condition:

$$hf > E_g + E_{FC} + E_{FV} \quad (55)$$

When a photon is absorbed, then electron is excited, which jumps on to the conduction band. When the electrons get excited, they follow relaxation by emitting acoustic and optic phonon to the bottom of the conduction band. The relaxation time for electron is 10^{-12} sec, but the relaxation time for electron to reach valence band again is $3 - 4 \times 10^{-9}$ sec. There is quite a probability that electron–hole recombination takes place, when electron jumps back to valence band. Hence, the lasing action of semiconductors is clear, when the quasi Fermi levels can be determined accurately for given excitation rate.

15.7.5 Lasing Action of Semiconductor Diode Laser

When p–n junction is formed, then excess electrons in n-type region flow across p-type region in n-type region, and excess holes flow from p-region to n-region. Near midway, they recombine to form depletion region. To obtain a laser radiation, the semiconductor or p–n junction diode is to be pumped. The pumping depends on the semiconductor material used. For p–n junction lasers, the junction region is most important as the population inversion occurs in this region.

The diode laser was first invented in 1962 by Robert Hall. Diode lasers are core devices in the field of electro-optics. The diode lasers are efficient and possess long lifetimes. In addition to this, they can give up to 200 mW of power despite being very small in size. They have potential role in laser disks and fiber-optic communication.

Construction

Figure 15.16 is GaAs p–n junction diode, n and p regions are doped in order to make them degenerate. Zinc atoms are diffused into n-type region and one face is polished so that it can be reflecting. Only the reflecting face will produce lasing action; other faces are kept rough to avoid any losses due to unwanted lasing action. The active layer is usually of $1 \mu\text{m}$ width.

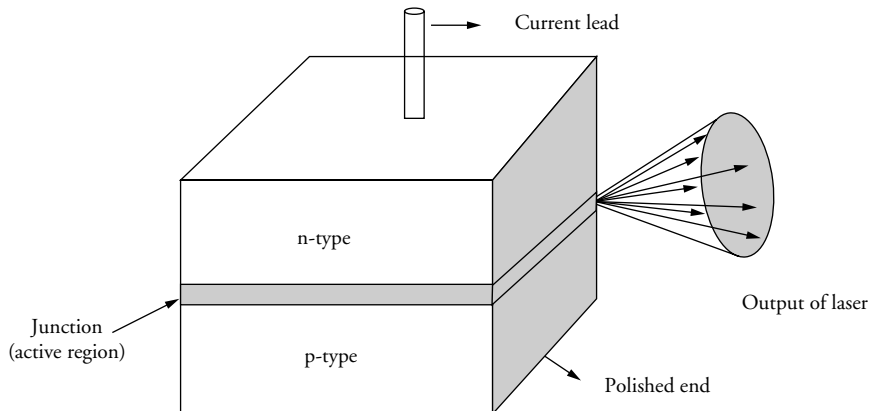


Figure 15.16 Semiconductor laser (GaAs).

Working

When electrons and holes recombine, then energy is released, and this is known as activation energy. Based on the type of energy released, the semiconductor diode can be two types:

- (i) **Direct semiconductor:** In these semiconductors, the energy released is in the form of heat, for example, group III and I elements such as gallium and arsenic.
- (ii) **Indirect semiconductor:** In these semiconductors, the energy is released in the form of light, for example, Si and Ge.

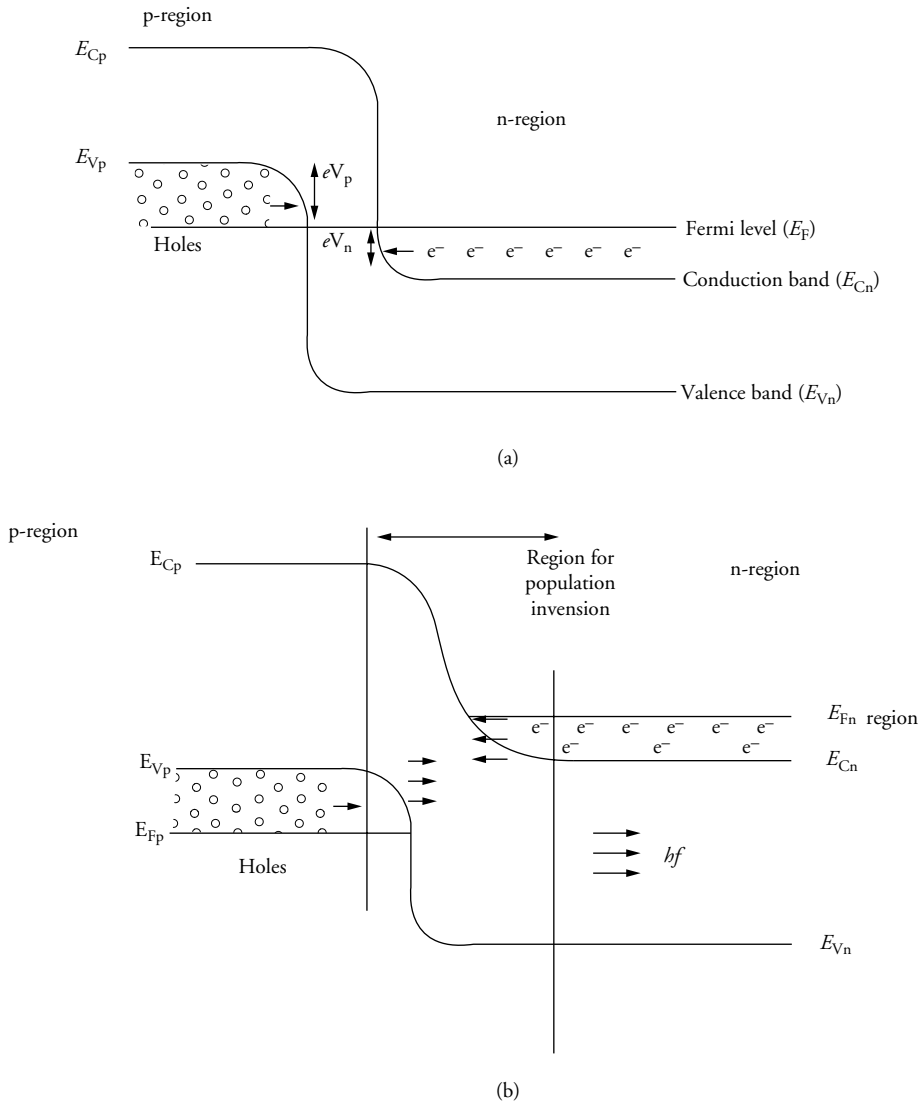


Figure 15.17 (a) p - n junction when the diode is in thermal equilibrium and (b) p - n Junction during forward biasing.

The semiconductor has to be forward biased in order to obtain lasing action. The junction has to be cleaned properly. The refractive index of semiconductor is almost 3.6. The wavelength required for lasing action is 8400–8500 Å. At first, the spontaneous emission dominates due to electron–hole pair recombination. Upon increasing diode current, the stage of population inversion is obtained. Then simulated emission begins corresponding to normal modes. The wavelength of normal mode is given by

$$\lambda = \frac{2L}{n} \quad (56)$$

At high current, population inversion occurs, and the output radiation of wavelength occurs in range 7000–25,000 Å. Figure 15.17 represents p–n junction energy band diagram.

When, there is no external applied voltage, then the two bands are separated by energy gap E_g . The contact potential developed is $e(V_n + V_p)$ Where V_n and V_p is the potential across n and p region respectively. When the diode is forward biased, then n-side is raised. Hence, the electrons start flowing toward the p-side and holes flow toward n-side. Hence, the depletion region contains higher concentration of electron and holes. Therefore, the condition of population inversion is attained. The total separation between E_{Fn} and E_{Fp} is $E_g + (eV_n + eV_p)$.

Mathematical Treatment

When light beam of frequency f is incident on eight semiconductors, then the absorbed quanta are given by

$$N_a = AB_{vc} P_v (1 - P_c) U(f) \quad (57)$$

where A is constant, P_v is probability of occupying a particular state. $(1 - P_c)$ represent probability that the conduction band is empty. B_{vc} is probability of transition from valence band to conduction band $U(f)$ is radiation density, which is function of frequency. The number of emitted light photons is given by

$$N = AB_{cv} P_c (1 - P_v) U(f) \quad (58)$$

The condition of amplification is

$$N > N_a$$

$$AB_{cv} P_c (1 - P_v) U(f) > AB_{vc} P_v (1 - P_c) U(f)$$

Let $B_{cv} = B_{vc}$

$$P_c (1 - P_v) > P_v (1 - P_c) \quad (59)$$

P_c and P_v can be written using Fermi–Dirac statistics:

$$P_c = \frac{1}{1 + \exp\left(\frac{E - E_c}{k_B T}\right)} \quad \text{and} \quad P_v = \frac{1}{1 + \exp\left(\frac{E - E_v}{k_B T}\right)}$$

Hence, Eqn. (59) becomes

$$E_c - E_v > hf > E_g \quad [hf > E_g] \quad (60)$$

The Schawlow–Townes condition is given by the following equation:

$$N_2 - N_1 = \frac{w^2}{2c^3 \mu \pi} \frac{t_s}{t_c} \Delta w$$

For population inversion, $N_2 = N_c$ and $N_1 = 0$:

$$N_c = \frac{w^2}{2c^3 \mu \pi} \frac{t_s}{t_c} \Delta w \quad (61)$$

The current density is given by

$$J = \frac{I}{A} = \frac{N_c A l e}{A t}$$

Where $Al \rightarrow$ volume of conductor of cross-section area A and length l , $t \rightarrow$ transition time for electrons to return to valence band. Hence

$$J = \frac{N_c l e}{t} \quad (62)$$

Semiconductor laser diodes cannot be operated for a longer duration because to obtain the required gain, the threshold current it to be increased. Increasing the current increases the temperature of material that is disadvantageous for diode operation.

Robert Hall was born in 1919 in New Haven, Connecticut. He got his BS in Physics from the California Institute of Technology. Then, he worked at the Research and Development Center of General Electric in Schenectady, New York where he invented semiconductor diode lasers in 1962. The major contribution of Hall was the development of technique used to purify germanium, which was further used to make transistors. He designed systems using continuous wave magnetrons, which could jam enemy radar. This was his major contribution to World War II. When the world war got over, Robert returned to CalTech in 1948 to obtain PhD in Nuclear Physics. He then spent the rest of his life in New York working for GE. In his career, he got 43 US patents.



ROBERT HALL

Semiconductor lasers are small and inexpensive, which have most applications for optical fiber communications systems, barcode readers compact disk players, and laser printers. Robert Hall also contributed in improving the power rectifiers used in electrical transmission devices. He also studied solar cells and photovoltaics.

SUMMARY

The chapter deals with the phenomena of light and electricity. Optical fibers and semiconductor diode lasers are important optoelectronic devices. Optical fiber is a cylindrical waveguide composed of core, cladding, and sheath; optical fibers work on the principle of total internal reflection. The rays inside the optical fiber propagate if they are within a required acceptance angle and cone. The numerical aperture lies between 0.13 and 0.3 for long-distance transmission and 0.3–0.5 for short-distance communication. Optical fibers can be classified as single-mode step index and multimode step index/graded index fibers. There are many power laser in optical fibers including Rayleigh scattering loss, microbend, macrobend, material losses, mode leaking, mode coupling loss, and temperature-dependent losses. The optical power decreases exponentially with distance. The attenuation coefficient is defined as the reciprocal of distance at which the power is reduced to $1/e$ times as that of initial power. Semiconductor diode lasers find potential application in the field of integrated circuits. For a solid structure, the Fermi energy corresponds to a Fermi level such that all the levels above fermi level are empty. The density of states is obtained to depend upon the fermi energy. The mass of electron is no longer 9.1×10^{-31} kg in crystal. Hence, effective mass of electron is taken “-ve” in valence band and “+ve” in conduction band). The Schawlow–Townes condition for lasers has been demonstrated, which illustrates that when average life time of photons is small, then the losses in resonant cavity are small. For the lasing action of GaAs p–n junction diode laser, the wavelength of 8000–8500 Å is required. During the forward biasing, n-side is raised and electrons start flowing toward the p-side. Hence, the condition of population inversion is achieved.

SOLVED PROBLEMS

Q. 1: The refractive index of core and cladding is 1.32 and 1.30, respectively. Obtain the numerical aperture of the optical fiber.

Ans: Numerical aperture = $\frac{1}{\mu_0} \sqrt{\mu_1^2 - \mu_2^2}$

Usually $\mu_0 \approx 1$, hence

$$NA = \sqrt{\mu_1^2 - \mu_2^2}$$

$$\mu_1 = \text{refractive index of care} = 1.32$$

$$\mu_2 = \text{refractive index of cladding} = 1.30$$

$$NA = \sqrt{(1.32)^2 - (1.30)^2}$$

$$NA = 0.2289$$

Q. 2: Obtain the acceptance angle and numerical aperture of optical fiber with refractive index of core and cladding to be 1.68 and 1.5, respectively.

Ans: $\mu_1 = 1.68$ and $\mu_2 = 1.5$

$$NA = \sqrt{\mu_1^2 - \mu_2^2}$$

$$= \sqrt{(1.68)^2 - (1.5)^2}$$

$$NA = 0.7565$$

$$\sin \theta_o = \sqrt{\mu_1^2 - \mu_2^2} \quad [\mu_o \approx 1]$$

$$\theta_o = \text{acceptance angle} = \sin^{-1}(NA)$$

$$\theta_o = \sin^{-1}(0.7565)$$

$$\theta_o = 49.15^\circ$$

Q. 3: Obtain the refractive index of core, if index of cladding is 1.5 and the fractional difference refractive index is 0.0007.

Ans: The fractional difference of refractive index is given by the following equation:

$$\Delta = \frac{\mu_1 - \mu_2}{\mu_1}$$

Here, $\mu_1 = 1.5$ and $\Delta = 0.0007$

$$0.0007 = \frac{1.5 - \mu_2}{1.5}$$

$$1.5 - \mu_2 = 1.5 \times 0.0007$$

$$1.5 - \mu_2 = 0.00105$$

$$\mu_2 = 1.5 - 0.00105$$

$$\mu_2 = 1.498$$

Q. 4: The refractive index of core and cladding is 1.45 and 1.42. Obtain the critical angle and acceptance angle.

Ans:

$$\sin \theta_c = \frac{\mu_2}{\mu_1}$$

$\mu_1 = 1.45$ and $\mu_2 = 1.42$

$$\sin \theta_c = \frac{1.42}{1.45}$$

$$\sin \theta_c = 0.9793$$

$$\theta_c = \sin^{-1}(0.9793)$$

$$\theta_c = 78.32^\circ$$

Hence, the critical angle (beyond which the total internal reflection takes place) is 78.32° .

Moreover,

$$\sin \theta_o = \sqrt{\mu_1^2 - \mu_2^2} \quad [\mu_o \approx 1]$$

$$\sin \theta_o = \sqrt{1.45^2 - (1.42)^2}$$

$$\sin \theta_o = \sqrt{0.0861}$$

$$\sin \theta_o = 0.2934$$

$$\theta_o = \sin^{-1}(0.2934)$$

$$\theta_o = 17.06^\circ$$

Q. 5: The numerical aperture of an optical fiber is 0.25 and the refractive index of core is 1.45. What would be the acceptance angle if the fiber is in water (refractive index of water = 1.33).

Ans:

$$NA = \sqrt{\mu_1^2 - \mu_2^2}$$

Here $NA = 0.25$

$$\mu_1 = 1.45,$$

$$\mu_2 = ?$$

$$0.25 = \sqrt{(1.45)^2 - \mu_2^2}$$

$$(0.25)^2 = (1.45)^2 - \mu_2^2$$

$$\mu_2^2 = (1.45)^2 - (0.25)^2$$

$$\mu_2^2 = 2.04$$

$$\mu_2 = \sqrt{2.04}$$

$$\mu_2 = 1.428$$

When the fiber is in water, then $\mu_o = 1.33$

$$\sin \theta_o = \frac{1}{\mu_o} \sqrt{\mu_1^2 - \mu_2^2}$$

$$\sin \theta_o = \frac{\sqrt{(1.45)^2 - (1.428)^2}}{\mu_o} = \frac{0.25}{1.33}$$

$$\sin \theta_o = 0.1879$$

$$\theta_o = \sin^{-1}(0.1879) = 10.83^\circ$$

Q. 6: An optical fiber has attenuation coefficient to be 4.2 dB/km . If the initial power is 0.7 mW, obtain the output power after 6 km.

Ans: Given
$$K = \frac{10}{r} \log_{10} \left(\frac{P_o}{P} \right)$$

Here $r = 6$ km
 $P_o = 0.7$ mW
 $K = 4.2$ dB/km

$$4.2 = \frac{10}{6} \log_{10} \left(\frac{0.7}{P} \right)$$

$$\frac{4.2 \times 6}{10} = \log_{10} \left(\frac{0.7}{P} \right)$$

$$2.52 = \log_{10} \left(\frac{0.7}{P} \right)$$

$$10^{(2.52)} = \frac{0.7}{P}$$

$$P = \frac{0.7}{(10)^{2.52}} = \frac{0.7}{331.131}$$

$$P = 2.11 \times 10^{-3} \text{ mW}$$

Q. 7: A metal has a density of 10.49 g/cm³ and atomic weight of 107 g. Obtain its Fermi energy.

Ans: Let us calculate N , that is, total number of electrons/volume.

$$107 \text{ g of metal has} = 6.023 \times 10^{23} \text{ electrons}$$

$$\frac{n}{M} = \frac{6.023 \times 10^{23}}{107}$$

$$\text{Mass} = \text{Volume} \times \text{density} = \rho V \quad [\text{Density } \rho = 10.49 \text{ g/cm}^3]$$

$$\frac{n}{\rho V} = \frac{6.023 \times 10^{23}}{107}$$

$$\frac{n}{V} = \frac{6.023 \times 10^{23}}{107} \times 10.49$$

$$N = \frac{n}{V} = 0.59 \times 10^{23} = 5.9 \times 10^{22} \text{ cm}^{-3}$$

$$N = 5.9 \times 10^{28} / \text{m}^3$$

The Fermi energy E_F is given by

$$E_F = \frac{\hbar^2}{2m} [3\pi^2 N]^{2/3}$$

Here, $m = 9.1 \times 10^{-31} \text{ kg}$

$$E_F = \frac{(6.62 \times 10^{-34})^2 (3 \times 3.14 \times 3.14 \times 5.9 \times 10^{28})^{2/3}}{8 \times 3.14 \times 3.14 \times 9.1 \times 10^{-31}}$$

$$E_F = 8.848 \times 10^{-19} \text{ J}$$

$$E_F = \frac{8.848 \times 10^{-19} \text{ eV}}{1.6 \times 10^{-19}} = 5.53 \text{ eV}$$

Q. 8: Obtain the Fermi energy for aluminum metal (atomic radius is 143 pm) when it is having face-centered cubic.

Ans: For face-centered cubic structure,

Number of electrons = 4

$$\text{Volume of cell} = a^3 = (2\sqrt{2}r)^3$$

$$= 16\sqrt{2} r \quad (r = 143 \text{ pm})$$

$$= 16 \times 1.44 \times (1.43 \times 10^{-10})^3$$

$$= 16 \times 1.44 \times 1.43 \times 1.43 \times 1.443 \times 10^{-30}$$

$$= 67.37 \times 10^{-20}$$

$$= 6.737 \times 10^{-29} \text{ m}^3$$

$$\text{Hence, } N = \frac{\text{Number of electrons}}{\text{volume}}$$

$$N = \frac{4}{6.737 \times 10^{-29}}$$

$$N = 0.593 \times 10^{29}$$

$$\begin{aligned}
 N &= 5.93 \times 10^{28} / \text{m}^3 \\
 \text{The Fermi energy is } E_F &= \frac{\hbar^2}{2m} (3\pi^2 N)^{2/3} \\
 &= \frac{h^2}{8m\pi^2} (3\pi^2 N)^{2/3} \\
 &= \frac{(6.63 \times 10^{-34})^2 (3 \times 3.14 \times 3.14 \times 5.93 \times 10^{28})^{2/3}}{8 \times 9.1 \times 10^{-31} \times 3.14 \times 3.14} \\
 &= \frac{43.95 \times 10^{-68} (175.40 \times 10^{28})^{2/3}}{717.77 \times 10^{-31}} \\
 &= \frac{43.95 \times 10^{-37}}{717.77} (30765.16 \times 10^{56})^{1/3} \\
 &= \frac{43.95 \times 10^{-37} \times 31.33 \times 4.64 \times 10^{18}}{717.77} \\
 E_F &= 8.901 \times 10^{-19} \text{ J} \\
 E_F &= \frac{8.901 \times 10^{-19} \text{ eV}}{1.6 \times 10^{-19}} = 5.56 \text{ eV}
 \end{aligned}$$

Hence, Fermi energy for aluminum is 5.56 eV.

OBJECTIVE QUESTIONS

- Optical fibers are same as coaxial cables. (Yes/No).
- What is the shape of optical fiber?

(a) Spherical	(b) Cylindrical
(c) Conical	(d) Triangular
- The dielectric constant of core is similar to

(a) wood	(b) ether
(c) glass	(d) silver
- The refractive index of cladding is _____ than the refractive index of core.

(a) less	(b) greater
(c) equal	(d) none of the above

5. Sheath is a _____ jacket surrounding cladding.
 (a) polybutylene (b) polyethylene
 (c) polypropylene (d) can be (a), (b), or (c)
6. The principle of communication in optical fibers is based on the
 (a) total internal reflection (b) dispersion
 (c) refraction (d) polarization
7. For the reflected ray to graze along the surface,
 (a) angle of incidence < critical angle
 (b) angle of incident > critical angle
 (c) angle of incidence > angle of refraction
 (d) angle of incidence = critical angle
8. Multimode is constituted by a set of
 (a) parallel rays (b) nonparallel rays
 (c) perpendicular rays (d) all of these
9. The acceptance angle is given by
 (a) $\sin \theta_o = \sqrt{\mu_1^2 + \mu_2^2}$ (b) $\sin \theta_o = \sqrt{\mu_2^2 - \mu_1^2}$
 (c) $\sin \theta_o = \frac{\sqrt{\mu_1^2 - \mu_2^2}}{\mu_o}$ (d) $\sin \theta_o = \frac{\mu_2}{\mu_1}$
10. The acceptance cone is given by
 (a) $2\theta_o$ (b) $3\theta_o$
 (c) θ_o (d) $\theta/2$
11. Fractional difference of refractive index is given by
 (a) $\Delta = \frac{\mu_2 - \mu_1}{\mu_1}$ (b) $\Delta = \frac{\mu_1}{\mu_2 - \mu_1}$
 (c) $\Delta = \frac{\mu_1 - \mu_2}{\mu_2}$ (d) $\Delta = \frac{\mu_1 - \mu_2}{\mu_1}$
12. Numerical aperture that is defined as sine of angle of acceptance of optical fiber is given by
 (a) $\frac{\sqrt{\mu_1^2 - \mu_2^2}}{\mu_o}$ (b) $\mu_1 \sqrt{2\Delta}$
 (c) none of these (d) Both (a) and (b)
13. For long-distance transmission, the numerical aperture lies between
 (a) 0.13 and 0.3 (b) 0.5 and 1
 (c) 0.4 and 0.5 (d) 0 and 1

14. Numerical aperture is independent of

- (a) refractive index change
 (b) refractive index of medium
 (c) acceptance angle
 (d) incidence and refractive angles

15. The V -parameter for fibers is given by

- (a) $V = \mu_1 k r$
 (b) $V = \mu_1 \sqrt{2\Delta} k r$
 (c) $V = \frac{\mu_1 r}{\sqrt{2\Delta} k}$
 (d) $V = \frac{\sqrt{2\Delta} k}{\mu_1 r}$

16. For single-mode operation, the value of V -parameter is

- (a) 3.808
 (b) 3.54
 (c) 2.405
 (d) 1.832

17. For step index fibers, the refractive index of core is

- (a) constant
 (b) varies as $\frac{1}{r}$
 (c) varies as $\frac{1}{r^2}$
 (d) varies as r

18. For step index fibers, the fraction refractive index is

- (a) 0.01 percent
 (b) 0.03 percent
 (c) 0.20 percent
 (d) 0.02 percent

19. The core of SMSIF is

- (a) thick
 (b) thin
 (c) 30–45 μm
 (d) 100 – 250 μm

20. For multimode step index fiber, the core diameter is

- (a) 50 – 200 μm
 (b) 100 – 250 μm
 (c) 2 – 15 μm
 (d) 60 – 70 μm

21. Maximum number of modes supported by MMSIF is

- (a) V
 (b) $\frac{V^2}{2}$
 (c) $\frac{V}{2}$
 (d) $2V$

22. The cut-off wavelength for MMSIF is

- (a) $\frac{2.405}{\lambda V}$
 (b) $\frac{V^2}{2}$
 (c) $\frac{\lambda}{2.405V}$
 (d) $\frac{\lambda V}{2.405}$

23. For parabolic profile of core, the profile function α is
 (a) 1 (b) 3
 (c) 2 (d) 1.405
24. Rayleigh scattering losses occur due to:
 (a) impurities (b) density variation
 (c) inhomogenities (d) all of these
25. Microbends hinder the
 (a) dispersion (b) refraction
 (c) total internal reflection (d) polarization
26. To modify the refractive index of fiber, which dopants are used?
 (a) P_2O_6, B_2O_3 (b) Na_2O
 (c) CaO (d) Al_2O_3
27. Skew rays change the plane of propagation on reflections. (Yes/No).
28. The relation between K_p and K is given by
 (a) $K = \frac{K_p}{4.343}$ (b) $K_p = 4.343 K$
 (c) $\frac{K_p}{K} = 1$ (d) $K_p = \frac{K}{4.343}$
29. The Fermi energy for a metal is directly proportional
 (a) $(3\pi^2 N)^{1/3}$ (b) $(3\pi^2 N)^{2/3}$
 (c) $\left(\frac{1}{3\pi^2 N}\right)$ (d) $\left(\frac{3\pi^2 N}{V}\right)^{2/3}$
30. The effective mass is given by
 (a) $m_{\text{eff}} = \hbar^2 \left[\frac{d^2 E}{dk^2} \right]^{-1}$ (b) $m_{\text{eff}} = \hbar^2 [d k^2]$
 (c) $m_{\text{eff}} = \hbar^2 \left[\frac{dE}{dk} \right]$ (d) $m_{\text{eff}} = \hbar^2 \left[\frac{dE}{dk} \right]^{-1}$
31. When $k_B T \ll E_F$, then the Fermi–Dirac distribution function $f(E)$ becomes
 (a) 1 (b) 0
 (c) $\frac{1}{2}$ (d) ∞

32. The threshold condition for sustained oscillations is

(a) $K = \frac{L}{\gamma}$

(b) $K = \frac{\gamma}{L}$

(c) $K = \gamma L$

(d) $K = 1$

33. In direct semiconductors, the energy is released in the form of

(a) heat

(b) electricity

(c) light

(d) all of these

34. For the lasing action of semiconductor lasers, the wavelength range is

(a) 1000 – 2000 Å

(b) 2000 – 2500 Å

(c) 8400 – 8500 Å

(d) 9000 – 9500 Å

35. The amplification condition is

(a) $E_c - E_v = E_g$

(b) $E_v - E_c = E_g$

(c) $E_v - E_c > E_g$

(d) $E_c - E_v > E_g$

ANSWERS

1. (No)

2. (b)

3. (c)

4. (a)

5. (b)

6. (a)

7. (d)

8. (b)

9. (c)

10. (a)

11. (d)

12. (d)

13. (a)

14. (d)

15. (b)

16. (c)

17. (a)

18. (c)

19. (b)

20. (a)

21. (b)

22. (d)

23. (c)

24. (d)

25. (c)

26. (a)

27. (Yes)

28. (d)

29. (b)

30. (a)

31. (c)

32. (b)

33. (a)

34. (c)

35. (d)

Micro-Assessment Questions

1. What are optical fibers?
2. List the uses of optical fibers.
3. What is core of optical fiber? Give its properties.
4. Which part of optical fiber is responsible for optical fiber?
5. What is cladding of optical fiber?
6. Explain the sheath for optical fiber.
7. What are modes of optical fibers?
8. Define the terms acceptance angle and cone.
9. Define fractional refractive index change.
10. What is numerical aperture?
11. Define V -parameter.
12. Give the cut-off wavelength for multimode step index fibers.
13. What are the maximum modes supported by multimode step index fibers.
14. Define the profile function.
15. Explain the induced losses due to radiations.
16. Define the temperature dependent losses.
17. What do you understand by mode leaking?
18. What are mode-coupling losses?
19. Define the attenuation coefficient in decibels/km.
20. What is the difference between fiber attenuation and attenuation coefficient?
21. What do you understand by density states?
22. What is Fermi energy?
23. What are direct semiconductors?
24. What are indirect semiconductors?
25. What is the active medium of lasers?
26. Why is one mirror of laser cavity partially silvered?
27. Show the typical propagation of light through MMGIF.

Critical Thinking Questions

1. Explain the parts of optical fibers with the help of a schematic diagram.
2. What is total internal reflection? What are the conditions for total internal reflection?
3. What is the difference between single-mode and multimode fibers?
4. Derive the expression for acceptance angle of fiber.
5. Derive figure of merit for optical fibers. Give the relation between figure of merit and fractional refractive index change.
6. What are single-mode step index fibers?
7. Define the multimode step index fibers. How do they differ from single-mode step index fibers?
8. Explain the multimode graded index fiber. How is the refractive index variation given for them?
9. How the multimode graded index fibers differ from single-mode step index fibers?
10. What are Rayleigh scattering losses? Give the variation of scattering loss with wavelength.
11. With the help of a neat sketch, differentiate between microbend and macrobend losses.

12. What are material losses?
13. Differentiate between mode leaking and mode-coupling loss.
14. Define the band structure and density of states.
15. Obtain the energy at Fermi level for semiconductors.
16. What is effective mass of electrons?
17. Derive the expression for density of states. Show that it depends upon Fermi energy.
18. What do you understand from the quasi Fermi levels for semiconductors?
19. What is the difference between direct and indirect semiconductors?
20. Why semiconductor diode lasers cannot be operated for longer durations?
21. Which condition should be satisfied to obtain intense laser beam?
22. Give the threshold condition for sustained oscillations.
23. Show that when kT approaches Fermi energy, then the distribution is no longer Fermi–Dirac distribution.

Graded Questions

1. List the different types of optical fibers along with the schematic representation.
2. Explain in detail acceptance angle, numerical aperture, and acceptance cone. Also derive the mathematical expression for them.
3. List the various types of power losses in optical fibers.
4. Derive the total attenuation losses in optical fibers.
5. What are semiconductor diode lasers? Explain in detail their working and construction.
6. What is Fermi–Dirac distribution? Explain the different cases taking Fermi-energy in consideration.
7. What is Schawlow–Townes condition for lasers? Explain in detail.
8. Explain the quasifermi levels for degenerate p-type levels.
9. Give in detail the lasing action of semiconductor lasers.
10. Give the schematic band gap diagram for p–n junction diode during thermal equilibrium and forward biasing.

Remember and Understand

1. Optical fiber is used in optical communication as a waveguide. It is cylindrical in shape and is made from transparent dielectric material.
2. Core is the innermost part of optical fiber and is responsible for signal propagation.
3. According to the principle of total internal reflection, whenever light ray travels from denser to rarer medium, then at a certain critical angle, the light ray is reflected in the same medium.
4. The maximum value of angle of incidence is at the launching end so that the ray just propagated through the core of optical fibers is known as acceptance angle.
5. The ratio of difference between refractive index of core and cladding to refractive index of core is known as fractional refractive index change.

6. Numerical aperture is the figure of merit for optical fiber. Numerical aperture is defined as the sine of angle of acceptance for optical fiber.
7. For SMSIF, the refractive index of core is constant, whereas for graded index fibers, it is not constant.
8. The profile function for MMGIF determines the shape of core profile.
9. The attenuation coefficient is defined as the reciprocal of distance at which the power is reduced to $1/e$ times as that of initial power.
10. For solid-state structure, the Fermi energy represents the energy corresponding to a Fermi level such that all the levels above it are empty at 0 K and the levels below Fermi level are filled.

Crystal Structure

Keywords: crystal lattice, Miller indices, Bravais lattice, close packing, packing fraction, coordination number, ionic radii, Bragg's law, Laue's theory, rotating crystal method, powder diffraction method, Brillouin zones, reciprocal lattice, atomic scattering factor, geometrical scattering factor

LEARNING OBJECTIVES

- ◆ To know about the difference between crystalline and amorphous solids on the basis of atomic arrangement
- ◆ To understand the crystal structure and its types
- ◆ To know about basis, motif, unit cells, and basic types of symmetry operations for crystal
- ◆ To gain insight of lattice parameters and Bravais lattices
- ◆ To learn about the crystal planes and Miller indices
- ◆ To calculate interplanar spacing for different types of lattices
- ◆ To know about cubic systems, that is, simple cubic, body-centered cubic (BCC), and face-centered cubic (FCC)
- ◆ To learn about the packing fraction and packing of spheres in crystals
- ◆ To know about X-ray diffraction pattern using Bragg's diffraction pattern
- ◆ To understand Laue's theory of X-ray diffraction
- ◆ To learn about different diffraction patterns
- ◆ To get an insight of reciprocal lattice for BCC, FCC, and simple cubic lattice
- ◆ To know about k -space
- ◆ To understand Brillouin zones
- ◆ To know about Brillouin zones for simple cubic, face-centered, and BCC lattice
- ◆ To learn about the importance of atomic scattering factor
- ◆ To learn about the importance and significance of geometrical scattering factor

16.1 Crystalline and Amorphous Solids

The basic states of matter are solids, liquids, and gases. Plasma is regarded as the fourth state of matter. Solids possess definite shape and size and are composed of well-described structural units. In case of liquid and gases, the atoms are usually in random motion due to large interatomic separations in

between them. The solids are also classified in two broad categories: crystalline and amorphous solids. These are discussed in the sections that follow.

16.1.1 Crystalline Solids

For crystalline solids, the atoms, ions, or molecules are arranged in definite three-dimensional array. Every atom or constituent ion occupies a well-defined position in space w.r.t. neighboring atoms. “Crystalline” is derived from Greek work “crystalles,” which means clear. The following are the salient features of crystalline solids.

- (i) The structural units of crystalline solids repeat themselves over regular intervals.
- (ii) Crystalline solids possess definite external geometry.
- (iii) All the bonds between atoms are of equal strength for crystalline solids.
- (iv) Crystalline solids have sharp melting and boiling point because all the bonds break at the same time.
- (v) Crystalline solids are anisotropic in nature; that is, they have different properties in different directions.

Some examples include calcite, mica, quartz, diamond, etc. Crystals can be monocrystal if it is a single crystal; it can be polycrystal, if it is an aggregation of large number of crystals. For polycrystals, the periodicity of the crystal is interrupted at the grain boundaries. The schematic of a crystalline solid is shown in Figure 16.1.



Figure 16.1 Crystalline pattern.

When we come across crystals, we should be familiar with the term “grain.” Grain is an array within which the structure is periodic. Grain can have macroscopic or microscopic dimensions.

16.1.2 Amorphous Solids

Solids in which the atoms or constituent ions are not arranged in regular or definite pattern are known as amorphous solids. The position of atoms or ions is not fixed w.r.t. each other. The following are the salient features of amorphous solids:

- (i) The structural units of amorphous solids do not repeat them over regular interval in space.
- (ii) They do not possess definite shape and size.
- (iii) The bonds between atoms of amorphous solids are not of equal strength.
- (iv) They do not exhibit sharp melting and boiling point because weaker bonds will break first and stronger bonds will break next.
- (v) Amorphous solids are isotropic in nature; that is, they exhibit same properties in all the directions.

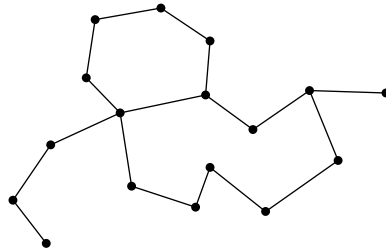


Figure 16.2 Amorphous solid structure.

Some examples include glass, plastic, rubber, etc. In amorphous solids, grains play an important role. For amorphous solids, the grain size becomes very small and comparable to unit. Figure 16.2 demonstrates the structure of amorphous solids. Crystallography deals with the geometric and physical properties of crystalline solids using neutron beams, electron beams, and X-rays.

16.2 Crystal Structure

In a crystal, atoms are arranged in periodic array. Every atom or molecule is represented by a representative unit; that is, the units are represented by mathematical points. These representative units are known as motifs (Figure 16.3). When these motifs are extended in space such that every mathematical point possesses identical surroundings, then this collection of infinite array of points constitutes lattice.

In Figure 16.3, \vec{a} and \vec{b} are translational vectors. If we see AB, then its magnitude is a and the magnitude of AC is also a . The magnitude of AD is $\sqrt{2}a$. If we consider any other point, then also the same distances are observed corresponding to the nearest neighbor and diagonal neighbor. Hence, every point has identical surroundings. The lattice represented in Figure 16.3 is a square lattice, but it can be either rectangular shaped or parallelogram shaped. In Figure 16.3, the square unit is repeating itself over regular space intervals.

Let us take \vec{T} as the translational vector, such that

$$\vec{T} = n_1\vec{a} + n_2\vec{b} \tag{1}$$

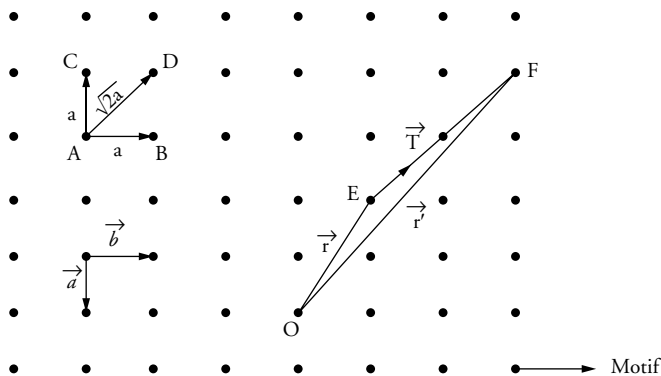


Figure 16.3 Lattice and motifs (in 2-D lattice).

n_1 and n_2 are integers and \vec{a} , \vec{b} are fundamental translational vectors. In 3-D, there is one more translational vector c , such that \vec{T} becomes

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad (2)$$

Two types of operations can be applied in ΔOEF , that is

$$\vec{r}' = \vec{r} + \vec{T}$$

$$\vec{r}' = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad (3)$$

Two cases may arise for Eqn. (3) as follows:

- (i) If n_1 , n_2 , and n_3 have integer values, then the fundamental translation vectors are primitive.
- (ii) If n_1 , n_2 , and n_3 have noninteger values, then the fundamental translation vectors are said to be non-primitive.

The crystal system can be very well defined using the translational vectors.

16.3 Basis and Symmetry Operations

In Section 16.2, we have studied about infinite array of atoms known as lattice to obtain a crystal structure; a group of atom should be added to every lattice point. This group of atoms is known as basis. To interpret physical structure of a crystal, every lattice point is associated to group of atoms. Basis may contain several atoms. Ionic crystals are associated with two types of ions: positive and negative. The relation between basis and crystal is shown in Figure 16.4.

In Figure 16.4, there are two basis atoms: positive and negative. The center of basis should coincide with every lattice point. The basis is usually regarded as the assembly of atoms that are identical in their arrangement, orientation, as well as composition. The number of basis atoms can be very large, but the number of space lattices is limited. There are 14 basic types of space lattices. For every crystal, there are some operations that leave the crystal unchanged. Hence, symmetry operations are defined as the operation that leaves crystal invariant, and the atoms yield identical features. Before we start for symmetry operations, we need to know about some basic symmetry element of the crystal as follows:

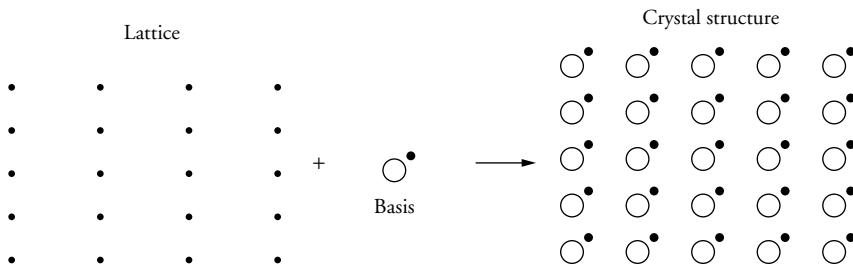


Figure 16.4 Lattice and crystal structure.

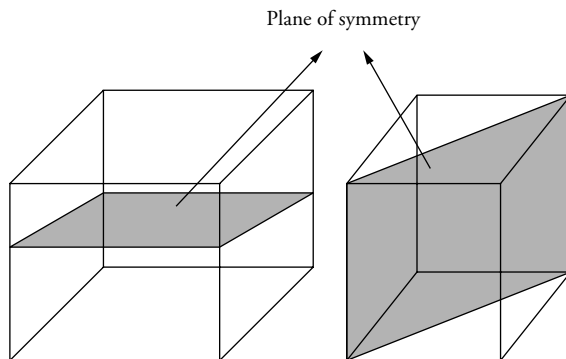


Figure 16.5 Planes of symmetry for cubic lattice.

16.3.1 Symmetry Plane

The symmetry plane is an imaginary plane that is supposed to divide the lattice into two equal halves. For a cube, there are three planes that are perpendicular to the parallel faces of cube and 6 diagonal planes as shown in Figure 16.5.

16.3.2 Symmetry Centre

Centre of symmetry is point in crystal so that for point \vec{r} , there also exists $-\vec{r}$ w.r.t. fixed position 0. The same point of crystal is obtained at \vec{r} and $-\vec{r}$.

16.3.3 Symmetry Axis

Let us suppose, there are four points: T , P , Q , and U (Figure 16.6). Let the system has n -fold symmetry operation such that if point T and U rotate at an angle θ , it yields points R and S , provided $RP = QS = QU = TP = a$. It can be mathematically represented as follows:

$$RS = RP' + P'Q' + Q'S$$

$$RS = a + a \cos \theta + a \cos \theta$$

$$RS = a(1 + 2 \cos \theta)$$

Let $RS = xa$, that is, translation of vector a .

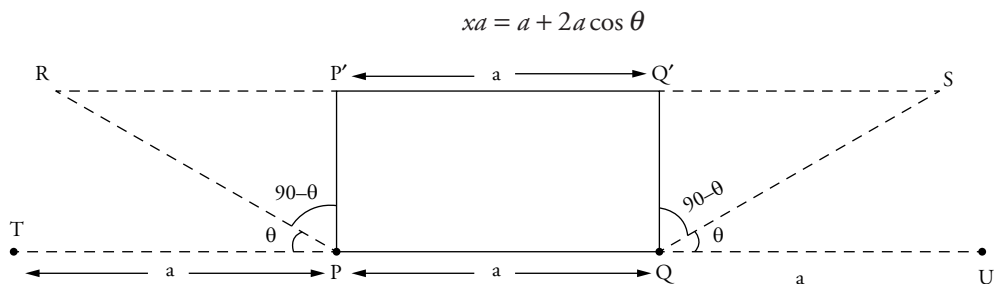


Figure 16.6 Rotation symmetry.

$$(x-1)a = 2a \cos \theta \quad [x]$$

$$\frac{(x-1)}{2} = \cos \theta$$

$$\cos \theta = \frac{N}{2} \quad [x-1 = N] \text{ also an integer} \quad (4)$$

as $-1 \leq \cos \theta \leq 1$, hence $-2 \leq N \leq 2$.

Hence, N can have values $-2, -1, 0, 1,$ and 2 .

We know that

$$n = \frac{360}{\theta} \quad (5)$$

For $\cos \theta = -1, 1/2, 0, 1, 2$ and 1 , we obtain $n = 2, 3, 4, 6$ and 1 , respectively. Hence, five-fold and seven-fold symmetry do not exist.

Now, we can discuss the symmetry operations; there are four different symmetry operations as discussed below:

- (i) **Rotation operation:** A body is said to possess rotational symmetry if it remains invariant after a rotation of angle (Figure 16.7). The crystal is said to exhibit n -fold symmetry, if after the rotation of $\frac{360}{n}$ angle, the crystal remains invariant. We have seen that five-fold and seven-fold symmetry axis does not exist.
- (ii) **Translational operation:** In this operation, the atoms repeat themselves after a distance a in given direction. The lattice remains invariant as shown in Figure 16.8.
- (iii) **Reflection operation:** The crystal is said to exhibit reflection operation such that if there is a plane dividing the crystal into two halves, then the system changes from left-handed system to right-handed system. In other words, the identical halves are mirror images of each other (Figure 16.9).
- (iv) **Inversion operation:** The inversion operation changes the system from left handed to right handed along with the change of position from \vec{r} to $-\vec{r}$ with respect to certain point known as inversion center (Figure 16.10).

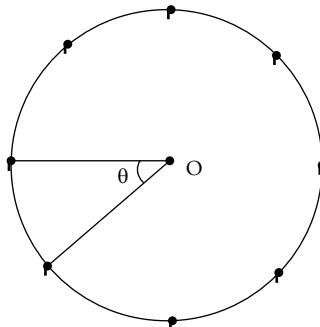


Figure 16.7 Rotational operation.



Figure 16.8 Translation operation.

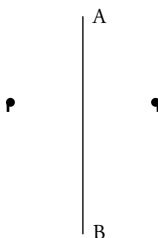


Figure 16.9 Reflection operation.

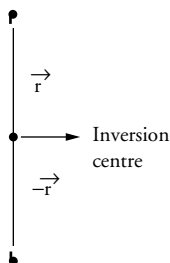


Figure 16.10 Inversion operation.

16.4 Unit and Primitive Cells

As demonstrated in Figure 16.11, if AB and CD is translated by vectors \vec{a} and \vec{b} , we may obtain an orthorhombic crystal, $[\alpha = \beta = 90^\circ]$. Hence, ABCD is the representative unit which when repeated will generate the whole lattice structure. Therefore, ABCD is regarded as the unit cell. If we take a 3-D case, such that there is a third vector \vec{c} also, then \vec{a} , \vec{b} , \vec{c} repeat themselves in space producing the entire crystal structure. Hence, the unit cell is defined as the smallest geometrical entity, which when repeated in space generates the entire crystal structure. It is the elementary building block of the lattice structure. There are two types of unit cells: primitive and non-primitive cells. The primitive unit cells possess minimum volume and the lattice points are present only at the corners. Hence, the primitive cells contain one complete unit of pattern. In the case of non-primitive cells, the lattice points can be at the center or face of unit cell. In Figure 16.11, EFGH represent a non-primitive cell. Orthorhombic has base-centered and body-centered cells, hence, they are doubly primitive cells. The volume of primitive cell is $\vec{a} \cdot (\vec{b} \times \vec{c})$.

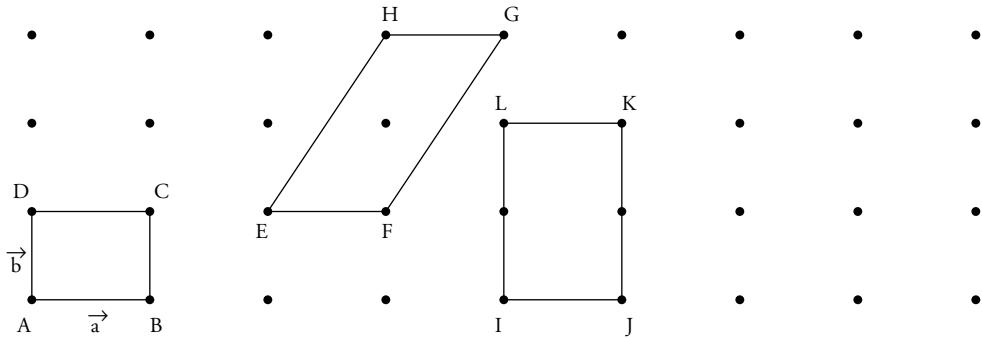


Figure 16.11 Two-dimensional lattice demonstrating unit cells.

16.5 Lattice Parameters and Types of Lattices

The unit cell is composed of three crystallographic axes and three interfacial angles. This collection of six parameters defines the lattice parameter for a unit cell. In Figure 16.12 OX, OY, and OZ are crystallographic axes. The crystallographic axes are drawn parallel to the line of intersection of two adjacent faces of the unit cell. The angles between these crystallographic axes are known as interfacial angle a , b , and c are the dimensions of unit cells and are known as primitives/intercepts. The angle between OX and OY is γ , between OX and OZ is β , and between OY and OZ is α , respectively. The points in the lattice can be arranged in different ways. But the symmetry operations and condition of identical surroundings should be kept in consideration. In 1848, Bravais introduced different types of lattice in two and three dimensions. There are five Bravais lattices in two dimensions and 14 Bravais lattices in three dimensions as demonstrated below:

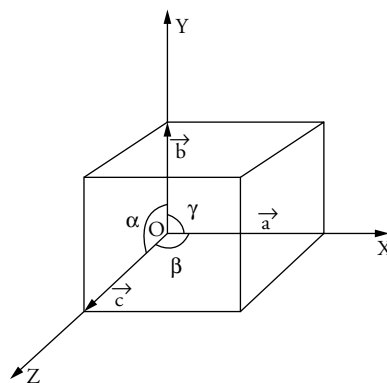


Figure 16.12 Lattice parameters for unit cell.

16.5.1 Two-Dimensional Lattices

The translations of \vec{a} and \vec{b} in two dimensions result in five Bravais lattices in two dimensions. Rectangular lattices are of two types: primitive (non-centered) and non-primitive (centered) as shown in Figure 16.13.

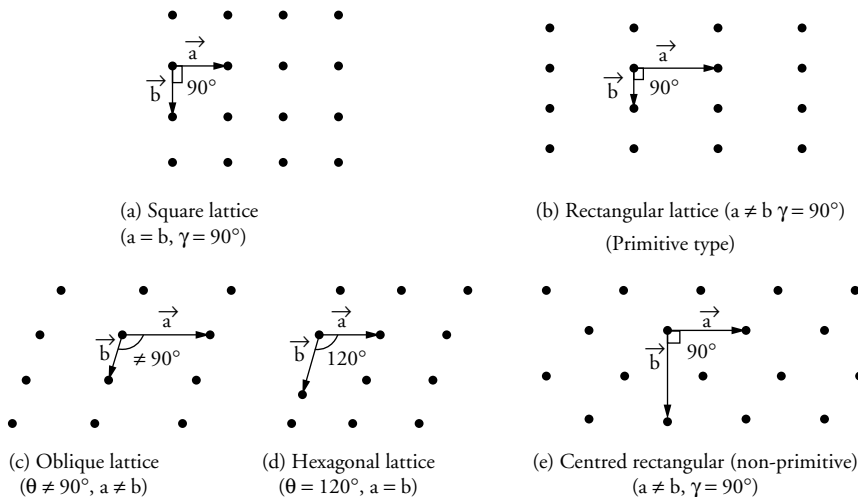


Figure 16.13 Bravais lattices in two dimensions.

16.5.2 Three-Dimensional Lattices

There are seven crystal systems and the points can be arranged into 14 ways, which are described as follows:

- (i) **Triclinic lattice:** This system exhibits only one Bravais lattice system. In triclinic arrangement, none of the interfacial angles is 90° and no intercept is equal (Figure 16.14(a)).

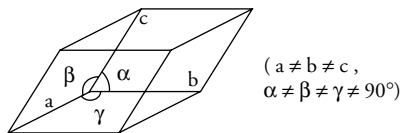


Figure 16.14(a) Triclinic arrangement (simple).

- (ii) **Trigonal lattice:** It is also known as rhombohedral arrangement, and it has one Bravais lattice. All the intercepts are equal, and all the interfacial angles are equal, but they are not equal to 90° (Figure 16.14(b)).

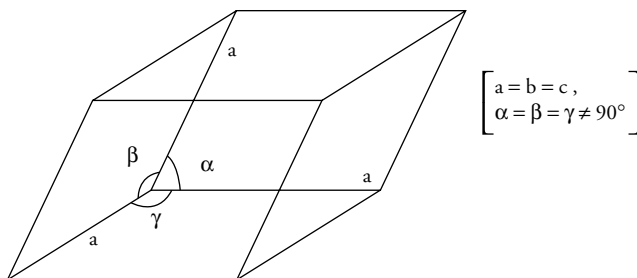


Figure 16.14(b) Trigonal lattice (simple).

- (iii) **Hexagonal lattice:** It has one Bravais lattice, two axes are coplanar, equal, and inclined at an angle of 120° to each other. The third axis is perpendicular to other two and is not equal to any of the axis, that is, $a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ (Figure 16.14(c)).

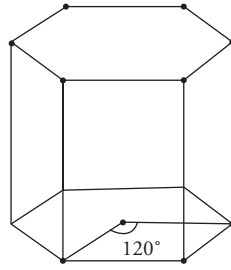


Figure 16.14(c) Hexagonal lattice (simple).

- (iv) **Monoclinic lattice:** It has two types of Bravais lattice: simple and base centered. In simple monoclinic lattice, the points occupy the corners only; whereas in base-centered lattice, there are two points that occupy the opposite faces of unit cell along with the corners. The axes are not equal for monoclinic lattice. Two interfacial angles are equal to 90° , and the third is not equal to 90° (Figure 16.14(d)).

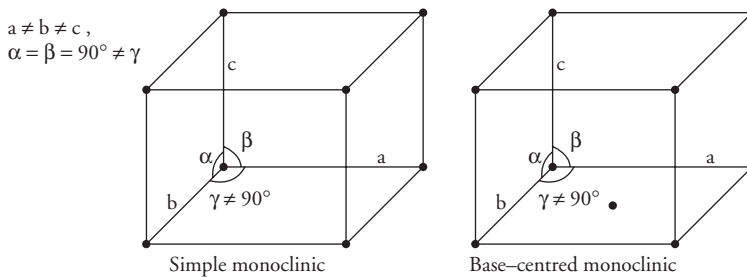


Figure 16.14(d) Monoclinic lattice.

- (v) **Tetragonal lattice:** It has two Bravais lattice: simple and base-centered. The three-crystallographic axes are perpendicular to each other. Two intercepts are equal to each other but are not equal to the third intercept. In simple tetragonal lattice, all the points occupy the corners; whereas in base-centered lattice, in addition to corners, the points are also present at the base, that is, $a = b \neq c$, and $\alpha = \beta = \gamma = 90^\circ$ (Figure 16.14(e)).

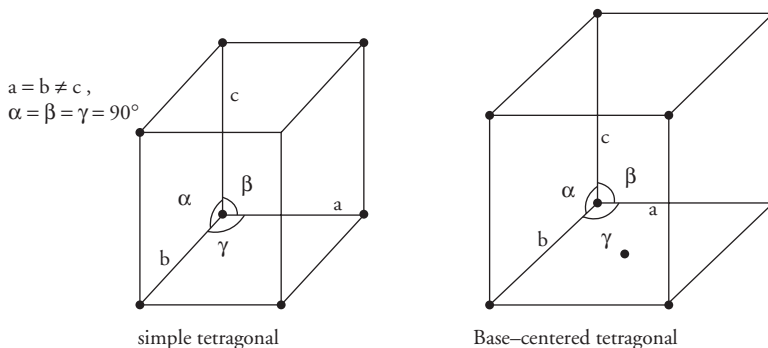


Figure 16.14(e) Tetragonal lattice.

- (vi) **Cubic lattice:** It has three Bravais lattices, that is, simple, body-centered, and face-centered. In face-centered lattice, points are present at the faces also in addition to corners. The axes are equal and are perpendicular to each other, that is, $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$ (Figure 16.14(f)).

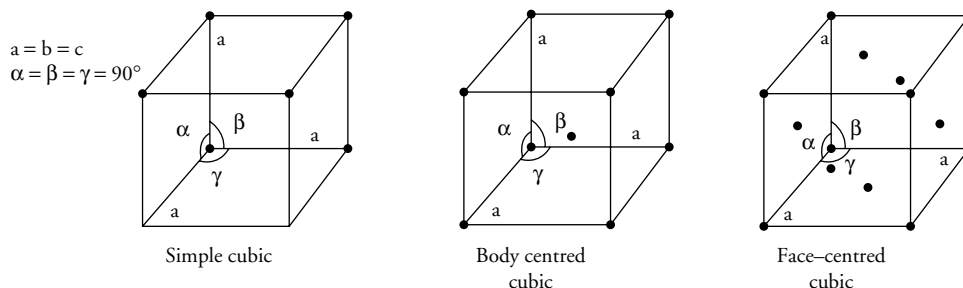


Figure 16.14(f) Cubic lattice.

- (vii) **Orthorhombic lattice:** It has four Bravais lattices: simple, body centered, base-centered, and face-centered. The axes are not equal, and all the angles are 90° , that is, $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$ (Figure 16.14(g)).

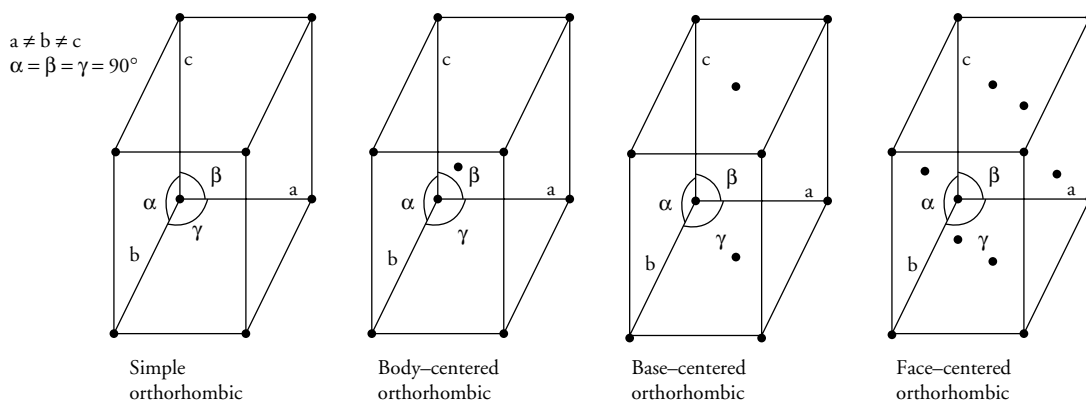


Figure 16.14(g) Orthorhombic lattices.

16.6 Introduction to Miller Indices and Crystal Planes

In Section 16.1, we have studied about crystalline and amorphous solids. Amorphous solids are isotropic, possessing similar properties in all the directions, but this is not the case with crystalline solids; crystalline solids are anisotropic in nature; that is, they have different properties in different directions. Hence, to understand the directions and planes for crystal is very important aspect. Miller devised a system of indices to represent different set of planes within the crystals known as Miller indices. Miller indices describe the directions and orientations of planes. For getting insight of Miller indices, we need to know about the reference system which we shall choose. The direction in general is denoted by $[uvw]$. The group of

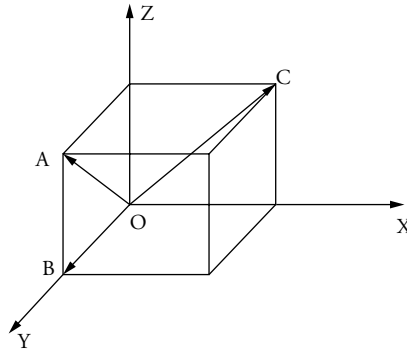


Figure 16.15 Crystal directions.

directions is given by $\langle uvw \rangle$. The Miller indices of a plane are denoted by (hkl) . A family or group of planes is given by $\{hkl\}$. In Figure 16.15, we can obtain the Miller directions that are given for OA, OB, and OC. OA is given by $[01\bar{1}]$, OB is given by $[0\bar{1}0]$, and OC is given by $[101]$. For $[01\bar{1}]$, the equivalent directions are $[100]$, $[001]$, $[\bar{1}00]$, $[0\bar{1}0]$, and $[00\bar{1}]$. The group of directions is given by $\langle 100 \rangle$.

To obtain Miller indices of crystal planes, we shall proceed as follows (using Figure 16.16).

- (i) Obtain point O as the origin and get the vectors in direction of X, Y, and Z w.r.t. origin.
- (ii) Obtain the intercepts of the plane whose Miller indices are to be determined on 3-D axis. In Figure 16.16, x , y , and z are the intercepts.
- (iii) Further, we have to express the intercepts in terms of primitive vectors, that is, $x = n_1a$, $y = n_2b$, and $z = n_3c$.

Here $x = 4a$, $y = 3b$, and $z = 4c$

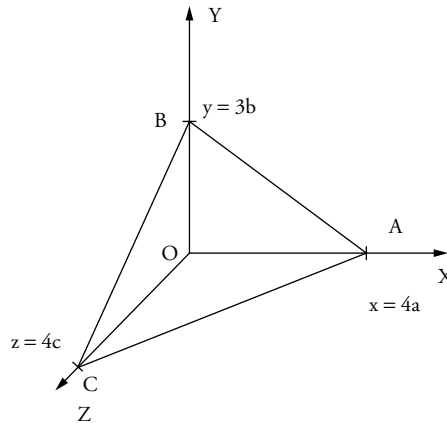


Figure 16.16 Determination of Miller indices for planes.

(iv) Obtain n_1 , n_2 , and n_3 and their reciprocals.

$$\text{That is, } \frac{1}{n_1} : \frac{1}{n_2} : \frac{1}{n_3} = \frac{1}{4} : \frac{1}{3} : \frac{1}{4}$$

- (v) Convert the reciprocals to smallest integers (hkl), that is, (3:4:3) which is obtained after taking LCM.
- (vi) (343) are the Miller indices of plane ABC. Hence, we can obtain a family of planes to be $\{343\}$.

16.7 Interplanar Spacing

Take a lattice point O as the origin of planes with Miller indices (hkl) (Figure 16.17). Using these Miller indices, draw the crystallographic axes OX, OY, and OZ. Let an adjacent plane possess the Miller indices (hkl). From origin O, draw a perpendicular $OP = d$ to this adjacent plane. “ d ” is known as the interplanar distance between the planes (hkl).

Let OP make angles α , β , and γ with OX, OY, and OZ, respectively. Here, α , β , and γ are not the interfacial angles.

For OP, the direction cosines are given by $\cos\alpha$, $\cos\beta$, and $\cos\gamma$. OA, OB, and OC are intercepts made by plane on the axes.

$$OA = \frac{a}{h}, \quad OB = \frac{b}{k}, \quad \text{and} \quad OC = \frac{c}{l} \quad (6)$$

a , b , and c are the lattice parameters.

In ΔOAP ,

$$\cos\alpha = \frac{OP}{OA} = \frac{d}{a/h} = \frac{hd}{a} \quad (7a)$$

In ΔOBP ,

$$\cos\beta = \frac{OP}{OB} = \frac{d}{b/k} = \frac{dk}{b} \quad (7b)$$

Similarly in ΔOCP ,

$$\cos\gamma = \frac{OP}{OC} = \frac{d}{c/l} = \frac{dl}{c} \quad (7c)$$

For planes, the sum of squares of all direction cosines is unity.

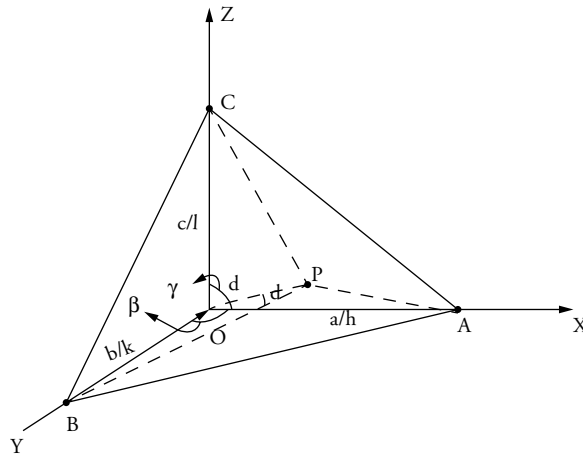


Figure 16.17 Interplanar spacing and Miller indices.

$$\Rightarrow \cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$$

$$\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{b}\right)^2 + \left(\frac{dl}{c}\right)^2 = 1$$

$$\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} = \frac{1}{d^2}$$

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad (8)$$

Equation (8) represents the interplanar distance between two planes.

For cubic system, $a = b = c$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (9)$$

There are some important noteworthy points for Miller indices as follows:

- (i) A set of planes could be defined using Miller indices.
- (ii) All the equidistant planes have the same Miller indices (hkl) .
- (iii) For a parallel plane, the intercept is ∞ , and hence the Miller index is zero.
- (iv) For a plane, (246) and (123) will represent the same set of planes.

16.8 Cubic Systems

The crystal system that exhibits the unit cell to be a cube is called cubic system. Depending on the number of atoms present in every cube, the unit cells can be distinguished into simple cubic, BCC, and FCC. Every cubic system possesses definite characteristics. That is, volume, number of atoms/unit cell, coordination number, atomic radius, density of unit cell, packing fraction. In this section, the unit cells and their characteristics are discussed.

16.8.1 Simple Cubic Crystal

For a simple cubic system, the atoms are present only at the corners of the cube as shown in Figure 16.18.

Every atom is shared by eight such cubes. Hence, the contribution of every atom at the corner is $\frac{1}{8}$.

For example, CsCl_2 , NH_4Cl , and polonium have such kind of unit cell.

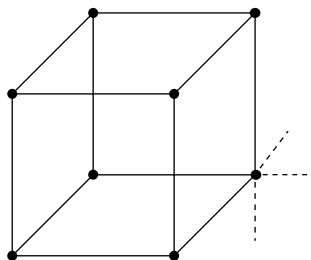


Figure 16.18 Simple cubic system.

Properties of Simple Cubic Crystal

- (i) **Volume:** The primitives of cube are equal yielding $a = b = c$, and hence the volume $V = a^3$ (10a)
- (ii) **Number of atoms/unit cell:** Every corner atom is shared by eight similar unit cells, and hence, the contribution of every atom is $\frac{1}{8}$. There are eight total atoms. Hence, N becomes

$$N = 8 \times \frac{1}{8} \quad (\text{contribution of every atom} = 1)$$

$$N = 1 \quad (\text{for simple cubic}) \quad (10b)$$

- (iii) **Coordination number:** The number of neighboring atoms that surround each atom in a lattice is known as coordination number. For simple cubic lattice, there are six neighbors that surround every corner atom. Hence,

$$\text{CN} = 6 \quad (\text{for simple cubic}) \quad (10c)$$

- (iv) **Atomic radius (r):** Usually, atoms are considered to be hard spheres surrounding each other. The atomic radius (Figure 16.19) is given by exactly half of the distance between two nearest neighbors (a). Hence, for simple cubic lattice

$$r = \frac{a}{2} \quad (10d)$$

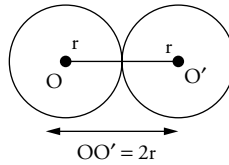


Figure 16.19 Atomic radius.

- (v) **Packing fraction (PF):** It is defined as the ratio of volume occupied by atoms to the total volume of unit cell. Hence,

$$\text{PF} = \frac{\text{Volume occupied by atoms in unit cell}}{\text{Total volume of unit cell}}$$

For simple cubic system,
$$\text{PF} = \frac{\text{Volume occupied by atoms}}{a^3}$$

Every atom has volume $\frac{4}{3}\pi r^3$

If there are N atoms, then the volume becomes $N \cdot \frac{4}{3}\pi r^3$. In simple cubic system, $N = 1$.

Hence, the volume occupied by atoms is $1 \cdot \frac{4}{3}\pi r^3$

$$\Rightarrow \text{PF} = \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 0.523 \quad [\text{using Eqn. (10d)}]$$

$$\therefore \text{PF} = 0.523$$

$$\text{PF} = 52.3\% \quad (10e)$$

Hence, in simple cubic systems, only 52.3 percent of volume of unit cells is occupied.

- (vi) **Density:** Let M be the molecular weight of crystal. Let there be N molecules/crystal. If N' is Avogadro's number, then

$$\text{Mass of } N' \text{ molecules} = M \text{ g}$$

$$\text{Mass of 1 molecule} = \frac{M}{N'} \text{ g}$$

$$\text{Mass of } N \text{ molecules} = \frac{M}{N'} N = m$$

$$m = \frac{M}{N'} N \quad (10f)$$

Let ρ be the density of crystal and a be the edge of unit cell, then

$$\frac{\text{mass}}{\text{volume}} = \text{density}(\rho)$$

$$\rho = \frac{m}{a^3}$$

Using Eqn. 10f,

$$\rho = \frac{MN}{N' a^3} \quad (10g)$$

Hence, Eqn. (10g) represents density for a crystal.

For simple cubic crystal, $N = 1$.

$$\Rightarrow \rho = \frac{M}{N' a^3} \quad (10h)$$

16.8.2 Body-Centered Cubic

For BCC, in addition to eight corner atoms, there is one additional atom present inside the body of the cube. For example, sodium, tungsten, tantalum, etc. possess BCC structure (Figure 16.20).

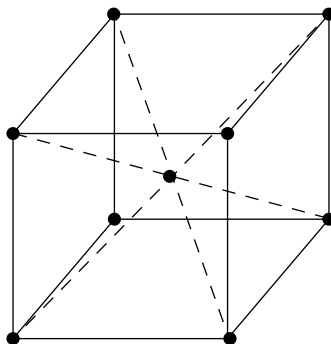


Figure 16.20 BCC unit cell.

Properties of BCC

(i) **Volume:** The primitives are equal, hence the volume is

$$\Rightarrow V = a^3 \quad (11a)$$

(ii) **Number of atoms/unit cell:** Corner atoms contribute to $\frac{1}{8}$ /unit cell, whereas the atom at center of unit cell belongs to one unit cell only.

$$N = \frac{1}{8} \times 8(\text{corner})\text{atoms} + 1(\text{atom at body centre})$$

$$N = 1 + 1 = 2$$

$$\Rightarrow N = 2 \quad (11b)$$

(iii) **Coordination number:** To every central atom, there are eight nearest neighbors. Hence,

$$\text{CN} = 8 \quad (11c)$$

(iv) **Atomic radius (r):** If we see along the diagonal, then we get Figure 16.21.
The diagonal $AD = 4r$

$$AC = \sqrt{AB^2 + BC^2}$$

$$AC = \sqrt{2a^2}$$

$$\Rightarrow AC = \sqrt{2}a \quad (11d)$$

In $\triangle ADC$,

$$AD^2 = AC^2 + CD^2$$

$$(4r)^2 = (\sqrt{2}a)^2 + a^2$$

$$\Rightarrow 16r^2 = 3a^2$$

$$\Rightarrow r^2 = \frac{3}{16}a^2$$

Hence, atomic radius $r = \frac{\sqrt{3}}{4}a$ (for BCC lattice) (11e)

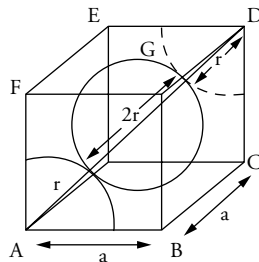


Figure 16.21 BCC diagonal.

(v) **Packing fraction (PF):** For BCC lattice, $N = 2$

Therefore, $PF = \frac{\text{Volume occupied by atoms in unit cell}}{\text{Total volume of unit cell}}$

$$\Rightarrow PF = \frac{N \cdot \frac{4}{3} \pi r^3}{a^3}$$

$$\Rightarrow PF = \frac{2 \times \frac{4}{3} \pi \left(\frac{\sqrt{3}}{4} a \right)^3}{a^3} \quad [\text{using Eqn. (11e)}]$$

$$\Rightarrow PF = \frac{\frac{8}{3} \pi \times \frac{3\sqrt{3}}{16 \times 4} a^3}{a^3} = \frac{\pi\sqrt{3}}{8} = \frac{3.14}{8} \times 1.73 = 0.68$$

$$\Rightarrow PF = 0.68$$

$$\Rightarrow PF = 68\% \quad (11f)$$

Hence, in BCC lattice, 68 percent of the volume is occupied/unit cell.

(vi) **Density:** From Eqn. (10g), the density is given by

$$\rho = \frac{M}{N' a^3} N$$

Here, $N = 2$

$$\rho = \frac{2M}{N' a^3} \quad (11g)$$

16.8.3 Face-Centered Cubic

In FCC, there are eight atoms at corners and six are present at faces. That is, every corner contains one atom and every face contains one atom. For example, aluminum, nickel, lead, and silver have FCC structure (Figure 16.22).

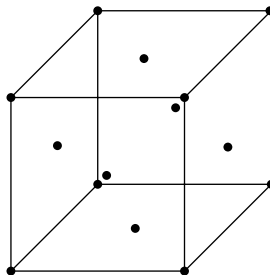


Figure 16.22 Face-centered cubic structure.

Properties of FCC

- (i) **Volume:** The primitives are same yielding:

$$\text{Volume } V = a^3 \quad (12a)$$

- (ii) **Number of atoms/unit cell:** In addition to eight corner atoms, there are six atoms present at face. Each corner atom is shared by eight atoms, whereas every face atom is shared by two unit cell. Hence,

$$N = 8 \times \frac{1}{8} (\text{shared at corners}) + 6 \times \frac{1}{2} (\text{shared at faces})$$

$$N = 1 + 3 = 4$$

$$\Rightarrow N = 4 \quad (\text{for FCC}) \quad (12b)$$

- (iii) **Coordination number:** Every face-centered atoms is touched by 4 corner atoms, 4 face-centered atoms of first unit cell and 4 face-centered atoms of second unit cell as shown in Figure 16.23. Hence,

$$\text{CN} = 12 \quad (12c)$$

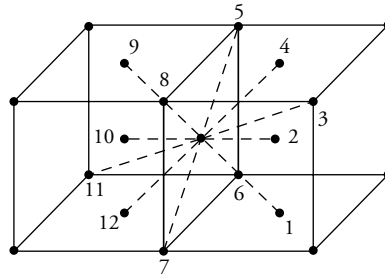


Figure 16.23 Coordination number for FCC.

- (iv) **Atomic radius (r):** The face can be interpreted as shown in Figure 16.24. In $\triangle ABC$

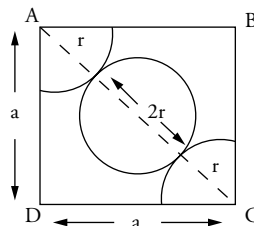


Figure 16.24 Face of FCC crystal.

$$\begin{aligned} AC^2 &= AD^2 + CD^2 \\ (4r)^2 &= a^2 + a^2 \\ 16r &= 2a^2 \\ \Rightarrow r^2 &= \frac{2}{16}a^2 \end{aligned}$$

Hence, atomic radius $r = \frac{\sqrt{2}}{4}a$ (for FCC lattice) (12d)

(v) **Packing fraction (PF):** For FCC lattice $N = 4$ and $r = \frac{\sqrt{2}}{4}a$

$$\begin{aligned} \Rightarrow \text{PF} &= \frac{N \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{4 \cdot \frac{4}{3}\pi \left(\frac{\sqrt{2}}{4}a\right)^3}{a^3} \\ \Rightarrow \text{PF} &= \frac{16\pi}{3a^3} \left(\frac{2\sqrt{2}a^3}{64}\right) = \frac{\sqrt{2}}{6}\pi = 0.74 \\ \Rightarrow \text{PF} &= 74\% \end{aligned} \quad (12e)$$

Hence, in FCC lattice, atoms occupy 74 percent of the available space.

(vi) **Density:** For FCC lattice, $N = 4$

Hence,

$$\begin{aligned} \rho &= \frac{MN}{N'a^3} \\ \Rightarrow \rho &= \frac{4M}{N'a^3} \end{aligned} \quad (12f)$$

16.9 Packing of Spheres in Crystals

Atoms are considered to be hard spheres of equal size. They can be arranged as shown in Figure 16.25(a). As is clear from Figure 16.25(a), every sphere is surrounded by six spheres. The center of spheres lies at the corners of equilateral triangle. Let this layer represent layer A. There are two ways in which we can proceed to stack other layers. They are described as follows: ABAB stacking and ABCABC stacking.

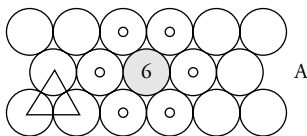


Figure 16.25 (a) Arrangement of atom.

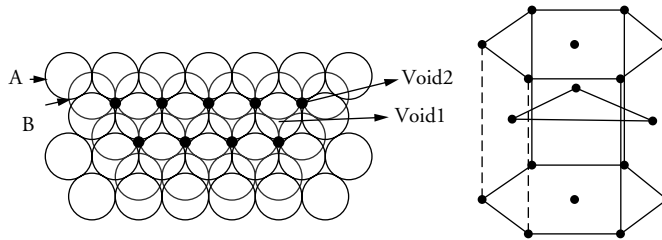


Figure 16.25(b) Stacking of B layer on A layer **Figure 16.25 (c)** Hexagonal arrangement is followed if ABAB ... is followed.

- (i) **ABAB stacking:** In Figure 16.25(b), it is clear that in between the spheres, there are voids (shown by black). If we place another layer over the voids, then B layer is formed (Figure 16.25(b)) two types of voids are formed over layer B. One is marked 1 and other 2. If we place atoms above the voids marked 1, then the center of symmetry of atoms match with those of A-layer atoms. Hence, we obtain A layer over B layer again. This type of arrangement is ABABAB ... and it leads to hexagonal close packing (HCP).
- (ii) **ABCABC stacking:** In Figure 16.25(c), two types of voids could be seen on the layer B, (one marked as 1 and the other as 2). If we place the third layer above voids marked 2, then we get another layer C. Hence, we get ABCABC arrangement. This type of layer has cubical symmetry.

16.10 Structure for Different Elements

There are different structures of elements that are discussed in the section that follows.

16.10.1 Diamond Cubic Structure

Diamond structure is made from two interpenetrating structures (Figure 16.26(a)). Diamond structure has two atoms/lattice point. Among two interpenetrating structures, one has the origin at $(0, 0, 0)$ and the second lattice has origin at $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$, where a is the lattice constant. Hence, the origin of the second lattice is at $\frac{1}{4}$ th of body diagonal. For diamond lattices, there are eight atoms/unit cell. The positives of atoms are given in Figure 16.26(b). $\frac{a}{2}$ and 0 are present on FCC, whereas $\frac{a}{4}$ and $\frac{3a}{4}$ are obtained by displacing the first lattice by $\frac{a}{4}$. Hence, $(0, 0, 0)$ and $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$, there are two identical atoms. Now we will calculate the packing fraction.

For diamond, $N = 8$

[3 are at faces, 4 inside the cell, and 1 at corner]

$$\text{PF} = \frac{N \cdot \frac{4}{3} \pi r^3}{a^3}$$

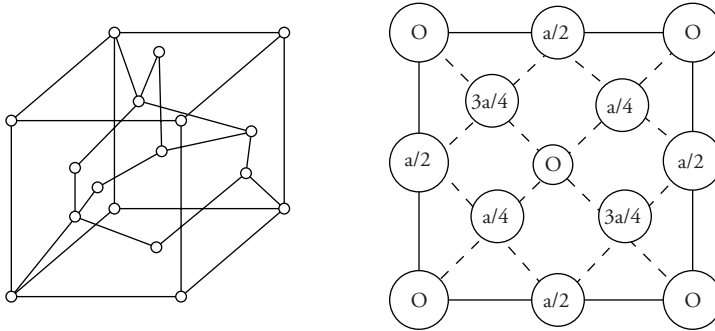


Figure 16.26(a) Diamond structure.

(b) Atomic position in diamond structure.

$$\Rightarrow \text{PF} = \frac{8 \times \frac{4}{3} \pi r^3}{a^3}$$

From Figure 16.26(b),

$$\Rightarrow r + 2r + 2r + 2r + r = \sqrt{3}a$$

$$\Rightarrow 8r = \sqrt{3}a$$

$$\Rightarrow r = \frac{\sqrt{3}a}{8} \quad (13)$$

Hence,
$$\text{PF} = \frac{32\pi}{3a^3} \left(\frac{\sqrt{3}a}{8} \right)^3 = \frac{32 \times 3 \sqrt{3} \pi a^3}{24a^3}$$

$$\text{PF} = \frac{\sqrt{3}\pi}{16} = 0.34$$

Hence,

$$\text{PF} = 34\% \quad (14)$$

Hence, in diamond cubic lattice, 34 percent of volume is occupied.

16.10.2 Sodium Chloride

Sodium chloride has FCC crystal structure as shown in Figure 16.27. Sodium and chloride ions are separated by half of the body diagonal of unit cell. Sodium ions occupy the octahedral voids and chloride ions are present at the FCC positions the position of sodium and chloride ions are given as follows:

$$\begin{array}{l} \text{Na}^+ \quad (000) \quad \left(\frac{a}{2}, \frac{a}{2}, 0 \right) \quad \left(0, \frac{a}{2}, \frac{a}{2} \right) \quad \left(\frac{a}{2}, 0, \frac{a}{2} \right) \\ \text{Cl}^- \quad \left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2} \right) \quad \left(0, 0, \frac{a}{2} \right) \quad \left(0, \frac{a}{2}, 0 \right) \quad \left(\frac{a}{2}, 0, 0 \right) \end{array}$$

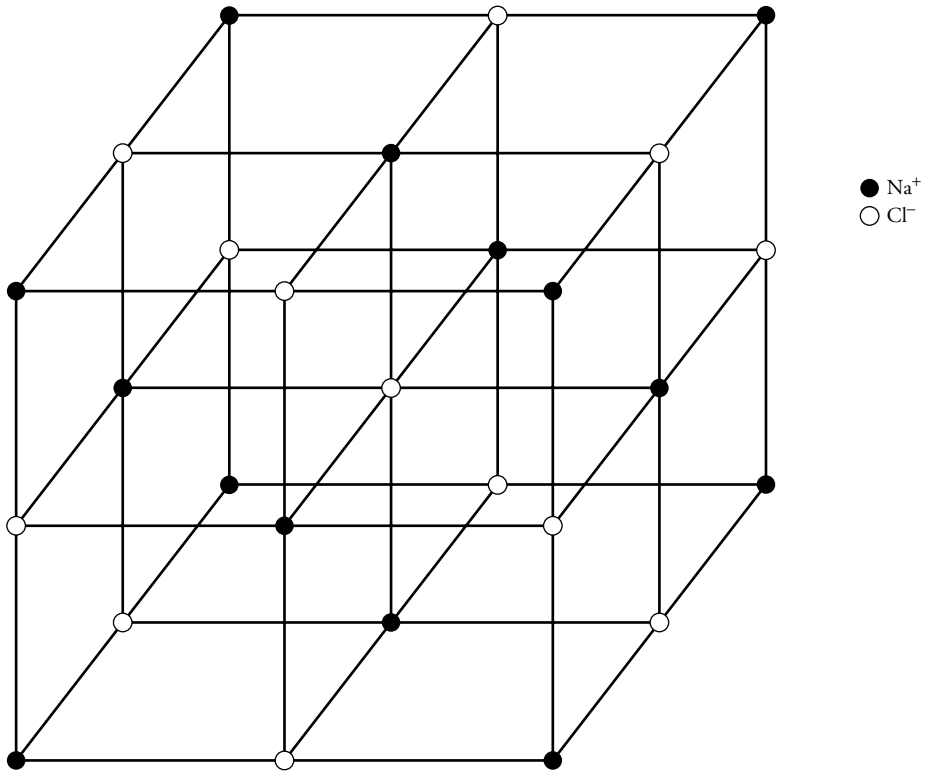


Figure 16.27 Sodium chloride structure.

16.10.3 Hexagonal Close Packing

In HCP, three atoms are present inside the hexagon body: one atom is present at the face and one atom is present at every corner Figure (16.28). Two atoms at basal planes are shared by two unit cells, and there are 12 corner atoms shared by 6 unit cells, hence

$$N = 12 \times \frac{1}{6} (\text{at corners}) + 2 \times \frac{1}{2} (\text{basal planes}) + 3 \text{ inside the hexagon}$$

$$\Rightarrow N = 6$$

The coordination number of atoms in HCP is 12. Every basal atom touches three atoms above and below its plane and six in its plane.

Therefore, $CN = 3(\text{atoms above its plane}) + 3(\text{below its plane}) + 6(\text{in its plane})$

$$\Rightarrow CN = 12$$

We will obtain the volume and packing fraction for HCP:

$$\text{Area of base for hexagon} = \frac{3\sqrt{3}a^2}{2}$$

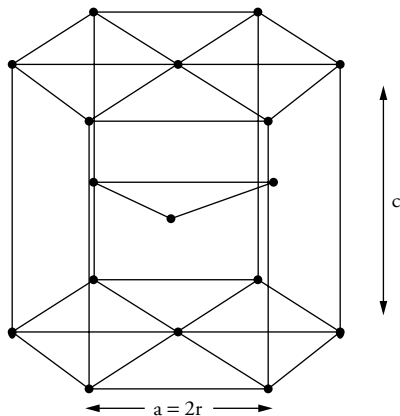


Figure 16.28 Hexagonal close-packed structure.

Hence,

$$\text{Volume} = \frac{3\sqrt{3}a^3c}{2}$$

For hexagon,

$$\Rightarrow r = \frac{a}{2}$$

Hence,

$$\text{PF} = \frac{N \times \frac{4}{3}\pi r^3}{\text{Volume}}$$

$$\Rightarrow \text{PF} = \frac{6 \times \frac{4}{3}\pi \left(\frac{a}{2}\right)^3}{\frac{3\sqrt{3}a^2c}{2}}$$

$$\Rightarrow \text{PF} = \frac{24\pi a^3 \times 2}{24 \times 3\sqrt{3}a^2c}$$

$$\Rightarrow \text{PF} = \frac{2\pi}{3\sqrt{3}} \left(\frac{a}{c}\right)$$

$$\left[\frac{c}{a} = \sqrt{\frac{8}{3}}\right]$$

(for HCP)

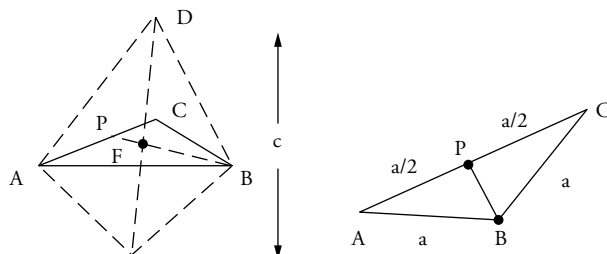


Figure 16.29 HCP unit cell.

$$PF = \frac{2\pi}{3\sqrt{3}} \left(\frac{\sqrt{3}}{8} \right) = 0.74 \quad (15)$$

$$PF = 74\%$$

Hence, in HCP, 74 percent of volume is occupied by the atoms,

In unit cell, $\frac{c}{a} = 1.633$, which can be derived using Figure. 16.29.

$$\frac{c}{a} = \frac{2DF}{AB} \quad (16)$$

We have to obtain DF,

$$DF = \sqrt{BD^2 - BF^2} \quad (17)$$

$$\text{As,} \quad BF = \frac{2}{3} BP \quad (18)$$

Now, we should find BP

$$\Rightarrow BP = \sqrt{AB^2 - AP^2} = \sqrt{a^2 - a^2/4} = \frac{\sqrt{3}a}{2}$$

$$\text{Using Eqs (18) and (19) in Eqn. (17), } BP = \frac{\sqrt{3}a}{2} \quad (19)$$

$$\Rightarrow DF = \sqrt{a^2 - \left[\frac{2}{3} \left(\frac{\sqrt{3}a}{2} \right) \right]^2} = \sqrt{a^2 - a^2/3}$$

$$\text{Hence,} \quad DF = \sqrt{\frac{2}{3}} a \quad (20)$$

Substituting Eqn. (20) in Eqn. (16)

$$\Rightarrow \frac{c}{a} = \frac{2 \times \sqrt{\frac{2}{3}} a}{a} = \sqrt{\frac{8}{3}}$$

$$\Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633 \quad (21)$$

16.11 Laue's Theory of X-ray Diffraction

Diffraction deals with bending of light around the corners of obstacle. X-rays are also diffracted provided the size of obstacle or aperture $\approx 1 \text{ \AA}$. Bragg obtained the X-ray diffraction from atomic planes of crystal (discussed in Chapter 2).

The Bragg's diffraction law is given by:

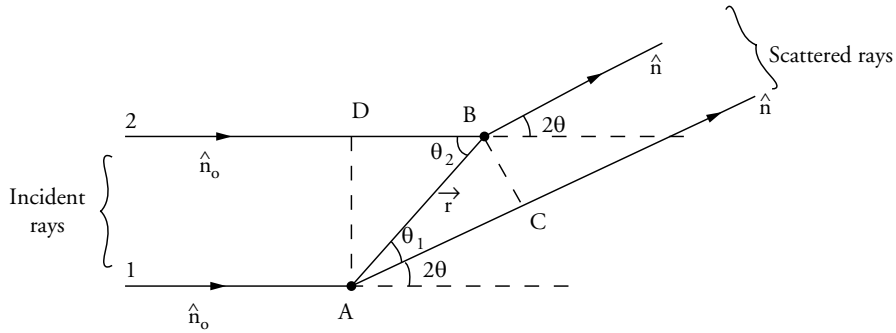


Figure 16.30 Laue's scattering of rays by scattered atoms.

$$2d \sin \theta = n\lambda \quad (22)$$

This is known as Bragg's law, d is the distance between two successive planes, θ is the glancing angle that incident ray makes with the plane of atoms. Bragg's law could establish the periodicity of space lattice. The basis composition determines relative intensity of various diffraction orders, although Bragg law do not provide any information regarding the intensity of scattering.

Bragg suggested that X-rays are scattered from the crystal planes, but Laue said that the reflection of X-rays occur from the individual atoms. Let A and B be the scattering centers separated by distance r as shown in Figure 16.30. Let parallel set of rays with unit vector \hat{n}_0 is incident on A and B. The unit vectors of scattered rays is \hat{n} . Let the angle between incident ray and scattered ray be 2θ . Draw perpendicular AD on the ray 2 and BC perpendicular to ray 1 (scattered ray 1).

The path difference between the rays scattered from A and B is given by the following equation:

$$\Delta = AC - BD \quad (23)$$

In $\triangle ABD$,

$$\cos \theta_2 = \frac{BD}{AB} \quad (24a)$$

$$BD = AB \cos \theta_2 = r \cos \theta_2$$

Similarly, in $\triangle ABC$

$$\cos \theta_1 = \frac{AC}{AB}$$

$$AC = AB \cos \theta_1 = r \cos \theta_1 \quad (24b)$$

Substituting Eqs (24a) and (24b) in Eqn. (23), we obtain

$$\Delta = r \cos \theta_1 - r \cos \theta_2$$

$$\Delta = \vec{r} \cdot \hat{n} - \vec{r} \cdot \hat{n}_o$$

$$\Delta = \vec{r} \cdot (\hat{n} - \hat{n}_o) = \vec{r} \cdot \vec{N} \quad (24c)$$

where $(N = \hat{n} - \hat{n}_o)$ represents the difference in unit vectors of the scattered and incident beams.

Further,

$$\begin{aligned} \vec{N} \cdot \vec{N} &= (\hat{n} - \hat{n}_o) \cdot (\hat{n} - \hat{n}_o) \\ N^2 &= |\hat{n}|^2 + |\hat{n}_o|^2 - 2\hat{n} \cdot \hat{n}_o \\ \Rightarrow N^2 &= 1 + 1 - 2 \cos 2\theta \\ \Rightarrow N^2 &= 2(1 - \cos 2\theta) = 2(2 \sin^2 \theta) \\ \Rightarrow N &= 2 \sin \theta \end{aligned} \quad (25)$$

N is also called scattering normal. Now, we will obtain the phase difference. The phase difference is given by

$$\Rightarrow \text{Phase difference } \phi = \frac{2\pi}{\lambda} (\text{path difference})$$

$$\Rightarrow \phi = \frac{2\pi}{\lambda} (\Delta) = \frac{2\pi}{\lambda} (\vec{r} \cdot \vec{N}) \quad (26)$$

For constructive pattern, or the condition of maxima, the phase difference should be multiple of 2π .

The crystal is periodic in nature. Hence, the atoms that are in same direction of A and B would also scatter the radiations in same direction as that of A and B. \vec{r} may coincide with any crystallographic axis. Hence, the following three conditions can be there:

$$\Rightarrow \phi_a = \frac{2\pi}{\lambda} (\vec{a} \cdot \vec{N}) = 2\pi h' = 2\pi n h \quad (27a)$$

$$\Rightarrow \phi_b = \frac{2\pi}{\lambda} (\vec{b} \cdot \vec{N}) = 2\pi k' = 2\pi n k \quad (27b)$$

$$\Rightarrow \phi_c = \frac{2\pi}{\lambda} (\vec{c} \cdot \vec{N}) = 2\pi l' = 2\pi n l \quad (27c)$$

h' , k' , and l' are integers, such that $h' = nh$, $k' = nk$, and $l' = nl$, (hkl) symbolizes the smallest vectors.

From Eqn. (27a), we can write

$$\vec{a} \cdot \vec{N} = nh\lambda \quad (28a)$$

$$\text{Similarly,} \quad \vec{b} \cdot \vec{N} = nk\lambda \quad (28b)$$

$$\text{and} \quad \vec{c} \cdot \vec{N} = nl\lambda \quad (28c)$$

Let \vec{N} makes angle α , β , and γ with \vec{a} , \vec{b} , and \vec{c} , respectively, then we can write Eqn. 28(a-c) as follows:

$$\Rightarrow aN \cos \alpha = nb\lambda \quad (29a)$$

$$\Rightarrow bN \cos \beta = nk\lambda \quad (29b)$$

$$\Rightarrow cN \cos \gamma = nl\lambda \quad (29c)$$

Substituting Eqn. (25) in Eqn. 29(a–c), then

$$\left. \begin{aligned} 2a \cos \alpha \sin \theta &= nb\lambda \\ 2a \cos \beta \sin \theta &= nk\lambda \\ 2a \cos \gamma \sin \theta &= nl\lambda \end{aligned} \right\} \quad (30)$$

The set of Eqn. (30) constitute Laue's equations. We can also obtain Bragg's law from the set of Eqn. (30). From Eqn. (30), we can write

$$\cos \alpha = \frac{nb\lambda}{2a \sin \theta}, \quad \cos \beta = \frac{nk\lambda}{2a \sin \theta}, \quad \cos \gamma = \frac{nl\lambda}{2a \sin \theta}$$

We can see from above equations that the direction cosines are proportional to $\frac{b}{a}$, $\frac{k}{b}$ and $\frac{l}{c}$, respectively.

Hence, the normal to (hkl) planes is similar to the scattering normal N . Hence, if d is the interplanar spacing between Bragg's planes, then

$$d = \frac{a}{n} \cos \alpha = \frac{b}{k} \cos \beta = \frac{c}{l} \cos \alpha \quad (31)$$

Substituting Eqn. (31) in Eqn. (30), we obtain

$$\Rightarrow 2d \sin \theta = n\lambda$$

Hence, Bragg's law could be obtained from the Laue's equations.

Max Laue was born at Pfaffendorf, Koblenz, on October 9, 1879. His father was an official in the German military administration. Laue was deeply influenced by Professor Goering, when he was at the Protestant school of Strassburg; Laue also joined military services for a year in 1898. He worked under Professor W. Voigt and Professor W. Abraham in University of Göttingen. In 1902, he worked under Professor Max Planck in University of Berlin and obtained his doctorate in 1903. He worked on the thermodynamic significance of the coherence of light waves and applications of entropy to radiation fields at the Institute for Theoretical Physics at Berlin under the supervision of Max Planck. He became Professor of Physics at the University of Zurich in 1912. He was appointed as a Professor of Physics at the University of Berlin, from 1919 to 1943. He wrote a paper on X-rays absorption during diffraction and submitted to the International Union of Crystallographers at Harvard University in 1948. Much of his research work was done on X-ray optics in collaboration with Borrmann at Fritz Haber Institute for Physical Chemistry at Berlin-Dahlem before his retirement in 1958. He received the Nobel Prize for diffraction of X-rays on crystals.



MAX LAUE

16.12 Diffraction Methods

X-rays is widely used to determine the crystal structure. X-rays spectroscopy is used for variety of applications. For a given value of “ d ”, λ and θ should match. Hence, the following three methods are generally used to identify the crystal structure depending on the variation of wavelength “ λ ” or orientation angle “ θ ”.

16.12.1 Laue's Method

Laue suggested that if the crystal behaves as a three-dimensional diffraction grating if crystals consist of regular order of atoms with interplanar spacing of the order of angstrom. Laue's experiment was performed on ZnS crystal, when an inhomogeneous X-rays was incident on it. Diffraction spots were obtained on photographic plate, which are named as Laue's spots as shown in Figure 16.31.

In this method, the single crystal is held on a goniometer. The crystal is fixed, and hence θ is fixed. A X-ray of wavelength range $0.2 - 2 \text{ \AA}$ is incident on single crystal. The dimensions of crystal are $1 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm}$. The beam usually falls perpendicular on the crystal. The X-rays fall on Bragg's planes with interplanar spacing d . For a particular set of θ , d , and λ , Bragg's condition is satisfied, which leads to constructive interference. The diffraction pattern is observed at the photographic plate. The photographic plate contains symmetrical arrangements of spots. The arrangement of spots depends on the crystal symmetry. In Laue's method due to continuous range of wavelengths, an overlapping pattern can be obtained, which makes the crystal structure difficult to determine.

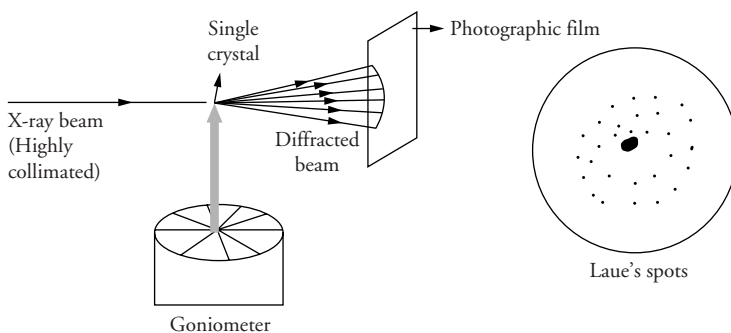


Figure 16.31 Laue's method and Laue's spots.

Von-Laue was famous as a motorist in Berlin as he used to ride the motor bicycle at high speed to his lectures. He used to love high speeds, but a fatal collision ended his life. He was driving to his laboratory on April 8, 1960, when a motorcyclist collided with von Laue's car. Von Laue's car overturned in the Berlin speedway and the Fire Brigade took him from beneath it. The motorcyclist who received his license just two days ago died on the spot. Due to the injuries, Von-Laue died on April 24, at the age of 80. Von-Laue also suffered from depression, which took away his sense of humor and joy. He took a theist who was very much interested in classical music. He had a desire that his tombstone should be engraved with the text "he died trusting firmly in the mercy of God."

16.12.2 Rotating Crystal Method

In this technique, the crystal is moving slowly with the help of a rotating shaft where monochromatic X-rays are used. During the rotation of crystal, it X-rays come across different set of planes. The single crystal used is almost of 1 mm dimension. The whole arrangement is within a hollow cylinder whose axis is collinear with the axis of rotation of single crystal (Figure 16.32). The cylindrical holder contains photographic plate to record the diffraction patterns. The X-rays will be diffracted. When the rotating crystals satisfy the Bragg's condition of $2d \sin \theta = n\lambda$. The plane that contains incident beam does not diffract any rays. The diffraction patterns are produced by all those planes that have some glancing angle w.r.t. the incident radiations. The rotation can be complete or oscillatory. During complete rotation, the overlapping of points can be obtained as each set of planes reflect four times, whereas the oscillatory motion can avoid this problem. If a is treated to be the axis of rotation, then we can directly find $a \sin \theta = \lambda$, because the distance d depends on the separation of lattice points on a -axis. Hence, a , b , and c can be obtained for a crystal using rotating crystal method.

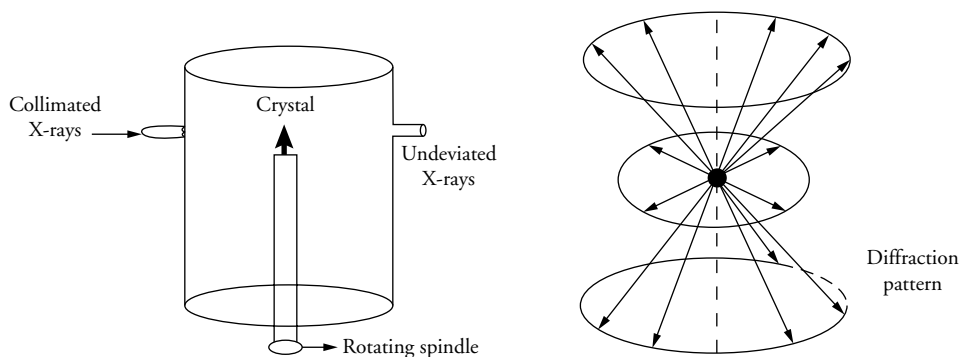


Figure 16.32 Rotating crystal methods and the pattern.

16.12.3 The Powder Crystal Method

Certain substances can be readily worked upon to obtain single crystals; but sometimes, it is difficult to obtain single crystals for certain substances. Debye, Scherrer, and Hull devised a formula to grow a crystalline material in powder form. The orientations of atoms are random by individual crystallites are ordered. Hence, a large number of crystallites are obtained by this method. The X-ray falls on powder sample and many diffraction planes are available for Bragg's diffraction. There are almost $10^{10} - 10^{12}$ crystals/mm of sample. Again, the diffraction will occur through set of parallel planes satisfying the condition $n\lambda = 2d \sin \theta$, such that the X-rays make certain glancing angle with lattice plane. The sample is usually taken in capillary tube made up of nondiffracting material inside a cylindrical Debye-Scherrer camera (Figure 16.33). The diffracted beams will form cone of photographic film with semivertical angle 2θ and θ is Bragg's angle. A series of concentric rings are obtained as shown in Figure 16.33. The glancing angle is given by

$$\theta_1 = \frac{90^\circ}{\pi D} x_1 \quad (32)$$

Where D is diameter of cylinder, and x_1 is the distance between symmetrical lines. Hence, we can obtain the distance between the planes of crystal using Bragg's angle.

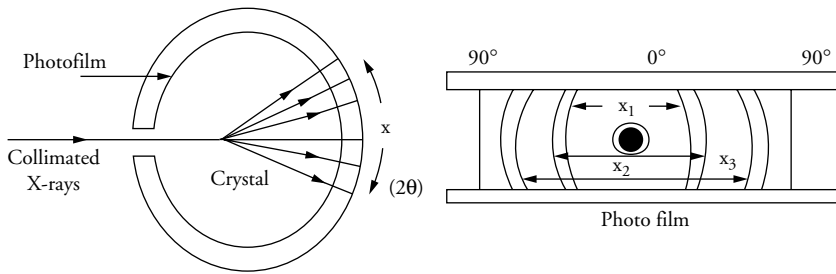


Figure 16.33 Powder crystal method and pattern obtained.

William Henry Bragg was born on July 2, 1862, in Cumberland, England. Sir William Lawrence Bragg (1890–1971) was the son of W.H. Bragg. W.H. Bragg was a very talented kid; he won many scholarships along with an exhibition to Trinity College, Cambridge. In 1886, Bragg joined as Professor of Pure and Applied Mathematics in Adelaide although he was had less knowledge in physics. He was a very good athlete and played tennis and golf. Slowly, he got interested in physics especially in electromagnetism. Bragg considered X-rays and γ -rays to be streams of neutral-pair particles instead of electromagnetic waves. This statement got him into controversy by his peers for several years. He was honored by the Rumford (1916) and Copley (1930) medals by the Royal Society. In 1931, he was also admitted to the Order of Merit. He died in London on March 12, 1942 due to heart trouble.



W.H. BRAGG

16.13 Reciprocal Lattice and \vec{k} -Space

The concept of reciprocal lattice was given by P.P. Ewald in 1923. Later on, its further improvization was done by Von Laue. X-ray diffraction from atomic planes generate patterns only when Bragg's condition is satisfied, that is, $n\lambda = 2d \sin\theta$. If we have to determine slope of a diffraction plane, we have to draw a normal to it. Every plane has different normals, and hence different slopes. To construct a set of reciprocal lattice, we need a set of planes.

Reciprocal lattice is the array of points that are obtained at the end of normals drawn to a common origin whose length is proportional to the reciprocal of interplanar spacing. The reciprocal lattice construction takes the following points in consideration:

- (i) The periodicity of crystal structure determines Laue's diffraction pattern.
- (ii) The direct lattice determines the position of diffraction spots.
- (iii) A set of planes can be represented by Miller indices. A normal can represent each set of planes by drawing normal from common origin whose length is proportional to reciprocal of interatomic spacing.

To construct a reciprocal lattice, we should proceed as follows:

- (i) Mark origin on the direct lattice.
- (ii) Construct normal to every plane in the direct lattice.

- (iii) Set the length of normals equal to 2π times the reciprocal of interplanar spacing for set of planes.
- (iv) Mark point at the end of all normals.
- (v) The collection of all these points constitute reciprocal lattice.

We will now define reciprocal lattice vector. It is defined as the vector with magnitude equal to reciprocal to interplanar spacing $\left(\frac{1}{d_{hkl}}\right)$. The direction of reciprocal lattice is parallel to normal of (hkl) plane.

\vec{a} , \vec{b} , and \vec{c} are primitives for direct lattice, \vec{a}^* , \vec{b}^* , and \vec{c}^* represent primitives for reciprocal lattice. \vec{a} is normal to \vec{b} and \vec{c} , hence

$$\vec{a}^* \cdot \vec{b} = \vec{a}^* \cdot \vec{c} = 0$$

and $\vec{a} \cdot \vec{a}^* = \vec{b} \cdot \vec{b}^* = \vec{c} \cdot \vec{c}^* = 2\pi$ (33a)
As \vec{c}^* is perpendicular to plane containing \vec{a} and \vec{b} , hence

$$\vec{c}^* = X(\vec{a} \times \vec{b}) \quad (33b)$$

Substituting Eqn. (33b) in Eqn. (33a), hence

$$\begin{aligned} \vec{c} \cdot \vec{c}^* &= 2\pi \\ \vec{c} \cdot X(\vec{a} \times \vec{b}) &= 2\pi \\ \Rightarrow X &= \frac{2\pi}{\vec{c} \cdot (\vec{a} \times \vec{b})} \end{aligned} \quad (33c)$$

Substituting Eqn. (33c) in Eqn. (33b),

$$\begin{aligned} \Rightarrow \vec{c}^* &= \frac{2\pi(\vec{a} \times \vec{b})}{\vec{c} \cdot (\vec{a} \times \vec{b})} = \frac{2\pi(\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \\ \Rightarrow \vec{c}^* &= \frac{2\pi(\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \end{aligned} \quad (34a)$$

$$\left[\begin{aligned} &\vec{a} \cdot (\vec{b} \times \vec{c}) \\ &= \vec{b} \cdot (\vec{a} \times \vec{c}) \\ &= \vec{c} \cdot (\vec{a} \times \vec{b}) \\ &= \text{Volume of unit cell} \end{aligned} \right]$$

Similarly,

$$\Rightarrow \vec{a}^* = \frac{2\pi(\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \quad (34b)$$

and
$$\Rightarrow \vec{b}^* = \frac{2\pi(\vec{c} \times \vec{a})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \quad (34c)$$

\vec{a}^* , \vec{b}^* , and \vec{c}^* have dimension of (length)⁻¹.

The reciprocal of reciprocal lattice yields direct lattice, that is, $(\vec{a}^*)^* = \vec{a}$. As d_{hkl} of normal plane lattice is equal to $\frac{1}{d_{hkl}}$ of reciprocal lattice. Similarly, volume V_{hkl} of normal lattice is equal to $\frac{1}{V_{hkl}}$ of reciprocal lattice.

The reciprocal lattice is an array of points such that the distance between points is inversely proportional to the interplanar spacing between (hkl) planes. As we have seen that reciprocal vector has dimensions of (length)⁻¹. Wavevector \vec{k} also has the same dimensions of (length)⁻¹ and is given by $\frac{2\pi}{\lambda}$.

If we get a reciprocal space such that $\frac{2\pi}{d_{hkl}}$ is the distance of separation between points, then \vec{k} -space is obtained. \vec{k} -space is also known as wave-number space. We have seen from Eqn. (2) that for direct lattice,

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

In \vec{k} -space, the reciprocal lattice vector is \vec{G} and is given by the following equation:

$$\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \quad (35)$$

Take dot product of T and G ,

$$\vec{T} \cdot \vec{G} = (n_1\vec{a} + n_2\vec{b} + n_3\vec{c}) \cdot (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$$

$$\Rightarrow \vec{T} \cdot \vec{G} = (n_1h + n_2k + n_3l)2\pi$$

$$\Rightarrow \vec{T} \cdot \vec{G} = 2\pi Z \quad (36)$$

where $Z = n_1h + n_2k + n_3l$.

Hence, vector \vec{G} drawn from origin to (hkl) of reciprocal lattice is normal to (hkl) plane of direct lattice. The Bragg's condition in reciprocal lattice becomes $2\vec{k} \cdot \vec{G} + G^2 = 0$, where \vec{k} is wave-vector.

16.13.1 Reciprocal Lattice for SC

The volume of the cell is $V = \vec{a} \cdot (\vec{b} \times \vec{c})$

Let $\vec{a} = a\hat{i}$, $\vec{b} = b\hat{j}$, and $\vec{c} = c\hat{k}$

$$V = a\hat{i} \cdot (b\hat{j} \times c\hat{k}) = a^3 \quad [\text{as } a = b = c]$$

The primitive lattice vectors are given by the following equation:

$$\vec{a}^* = \frac{2\pi \cdot (\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} = \frac{2\pi a^2 \hat{i}}{a^3} = \frac{2\pi}{a} \hat{i}$$

Similarly, $\vec{b}^* = \frac{2\pi}{a} \hat{j}$ and $\vec{c}^* = \frac{2\pi}{a} \hat{k}$

Hence, the reciprocal lattice for simple cubic lattice is itself a simple cubic lattice with the lattice constant $\frac{2\pi}{a}$. These reciprocal lattice vectors are directed along the crystallographic axis.

16.13.2 Reciprocal Lattice for BCC Lattice

The primitive translation vectors for BCC lattice are given by

$$\vec{A} = \frac{a}{2}(-\hat{i} + \hat{j} + \hat{k}), \vec{B} = \frac{a}{2}(\hat{i} - \hat{j} + \hat{k}), \text{ and } \vec{C} = \frac{a}{2}(\hat{i} + \hat{j} - \hat{k})$$

where a is the lattice constant, the volume of primitive cell is given by the following equation:

$$\vec{A} \cdot (\vec{B} \times \vec{C}) = \frac{a^3}{2} [(-\hat{i} + \hat{j} + \hat{k}) \cdot (\hat{i} - \hat{j} + \hat{k}) \times (\hat{i} + \hat{j} - \hat{k})] \quad (37)$$

Let us obtain

$$\begin{aligned} (\hat{i} - \hat{j} + \hat{k}) \times (\hat{i} + \hat{j} - \hat{k}) &= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} \\ &= \hat{i}[1-1] - \hat{j}[-1-1] + \hat{k}[1+1] \\ &= 2\hat{j} + 2\hat{k} \end{aligned} \quad (38)$$

Substituting Eqn. (38) in Eqn. (37), we obtain

$$\begin{aligned} \vec{A} \cdot (\vec{B} \times \vec{C}) &= \frac{a^3}{8} [(-\hat{i} + \hat{j} + \hat{k}) \cdot (2\hat{j} + 2\hat{k})] = \frac{a^3}{2} \\ \vec{A} \cdot (\vec{B} \times \vec{C}) &= \frac{a^3}{2} \end{aligned} \quad (39)$$

Hence,

$$\begin{aligned} \vec{a}^* &= \frac{2\pi \cdot (\vec{B} \times \vec{C})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi \cdot \frac{a^2}{4} (2\hat{j} + 2\hat{k})}{a^3 / 2} \\ \vec{a}^* &= \frac{2\pi}{a} (\hat{j} + \hat{k}) \end{aligned} \quad (40a)$$

Similarly,

$$\vec{b}^* = \frac{2\pi \cdot (\vec{C} \times \vec{A})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{k} + \hat{i}) \quad (40b)$$

and

$$\vec{c}^* = \frac{2\pi \cdot (\vec{A} \times \vec{B})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{i} + \hat{j}) \quad (40c)$$

Equations 40(a–c) represent the reciprocal lattice for BCC lattice. The reciprocal lattice to BCC lattice represents the direct lattice for FCC lattice with lattice constant $\left(\frac{2\pi}{a}\right)$.

16.13.3 Reciprocal Lattice for FCC Lattice

The primitive translational vectors for FCC lattice are given as follows:

$$\vec{A} = \frac{a}{2}(\hat{j} + \hat{k}), \quad \vec{B} = \frac{a}{2}(\hat{k} + \hat{i}), \quad \text{and} \quad \vec{C} = \frac{a}{2}(\hat{i} + \hat{j})$$

The volume of primitive cell of FCC lattice is given by the following equation:

$$\begin{aligned} \vec{A} \cdot (\vec{B} \times \vec{C}) &= \frac{a^3}{8} [(j+k) \cdot (k+i) \times (i+j)] \\ \Rightarrow \vec{A} \cdot (\vec{B} \times \vec{C}) &= \frac{a^3}{8} (j+\hat{k}) \cdot (\hat{j}-\hat{i}+\hat{k}) = \frac{a^3}{4} \end{aligned} \quad (41)$$

Hence,

$$\begin{aligned} \Rightarrow \vec{a}^* &= \frac{2\pi(\vec{B} \times \vec{C})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi \cdot \frac{a^2}{4}(j-i+k)}{a^3/4} \\ \Rightarrow \vec{a}^* &= \frac{2\pi}{a}(-i+j+\hat{k}) \end{aligned} \quad (42a)$$

Similarly,

$$\vec{b}^* = \frac{2\pi(\vec{C} \times \vec{A})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a}(i-j+k) \quad (42b)$$

and

$$\vec{c}^* = \frac{2\pi(\vec{A} \times \vec{B})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a}(i+j-k) \quad (42c)$$

Equations 42(a–c) represent the reciprocal lattice vectors for FCC lattice. The reciprocal lattice vectors for FCC lattice are same as that of primitive vectors of direct BCC lattice with lattice constant $\frac{2\pi}{a}$.

16.14 Brillouin Zones

The primitive cell in reciprocal lattice represents the Brillouin zones. The Brillouin zones consist of all the Bragg diffracted k -vectors. Let us construct Brillouin zones, using primitive translation vectors \vec{a} and \vec{b} , such that $\vec{a} = a\hat{i}$ and $\vec{b} = b\hat{j}$ (for square lattice)

Hence, corresponding $\vec{a}^* = \frac{2\pi}{a}\hat{i}$ and $\vec{b}^* = \frac{2\pi}{b}\hat{j}$

$$\vec{G} = h\vec{a}^* + k\vec{b}^* \quad [\text{from Eqn. (35)}]$$

$$\vec{G} = \frac{2\pi}{a} (h\hat{i} + k\hat{j}) \tag{43}$$

From Bragg's law in reciprocal space,

$$2\vec{k} \cdot \vec{G} + G^2 = 0 \quad \left[\begin{array}{l} \vec{k} = k_1\hat{i} + k_2\hat{j} \\ \text{is wavevector} \end{array} \right]$$

$$2(k_1\hat{i} + k_2\hat{j}) \cdot \left(\frac{2\pi}{a} (h\hat{i} + k\hat{j}) \right) + \frac{4\pi^2}{a^2} (h^2 + k^2) = 0$$

$$hk_1 + kk_2 = \frac{-\pi}{a} (h^2 + k^2) \tag{44}$$

Equation (44) represents family of straight lines in $k_1 - k_2$ plane.

$$k_1 = -\frac{\pi}{a} \frac{h^2 + k^2}{h} \quad \text{and} \quad k_2 = -\frac{\pi}{a} \frac{h^2 + k^2}{k}$$

We obtain four lines $k_1 = \pm\pi/a, k_2 = \pm\pi/a$, which are plotted in Figure 16.34.

Figure 16.34 also shows $\pm k_1 \pm k_2 = \frac{2\pi}{a}$ set of lines $k_1 = \pm\frac{\pi}{a}$ and $k_2 = \pm\frac{\pi}{a}$ represents 1st Brillouin zone; whereas $k_1 = \pm\frac{2\pi}{a}$ and $k_2 = \pm\frac{2\pi}{a}$ represent 2nd Brillouin zone.

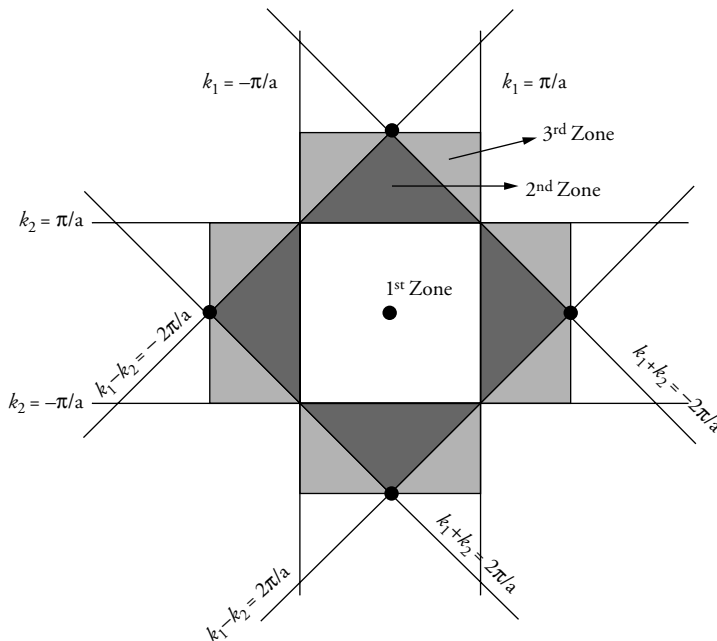


Figure 16.34 Brillouin zones.

16.14.1 Brillouin Zone of SC Lattice

A cube is obtained from the first Brillouin zone of simple cubic lattice. The primitive translation vector for simple cubic lattice are (Figure 16.35)

$$\vec{a} = a\hat{i}, \vec{b} = b\hat{j} \text{ and } \vec{c} = c\hat{k}$$

(for cubic lattice $a = b = c$)

The reciprocal lattice vectors are

$$\vec{a}^* = \frac{2\pi}{a}\hat{i}, \vec{b}^* = \frac{2\pi}{a}\hat{j}, \text{ and } \vec{c}^* = \frac{2\pi}{a}\hat{k}$$

k vector for X-ray is given by the following equation:

$$\vec{k} = k_1\hat{i} + k_2\hat{j} + k_3\hat{k} \quad (45a)$$

and G vector is written as follows:

$$\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \quad (45b)$$

The Bragg's law in reciprocal lattice is given by the following equation:

$$\begin{aligned} 2\vec{k} \cdot \vec{G} + G^2 &= 0 \\ \frac{2\pi}{a}(k_1h + k_2k + k_3l) + \frac{4\pi^2}{a^2}(h^2 + k^2 + l^2) &= 0 \\ hk_1 + kk_2 + lk_3 &= -\frac{\pi}{a}(h^2 + k^2 + l^2) \end{aligned} \quad (45c)$$

$$\left. \begin{array}{l} \text{If } h = \pm 1, k = 0, \text{ and } l = 0, \text{ then } k_1 = \pm \frac{\pi}{a} \\ \text{If } h = 0, k = \pm 1, \text{ and } l = 0, \text{ then } k_2 = \pm \frac{\pi}{a} \\ \text{If } h = 0, k = 0, \text{ and } l = \pm 1, \text{ then } k_3 = \pm \frac{\pi}{a} \end{array} \right\} \quad (46)$$

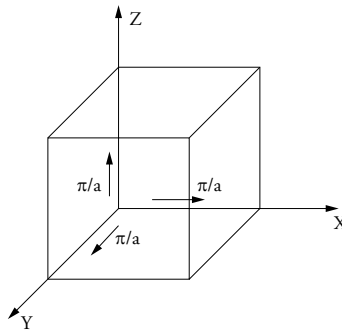


Figure 16.35 Brillouin zone for SC lattice.

Equation (46) represents the planes and space occupied and represents 1st Brillouin zones. The space between the planes represented by Eqn. (46) is a cube, and its side is $\frac{2\pi}{a}$.

16.14.2 Brillouin Zones for BCC

For BCC lattice, the primitive translation vectors in reciprocal are lattice given by the following equation:

$$\vec{a}^* = \frac{2\pi}{a}(\hat{j} + \hat{k}), \vec{b}^* = \frac{2\pi}{a}(\hat{k} + \hat{i}), \text{ and } \vec{c}^* = \frac{2\pi}{a}(\hat{i} + \hat{j})$$

The reciprocal lattice vector is

$$\begin{aligned} \vec{G} &= h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \\ \vec{G} &= h\left(\frac{2\pi}{a}(\hat{j} + \hat{k})\right) + k\left(\frac{2\pi}{a}(\hat{k} + \hat{i})\right) + l\left(\frac{2\pi}{a}(\hat{i} + \hat{j})\right) \\ \vec{G} &= \frac{2\pi}{a}\left[(k+l)\hat{i} + (h+k)\hat{j} + (h+l)\hat{k}\right] \end{aligned} \quad (47a)$$

Using the Bragg's condition,

$$2\vec{k} \cdot \vec{G} + G^2 = 0$$

$$\begin{aligned} &\frac{2\pi}{a}\left[k_1(k+l) + k_2(h+k) + k_3(h+l)\right] \\ &+ \frac{4\pi^2}{a^2}\left[(k+l)^2 + (h+k)^2 + (h+l)^2\right] = 0 \\ \Rightarrow &(k+l)k_1 + (h+k)k_2 + (h+l)k_3 = -\frac{\pi}{a}\left[(k+l)^2 + (h+k)^2 + (h+l)^2\right] \end{aligned} \quad (47b)$$

$$\text{If } h = \pm 1 \text{ and } k = 0 = l, \text{ then } \pm k_3 \pm k_2 = -\frac{2\pi}{a} \quad (48a)$$

$$\text{If } h = 0, k = \pm 1, \text{ and } l = 0, \text{ then } \pm k_1 \pm k_3 = -\frac{2\pi}{a} \quad (48b)$$

$$\text{If } h = 0, k = 0, \text{ and } l = \pm 1, \text{ then } \pm k_1 \pm k_2 = -\frac{2\pi}{a} \quad (48c)$$

The set of Eqn. 48(a–c) represents set of 12 planes. The region enclosed inside the 12 planes will represent dodecahedron.

16.14.3 Brillouin Zone for FCC

The primitive translation vectors for FCC are

$$\vec{a}^* = \frac{2\pi}{a}(-\hat{i} + \hat{j} + \hat{k}), \vec{b}^* = \frac{2\pi}{a}(\hat{i} - \hat{j} + \hat{k}), \text{ and } \vec{c}^* = \frac{2\pi}{a}(\hat{i} + \hat{j} - \hat{k})$$

From Bragg's condition,

$$2\vec{k} \cdot \vec{G} + G^2 = 0 \quad \left[\begin{aligned} \vec{G} &= h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \\ \vec{k} &= k_1\hat{i} + k_2\hat{j} + k_3\hat{k} \end{aligned} \right]$$

$$\frac{4\pi}{a} \left[k_1(-\hat{i} + \hat{j} + \hat{k}) + k_2(\hat{i} - \hat{j} + \hat{k}) + k_3(\hat{i} + \hat{j} - \hat{k}) \right]$$

$$= -\frac{4\pi^2}{a^2} \left[(-h+k+l)^2 + (h-k+l)^2 + (h+k-l)^2 \right]$$

$$(-h+k+l)k_1 + (h-k+l)k_2 + (h+k-l)k_3$$

$$= -\frac{\pi}{a} \left[(-h+k+l)^2 + (h-k+l)^2 + (h+k-l)^2 \right] \quad (49)$$

when	h = ±1, k = 0, l = 0	then	±k ₁ ± k ₂ ± k ₃ = 3π/a	} (50)
when	h = 0, k = ±1, l = 0	then	±k ₁ ± k ₂ ± k ₃ = 3π/a	
when	h = 0, k = 0, l = ±1	then	±k ₁ ± k ₂ ± k ₃ = 3π/a	

The Eqn. (50) represents the set of planes. The space between the planes form truncated octahedron whose reciprocal lattice vectors are given by

$$\frac{2\pi}{a}(\pm 2\hat{i}), \frac{2\pi}{a}(\pm 2\hat{j}), \frac{2\pi}{a}(\pm 2\hat{k})$$

16.15 Atomic Scattering Factor

Till now, we are familiar with Bragg's condition of $2d \sin\theta = n\lambda$. In Bragg's law, we assumed the scattering of X-rays from electrons; but in actual practice, the scattered X-rays are obtained from the atoms or in unit cell. The extent of scattering depends upon the scattering power of atoms. It is given by

$$f = \frac{\text{Amplitude of radiations which scattered from the atom}}{\text{Amplitude of radiation which are scattered from the electron}}$$

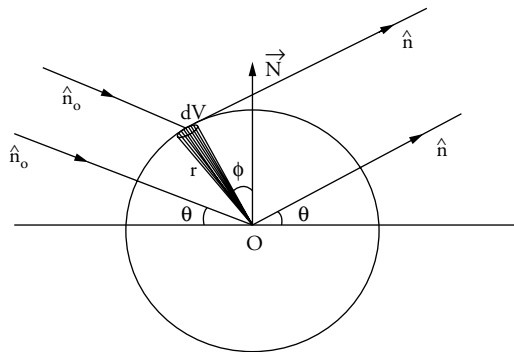


Figure 16.36 Scattered and incident radiations.

From Figure 16.36, let O be the scattering center and electrons are arranged uniformly around the center. Let \vec{r} be the radius of atom and consider a small volume element dV at vector \vec{r} , (Figure 16.36), such that

$$\text{Charge at } \vec{r} = \rho(\vec{r})dV \quad (51)$$

(where $\rho(r)$ is the volume charge density at \vec{r})

\hat{n}_o is the direction of incident X-ray and \hat{n} is the direction of scattered X-ray. As discussed in Section 16.11, Eqn. (26), the phase difference between the scattered radiations from point O and volume element dV is given by the following equation:

$$\phi_o = \frac{2\pi}{\lambda} (\vec{r} \cdot \vec{N}) \quad \text{and} \quad \left[\begin{array}{l} \vec{N} = \hat{n} - \hat{n}_o, \\ N = 2 \sin \theta \end{array} \right]$$

$$\begin{aligned} \Rightarrow \phi_o &= \frac{2\pi}{\lambda} rN \cos \phi \\ \Rightarrow \phi_o &= \frac{2\pi}{\lambda} r \cos \phi (2 \sin \theta) = \frac{4\pi r}{\lambda} \sin \theta \cos \phi \end{aligned} \quad (52a)$$

Put $\Rightarrow \mu = \frac{4\pi}{\lambda} \sin \theta$ (52b)

then Eqn. (52a) becomes

$$\phi_o = \mu r \cos \phi \quad (53)$$

The volume element dV for a ring of radius $r \sin \phi$, thickness dr , and width $rd\phi$ is given by the following:

$$\begin{aligned} dV &= \text{circumference} \times \text{width} \times \text{thickness} \\ dV &= 2\pi r \sin \phi (rd\phi) dr \\ dV &= 2\pi r^2 \sin \phi dr d\phi \end{aligned} \quad (54)$$

We will consider amplitude of scattered radiations for an electron and an atom. Let the amplitude of scattered radiations from point electron at O along \hat{n} is $Ae^{i(kx - \omega t)}$ where k is wavevector, and x is distance covered along \hat{n} . Let the amplitude of scattered radiations from atom (constituted by volume dV with charge $\rho(\vec{r})dV$, along \hat{n} is $Ae^{i(kx - \omega t + \phi_o)} \rho(r)dV$). Hence, the ratio of amplitude of scattered radiations by volume dV to amplitude of scattered radiations by electrons is given by the following equation:

$$\begin{aligned} df &= \frac{Ae^{i(kx - \omega t + \phi_o)} \rho(\vec{r})dV}{Ae^{i(kx - \omega t)}} = e^{i\phi_o} \rho(\vec{r})dV \\ df &= e^{i\phi_o} \rho(\vec{r})dV \end{aligned} \quad (55)$$

Hence,

$$f = \int df = \int e^{i\phi_o} \rho(\vec{r})dV$$

$$f = \int_{r=0}^{\infty} \int_{\phi_0=0}^{\pi} \rho(\vec{r}) e^{i\mu r \cos \phi} 2\pi r^2 \sin \phi d\phi dr$$

[using Eqs (53) and (54)]

$$f = \int_{\phi=0}^{\pi} \underbrace{e^{i\mu r \cos \phi} \sin \phi d\phi}_{\downarrow \frac{2 \sin \mu r}{\mu r}} \int_{r=0}^{\infty} 2\pi r^2 \rho(r) dr$$

$$f = \int_0^{\infty} 4\pi r^2 \rho(\vec{r}) \frac{\sin \mu r}{\mu r} dr$$

For $\theta \rightarrow 0$, $\mu \rightarrow 0$, and $\frac{\sin \mu r}{\mu r} \rightarrow 1$

$$f = \int_0^{\infty} 4\pi r^2 \rho(\vec{r}) dr \quad (56)$$

$4\pi r^2 \rho(\vec{r}) dr \rightarrow$ represents total charge in spherical shell of radius r and thickness dr .

$$f = Z \quad (57)$$

Hence, f denotes total charge of atom. For $\theta = 0$, $f = Z$ and for all other values of θ , $f < Z$. The f can determine exact charge distribution in the atom. Batterman et al. have determined the scattering factors for Fe, Cu, and aluminum.

16.16 Geometrical Structure Factor

The atomic scattering factor determines the relative intensity of scattered amplitudes by atom and electron. The scattering of X-rays depends on the nature of the crystal also, that is, atoms and their distribution. To obtain, the total scattering, the amplitudes of all the scattered wavelengths by each atom are added up to get geometrical structure factor.

Let a cell contains n -atoms such that the position of i th atoms is given by (Figure 16.37)

$$\vec{r}_i = u_i \vec{a} + v_i \vec{b} + w_i \vec{c} \quad (58a)$$

(where u_i , v_i , and w_i are constants)

Let f_i is the scattering fraction for i th atom. We have supposed that all the electrons of i th atoms are concentrated at \vec{r}_i . The total scattering amplitude is

$$F = \sum_i f_i e^{-i\phi}$$

$$F = \sum_i f_i e^{-i\left(\frac{2\pi}{\lambda}(\vec{r} + \vec{r}_i) \cdot N\right)} \quad (58b)$$

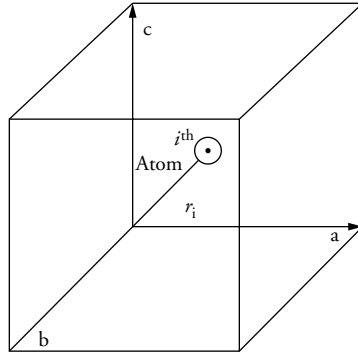


Figure 16.37 Position of i th atom.

$$F = e^{-\frac{2\pi}{\lambda}(\vec{r} \cdot \vec{N})} \sum_i f_i e^{-\frac{2\pi}{\lambda}(\vec{r}_i \cdot \vec{N})} \quad (58c)$$

In Eqn. (58c), we shall calculate $\vec{r}_i \cdot \vec{N}$, [ϕ_i is the phase difference between the scattered radiations from i th atom and at origin, N is the direction of normal to the plane].

$$\begin{aligned} \vec{r}_i \cdot \vec{N} &= (u_i \vec{a} + v_i \vec{b} + w_i \vec{c}) \cdot \vec{N} \\ \vec{r}_i \cdot \vec{N} &= u_i (\vec{a} \cdot \vec{N}) + v_i (\vec{b} \cdot \vec{N}) + w_i (\vec{c} \cdot \vec{N}) \quad \left[\begin{array}{l} \text{Using} \\ \text{Eqn. 28(a-c)} \end{array} \right] \\ \vec{r}_i \cdot \vec{N} &= u_i (\lambda h) + v_i (\lambda k) + w_i (\lambda l) \\ \vec{r}_i \cdot \vec{N} &= \lambda (u_i h + v_i k + w_i l) \quad (59) \end{aligned}$$

Using Eqn. (59) in Eqn. (58c),

$$\begin{aligned} F &= e^{-\frac{2\pi i}{\lambda}(\vec{r} \cdot \vec{N})} \sum_i f_i e^{-2\pi i(u_i h + v_i k + w_i l)} \\ \vec{F} &= e^{-\frac{2\pi i}{\lambda}(\vec{r} \cdot \vec{N})} S \quad (60) \end{aligned}$$

where

$$S = \sum_i f_i e^{-2\pi i(u_i h + v_i k + w_i l)} \quad (61)$$

S is known as geometrical structure factor. We can calculate structure factor for some simple lattice.

- (i) **SC lattice:** It contains one atom at $(0, 0, 0)$ /unit cell.

Hence,

$$S = \sum f_i e^0 = f \quad (62a)$$

Hence, all the Bragg lines will occur.

- (ii) **BCC lattice:** It contains atom at $(0, 0, 0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

$$S = f \left[e^0 + e^{-2\pi i(\frac{1}{2} + \frac{1}{2} + \frac{1}{2})} \right] = f \left[1 + e^{-\pi i(b+k+l)} \right]$$

$$\left. \begin{array}{l} \text{If } (h+k+l) = \text{odd, then } e^{-\pi i(h+k+l)} = -1 \\ \text{If } (h+k+l) = \text{even, then } e^{-\pi i(h+k+l)} = 1 \end{array} \right\} \quad (62b)$$

Hence, for odd $(h+k+l)$, $S = 0$. Hence, the reflection like (100), (221), (210), (111), are missing for BCC lattice.

For even $(h+k+l)$, $S = 2f$. Hence the reflections such as (2, 0, 0), (3, 1, 0), (2, 2, 2), (110) are present.

(iii) **FCC lattice:** The atoms are present at $(0, 0, 0)$ and $(\frac{1}{2}, \frac{1}{2}, 0)$, $(0, \frac{1}{2}, \frac{1}{2})$, and $(\frac{1}{2}, 0, \frac{1}{2})$.

$$S = f \left[e^0 + e^{-\pi i(h+l)} + e^{-\pi i(h+k)} + e^{-\pi i(k+l)} \right]$$

If $(h+l)$, $(h+k)$, and $(k+l)$ are odd or even, then

$$S = 4f \quad (62c)$$

If one is odd and other are even or one is even and other are odd, then

$$S = 0 \quad (62d)$$

Hence, no reflection occurs for (211), (324), and (100) planes of FCC lattice.

SUMMARY

This chapter deals with the crystal structure, basis, crystal lattice, motif, unit cell, and primitive cell. There are 14 Bravais crystal lattices. The planes and directions of crystal structure are represented by Miller indices (hkl) . Cubic crystal is the most ordered one and triclinic is the most disordered. Cubic crystal has three Bravais lattices, that is, simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC). The coordination number of FCC, BCC, and SC is 12, 8, and 6, respectively. The packing fraction is highest for FCC lattice to be 74 percent. The HCP structure has packing fraction of 74 percent and coordination number 12. Diamond structure is made of two interpenetrating FCC lattice, whereas NaCl has FCC lattice. With the help of Bragg's law, crystal structure could be determined. It assumes scattering by lattice; whereas, Laue's theory says the diffraction occurs due to every atom. Laue's method, rotating crystal method, and powder diffraction methods are used to obtain the primitives of crystals. Ewald gave the concept of reciprocal lattice, the reciprocal lattice vector is inversely proportional to d_{hkl} , that is, interplanar spacing. FCC is reciprocal lattice for BCC and vice versa; whereas, SC is its own reciprocal lattice. With the help of Bragg's law in reciprocal lattice, that is, $2\vec{k} \cdot \vec{G} + G^2 = 0$ and wavevector, Brillouin zones are obtained. The Brillouin zone for SC is cubic itself, BCC possesses dodecahedron; whereas for FCC, it is truncated octahedron. The atomic scattering factor is equal to atomic number of an atom. Through geometrical structure factor $S = \sum f_i e^{-2\pi i(u_i h + v_i k + w_i l)}$ helps in determining the missing reflections.

SOLVED PROBLEMS

Q.1: Identify the lattice

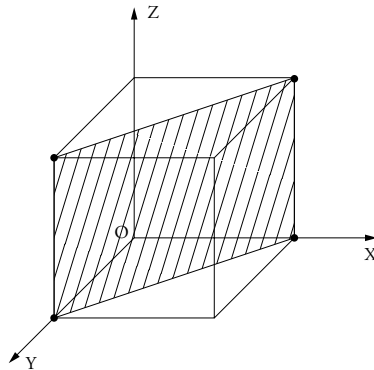
(i) $a = 9.4 \text{ \AA}$, $b = 8 \text{ \AA}$, $c = 10.2 \text{ \AA}$, $\alpha = \beta = \gamma = 90^\circ$

(ii) $a = 3 \text{ \AA} = b = c$
 $\alpha = \beta = \gamma = 85^\circ$

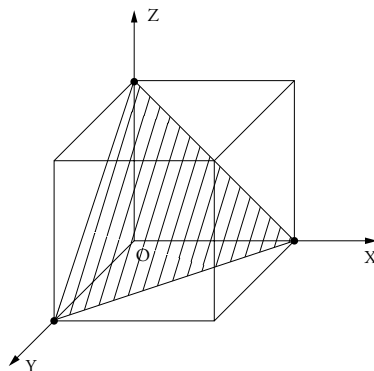
Ans: (i) It is orthorhombic lattice.
(ii) It is trigonal lattice.

Q.2: Obtain the plane (i) (110), (ii) (111), (iii) (010), (iv) (100), (v) (011), and (vi) $(0\bar{1}0)$ for cubic systems.

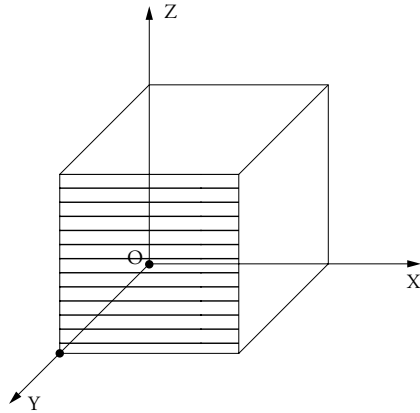
Ans: (i) (110)



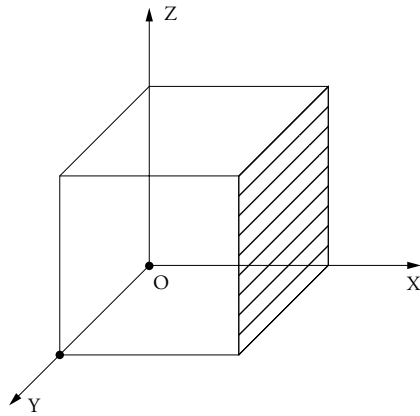
If the Miller index for an axis is 0, then its intercept is made at $\frac{1}{0} = \infty$. Here, z will meet at infinity.
(ii) (111)



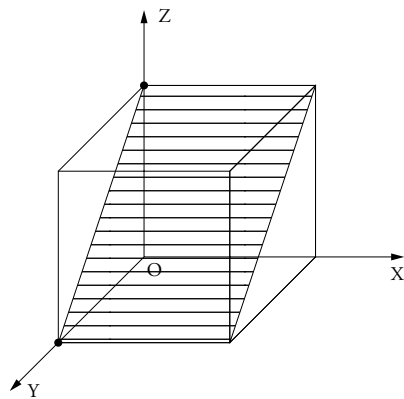
(iii) (010)

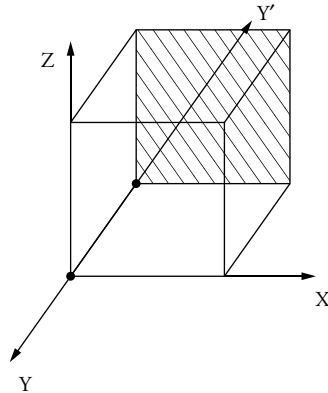


(iv) (100)



(v) (011)



(vi) $(0\bar{1}0)$ 

Q.3: A plane intercepts at $2a$, $3b$, and $\frac{c}{3}$ in simple cubic cell. Obtain the Miller indices for plane.

Ans: The intercepts are $\left(2, 3, \frac{1}{3}\right)$

Reciprocal gives $\left(\frac{1}{2}, \frac{1}{3}, 3\right)$

Smallest integers yield $(3, 2, 18)$

Hence, Miller indices are $(3, 2, 18)$.

Q.4: A plane makes intercept of 4 \AA , 6 \AA , and 3 \AA for monoclinic lattice such that $a : b : c = 4 : 2 : 3$. Obtain the Miller indices for the system.

Ans: $a : b : c = 4 : 2 : 3$

We know $n_1 a = 4$, $n_2 b = 6$, and $n_3 c = 3$

$$n_1 = \frac{4}{a} = \frac{4}{4} = 1$$

$$n_2 = \frac{6}{b} = \frac{6}{2} = 3$$

$$n_3 = \frac{3}{c} = \frac{3}{3} = 1$$

Hence, $n_1 = 1$, $n_2 = 3$, and $n_3 = 1$

Reciprocals are $\left(1, \frac{1}{3}, 1\right)$

Smallest integers are $(3, 1, 3)$

Hence, Miller indices are $(3, 1, 3)$.

Q.5: For lead, obtain the spacing of (011), (111), and (112) planes for FCC structure ($a = 4.95 \text{ \AA}$).

Ans:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{011} = \frac{4.95}{\sqrt{2}} = \frac{4.95}{1.41} = 3.51 \text{ \AA}$$

$$d_{111} = \frac{4.95}{\sqrt{3}} = \frac{4.95}{1.73} = 2.86 \text{ \AA}$$

$$d_{112} = \frac{4.95}{\sqrt{6}} = \frac{4.95}{2.44} = 2.02 \text{ \AA}$$

Q.6: For orthorhombic system, calculate lattice spacing of (110) planes for $a = 4.5 \text{ \AA}$, $b = 3.5 \text{ \AA}$, and $c = 2.5 \text{ \AA}$.

Ans:

$$d = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}$$

$$d = \left(\left(\frac{1}{4.5} \right)^2 + \left(\frac{1}{3.5} \right)^2 + 0 \right)^{-1/2}$$

$$d = (0.04938 + 0.081632)^{-1/2}$$

$$d = 2.77 \text{ \AA}$$

Q.7: The silver has FCC structure (mass number = 108). Obtain the density, if its lattice constant is 4.077 \AA .

Ans: For FCC,

$$\rho = \frac{4M}{N' a^3}$$

$$a = 4.077 \text{ \AA}, \quad N' = 6.023 \times 10^{23}, \quad M = 108$$

$$\rho = \frac{4 \times 108}{6.023 \times 10^{23} \times (4.077 \times 10^{-8})^3}$$

$$\rho = \frac{432}{408.16 \times 10^{23} \times 10^{-24}}$$

$$\rho = 10.58 \text{ g/cm}^3$$

Q.8: Copper has atomic radius of 1.278 Å and FCC structure. Obtain its density ($M = 63.54 \text{ g}$)

Ans: For FCC,

$$\rho = \frac{4M}{N' a^3}$$

Here,

$$r = 1.278 \text{ Å}$$

for FCC

$$r = \frac{\sqrt{2}}{4} a$$

$$a = \frac{4r}{\sqrt{2}} = \frac{4 \times 1.278}{\sqrt{2}}$$

$$a = 3.625 \text{ Å}$$

Hence,

$$\rho = \frac{4 \times 63.54}{6.023 \times 10^{23} \times (3.625 \times 10^{-8})^3}$$

$$\rho = \frac{254.16}{286.9 \times 10^{-1}} = 8.85 \text{ g/cm}^3.$$

Q. 9: A wavelength of 0.63 Å is used for first order diffraction and the glancing angle of 12°. What should be the glancing angle for second-order diffraction?

Ans: $\theta_1 = 12^\circ$, $\lambda = 0.63 \text{ Å}$, $n_1 = 1$, and $n_2 = 2$

According to Bragg's law $2d \sin \theta_1 = n_1 \lambda$,

$$2d \sin 12^\circ = 0.63$$

$$2d = \frac{0.63}{\sin 12^\circ} \quad (\text{a})$$

For second order diffraction,

$$2d \sin \theta_2 = n_2 \lambda$$

$$2d = \frac{2 \times 0.63}{\sin \theta_2} \quad (\text{b})$$

From Eqs (a) and (b),

$$\frac{0.63}{\sin 12^\circ} = \frac{2 \times 0.63}{\sin \theta_2}$$

$$\sin \theta_2 = 2 \times \sin 12^\circ = 2 \times 0.2079 = 0.414$$

$$\theta_2 = \sin^{-1}(0.414)$$

$$\theta_2 = 24.45^\circ$$

Q.10: Calculate the glancing angle for NaCl [001] corresponding to second-order diffraction maximum. The lattice constant is 2.814 \AA and wavelength of X-rays is 0.72 \AA .

Ans: First of all, we shall obtain “ d ”

$$a = 2.814 \text{ \AA}$$

$$d_{001} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{2.814}{1} = 2.814 \text{ \AA}$$

Now, according de Bragg’s law,

$$2d \sin \theta = n\lambda$$

Here, $n = 2$, $\lambda = 0.72 \text{ \AA}$, and $d = 2.814$:

$$\sin \theta = \frac{2 \times 0.72}{2 \times 2.814} = 0.2558^\circ$$

$$\theta = \sin^{-1}(0.2558) = 14.82^\circ$$

$$\theta = 14.82$$

Q.11: For BCC crystal, X-rays of wavelength 1.54 \AA irradiate (101) planes. If the interplanar separation is 1.181 \AA , obtain the orders of Bragg reflection:

Ans: According to Bragg’s condition,

$$2d \sin \theta = n\lambda$$

For maximum, $\sin \theta \rightarrow 1$

$$n = \frac{2d}{\lambda} = \frac{2 \times 1.181}{1.54} = 1.534$$

“ n ” should be a whole number, for $\theta < 90^\circ$, $n \approx 1$. Hence, only the first-order diffraction occurs.

Q.12: Sodium chloride crystal has lattice constant of 5.6 \AA . If the interplanar separation $d = \frac{a}{\sqrt{5}}$ and wavelength of 1.1 \AA fall on the planes, how many diffraction orders can be observed?

Ans: We know $2d \sin \theta = n\lambda$

$$d = \frac{a}{\sqrt{5}} = \frac{5.6}{\sqrt{5}} = 2.504 \text{ \AA}$$

$\lambda = 1.1 \text{ \AA}$, for maximum, $\sin \theta \rightarrow 1$

$$n = \frac{2d}{\lambda} = \frac{2 \times 2.504}{1.1} = 4.55$$

As n can be whole number only, $n = 4$ for $\theta < 90^\circ$.

Q.13: Find different orders of Bragg's reflection, if the crystal spacing is 2.384 \AA and wavelength of 1.54 \AA is incident on it.

Ans: $\lambda = 1.54 \text{ \AA}$ and $d = 2.384 \text{ \AA}$

From Bragg's law of diffraction,

$$2d \sin \theta = n\lambda$$

For $n = 1$,

$$\sin \theta_1 = \frac{n\lambda}{2d} = \frac{1.54}{2 \times 2.384}$$

$$\sin \theta_1 = 0.3229$$

$$\theta_1 = 18.83^\circ$$

For $n = 2$,

$$\sin \theta_2 = 0.645$$

$$\theta_2 = 40.23^\circ$$

For $n = 3$,

$$\sin \theta_3 = 0.9689$$

$$\theta_3 = 75.67^\circ$$

For $n = 4$,

$$\sin \theta_4 = 1.311$$

$$\sin \theta_4 > 1$$

Hence, $n = 4$ is not possible. Only three orders of diffraction are observed.

Q.14: Obtain the reciprocal lattice vector for $\vec{a} = 2\hat{x}$ and $\vec{b} = \hat{x} + 2\hat{y}$, two-dimensional lattice.

Ans: Let us suppose $\vec{c} = \hat{z}$

$$\vec{a}^* = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = 2\pi \frac{(\hat{x} + 2\hat{y}) \times \hat{z}}{2\hat{x} \cdot (\hat{x} + 2\hat{y} \times \hat{z})}$$

$$\vec{a}^* = \pi \hat{x} - \frac{\pi}{2} \hat{y}$$

Similarly,

$$\begin{aligned} \vec{b}^* &= \frac{2\pi \cdot \vec{c} \times \vec{a}}{(\vec{a} \cdot \vec{b} \times \vec{c})} \\ &= \frac{2\pi \cdot (\hat{z} \times 2\hat{x})}{2\hat{x} \cdot ((\hat{x} + 2\hat{y}) \times \hat{z})} = \pi \hat{y} \end{aligned}$$

Q.15: The primitive lattice vectors of hexagonal space lattice are as follows:

$$\vec{a} = \frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j}$$

$$\vec{b} = -\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j}$$

$$\vec{c} = c \hat{k}$$

Obtain the volume of primitive cell and primitive translation of reciprocal lattice:

Ans: Volume,

$$V = \vec{a} \cdot (\vec{b} \times \vec{c})$$

$$V = \left(\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \cdot \left(\left(-\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \times c \hat{k} \right)$$

$$V = \left(\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \cdot \left(\frac{ac}{2} \hat{j} + \frac{\sqrt{3}}{2} ac \hat{i} \right)$$

$$V = +\frac{\sqrt{3}}{4} a^2 c + \frac{\sqrt{3}}{4} a^2 c = \frac{\sqrt{3}}{2} a^2 c$$

Hence, volume, $V = \frac{\sqrt{3}}{2} a^2 c$

The primitive translation of reciprocal lattice is given by the following equation:

$$\vec{a}^* = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = \frac{2\pi \left[\left(-\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \times c \hat{k} \right]}{\frac{\sqrt{3}}{2} a^2 c}$$

$$\vec{a}^* = \frac{2\pi \left[\frac{ac}{2} \hat{j} + \frac{\sqrt{3}}{2} ac \hat{i} \right]}{\frac{\sqrt{3}}{2} a^2 c}$$

$$\vec{a}^* = \frac{2\pi}{a} \left(\hat{i} + \frac{1}{\sqrt{3}a} \hat{j} \right)$$

Similarly,

$$\vec{b}^* = \frac{2\pi \cdot (\vec{c} \times \vec{a})}{\vec{a} \cdot (\vec{b} \times \vec{c})} = \frac{2\pi \cdot \left(c \hat{k} \times \left(\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \right)}{\sqrt{3} / 2 a^2 c}$$

$$\vec{b}^* = \frac{2\pi \left[\frac{ac}{2} \hat{j} - \frac{\sqrt{3}ac}{2} \hat{i} \right]}{\frac{\sqrt{3}}{2} a^2 c}$$

$$\vec{b}^* = \frac{2\pi}{a} \left[-\hat{i} + \frac{1}{\sqrt{3}a} \hat{j} \right]$$

and

$$\vec{c}^* = \frac{2\pi \cdot (\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{c}^* = \frac{2\pi \left(\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right) \times \left(-\frac{a}{2} \hat{i} + \frac{\sqrt{3}}{2} a \hat{j} \right)}{\frac{\sqrt{3}}{2} a^2 c}$$

$$\vec{c}^* = \frac{2\pi}{c} \hat{k}$$

OBJECTIVE QUESTIONS

1. Primitive cell has

- (a) zero volume (b) maximum volume
(c) negative volume (d) minimum volume

2. Coordination number of SC lattice is

- (a) 8 (b) 6
(c) 12 (d) 10

3. Atomic radius for BCC lattice is

- (a) $\frac{a}{2}$ (b) $\frac{\sqrt{3}}{2}a$
(c) $\frac{\sqrt{3}a}{4}$ (d) $\frac{\sqrt{2}a}{4}$

4. Atomic radius for FCC lattice is

- (a) $\frac{\sqrt{2}a}{4}$ (b) $\frac{\sqrt{3}a}{4}$
(c) $\frac{\sqrt{3}a}{2}$ (d) $\frac{a}{2}$

5. Number of atoms in FCC lattice are

- (a) 1 (b) 12
(c) 4 (d) 2

6. The coordination number in HCP lattice is

- (a) 15 (b) 12
(c) 8 (d) 6

7. The ratio c/a for HCP lattice is

- (a) $\sqrt{\frac{6}{5}}$ (b) $\sqrt{\frac{6}{7}}$
(c) $\sqrt{\frac{4}{3}}$ (d) $\sqrt{\frac{8}{3}}$

8. Atomic radius for SC lattice is

- (a) $\frac{a}{2}$ (b) $\frac{\sqrt{3}a}{4}$
(c) $\frac{\sqrt{2}a}{4}$ (d) $\frac{a}{4}$

9. The packing fraction of FCC lattice is
(a) 58 percent (b) 64 percent
(c) 74 percent (d) 50 percent
10. Packing fraction of BCC lattice is
(a) 52 percent (b) 68 percent
(c) 74 percent (d) 90 percent
11. Sodium chloride has _____ structure
(a) FCC (b) BCC
(c) HCP (d) SC
12. For monoclinic crystal
(a) $\alpha = \beta = \gamma = 90^\circ$ (b) $\alpha \neq \beta \neq \gamma \neq 90^\circ$
(c) $\alpha = \beta = 90^\circ \neq \gamma$ (d) $\alpha = \beta = 120^\circ, \gamma = 90^\circ$
13. A crystal cannot have _____ symmetry
(a) 5 (b) 7
(c) both (a) and (b) (d) none of these
14. BCC lattice is the reciprocal of
(a) SC (b) FCC
(c) BCC (d) HCP
15. (300) reflection is absent for
(a) BCC (b) FCC
(c) SC (d) HCP
16. FCC lattice is the reciprocal of
(a) SC (b) FCC
(c) HCP (d) BCC
17. The Brillouin zones obtained by BCC lattice is
(a) cubic (b) octahedron
(c) dodecahedron (d) HCP
18. The Brillouin zone obtained by FCC lattice is
(a) cubic (b) octahedron
(c) dodecahedron (d) truncated octahedron
19. The structure factor $S = 4f$ exists for FCC, if all indices are
(a) all even or odd (b) one even and two odd
(c) one odd and two even (d) all of these

ANSWERS

- | | | |
|--------|---------|---------|
| 1. (d) | 8. (a) | 15. (a) |
| 2. (b) | 9. (c) | 16. (d) |
| 3. (c) | 10. (b) | 17. (c) |
| 4. (a) | 11. (a) | 18. (d) |
| 5. (c) | 12. (c) | 19. (a) |
| 6. (b) | 13. (c) | |
| 7. (d) | 14. (b) | |

Micro-Assessment Questions

1. What are crystalline solids? Give their properties along with examples.
2. Define amorphous materials with examples.
3. Define lattice ad motifs for crystal plane.
4. What are the translational vectors?
5. Explain basis for a crystal lattice.
6. Define plane of symmetry and center of symmetry.
7. How does reflection operation differ from rotation operation?
8. Explain the translational operation.
9. What is inversion operation?
10. What is unit cell?
11. Define the lattice parameters for crystal structure.
12. Give the parameters for oblique lattice and primitive rectangular lattice.
13. Draw base-centered tetragonal lattice.
14. Give the lattice parameters for hexagonal and monoclinic lattice.
15. Define interplanar spacing for planes.
16. What is the miller index, when the intercept is infinity?
17. What is the coordination number for SC, BCC, and FCC system?
18. Explain the crystal structure for sodium chloride.
19. Give the c/a ratio for HCP.
20. What is Bragg's equation?
21. Define reciprocal lattice.
22. Give the dimensions of reciprocal vector.

Critical Thinking Questions

1. State the differences between crystalline and amorphous materials.
2. Define crystal structure. Which quantities are required to make a crystal?
3. Give the basic symmetry elements of a lattice.
4. Show that five- and seven-fold symmetry does not exist for crystal structure.
5. Describe the basic symmetry operations for crystal lattice, which leaves the lattice invariant.
6. List the differences between translational and rotational operation for crystal.
7. How does unit cell differ from primitive cell?
8. Give the different types of lattices in two-dimensional systems.
9. Draw the two Bravais lattice for the monoclinic lattice.
10. How many types of orthorhombic lattices are possible? Explain.
11. Draw the plane (111) and (101).
12. Obtain the Miller indices, given the intercepts are $3a$, $3b$, and $2c$ for simple cubic cell.
13. Obtain the lattice spacing for 111 plane of orthorhombic system with $a = 0.35$ nm, $b = 0.25$ nm, and $c = 0.55$ nm.
14. Derive the atomic radius for FCC system.
15. Derive the packing fraction and atomic radius for BCC system.
16. Explain in detail all the properties for simple cubic system.

17. Obtain the density for iron and copper.
18. What is ABC stacking? Explain with diagram.
19. Give the crystal structure for sodium chloride crystal.
20. Explain the scattering normal for crystal.
21. Derive the Bragg's law of diffraction from the Laue's equations.
22. What is rotating crystal method to determine crystal structure?
23. Explain the Laue's method of crystal structure determination.
24. Describe the powder crystal method of crystallography.
25. Obtain the reciprocal lattice for simple cubic system.
26. Derive the reciprocal lattice for simple cubic lattice.
27. Obtain the Brillouin zones for BCC.
28. Derive the Brillouin's zones for FCC lattice.
29. What is atomic scattering factor? How does it differ from geometrical scattering factor?

Graded Questions

1. Explain in detail the types of Bravais lattices in three dimensions.
2. What are Miller indices? How can we obtain Miller indices for a plane? Draw a plane for (110).
3. Define interplanar spacing. Derive the interplanar spacing for tetragonal system.
4. Explain the cubic systems in detail along with their coordination number, atomic radius, and packing fraction.
5. Describe the packing of spheres in ABAB and ABCABC stacking in detail.
6. Explain in detail with diagram the crystal structure for diamond. Also obtain the packing fraction, atomic radius, and coordination number.
7. What is hexagonal close packing? Obtain its packing fraction. Show that for HCP the c/a is 1.633.
8. State the Laue's method of X-ray diffraction. Derive the Laue's equations for crystals.
9. List the various X-ray diffraction techniques for determination of crystal structure.
10. Define the reciprocal vector. Obtain the reciprocal vectors from primitive lattice vectors.
11. Obtain the reciprocal lattice for BCC and FCC systems. Show that FCC and BCC lattices are reciprocal lattices of each other.
12. Derive the first and second Brillouin zones for crystal.
13. What is atomic scattering factor? Show that the atomic scattering factor denotes the total charge of atom.
14. Define geometrical factor. Derive the geometrical structure factor.
15. Obtain the geometrical structure factor for SC, BCC, and FCC lattice. Why (211), (342), and (100) planes do not exist for FCC lattice?

Remember and Understand

1. In crystals, atoms occupy well-defined positions in space; whereas in amorphous solids, the arrangement does not follow any regular arrangement. Crystals are anisotropic, whereas amorphous solids are isotropic.

2. In the crystals, every atom or molecule is represented by a representative unit which is mathematical points known as motifs.
3. To obtain a crystal structure, a group of atom should be added to every lattice point. This group of atoms is known as basis. Basis may contain several atoms.
4. The symmetry plane is an imaginary plane, which is supposed to divide the lattice into two equal halves.
5. Symmetry center is point in crystal so that for point r , there exists $-r$ w.r.t. fixed position O. Five- and seven-fold-symmetry do not exist.
6. There are four different symmetry operations, that is, rotational, translation, reflection, and inversion.
7. Unit cells are the smallest entities which when repeated will generate the whole crystal lattice in space. Unit cells are of two types: primitive and nonprimitive. Primitive cell has minimum volume. In nonprimitive cell, the lattice point can be at the center of cell also.
8. The intercepts for unit cell are a , b , and c . There are five types of crystal lattice in two-dimensional space and 14 types of crystal lattice in three-dimensional space. The most symmetric lattice is cubic system.
9. Miller devised a set of indices to represent different set of planes within the crystals. Miller indices describe the directions and orientations of planes. The direction in general is denoted by $[uvw]$ and direction by $\langle uvw \rangle$. The Miller indices of a plane are denoted by (hkl) .
10. The interplanar spacing “ d ” between planes is given by the following equation:

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

11. The cubic unit cells are of three types: simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC). All of these have the same volume. The coordination number for SC, BCC, and FCC is 6, 8, and 12, respectively. The packing fraction of SC, BCC, and FCC is 52.3 percent, 68 percent, and 74 percent, respectively.
12. Diamond cubic structure is made of two interpenetrating lattices: one lattice having the origin at $(0, 0, 0)$ and other lattice having the origin at $(a/4, a/4, a/4)$. There are a total of eight atoms/unit cell and the packing fraction is 34 percent for diamond cubic lattice.
13. In hexagonal close packing (HCP), three atoms are present inside the hexagon body, two at basal planes and one at every corner. The packing fraction is 74 percent for HCP and the coordination number is 12. The c/a ratio for HCP is 1.633.
14. Bragg suggested that X-rays are scattered from the crystal planes, but Laue said that the reflection of X-rays occur from the individual atoms. Laue gave set of three equations from which Bragg's equation can be obtained:

$$2a \cos \alpha \sin \theta = nh\lambda$$

$$2a \cos \beta \sin \theta = nk\lambda$$

$$2a \cos \gamma \sin \theta = nl\lambda$$

15. There are three methods to determine the crystal structure: (i) Laue's method in which the position of crystal is fixed, (ii) rotating crystal method in which the crystal rotates, and (iii) powder diffraction method that uses the sample in powdered form.
16. Reciprocal lattice is the array of points that are obtained at the end of normal drawn to a common origin whose length is proportional to the reciprocal of interplanar spacing. The magnitude of reciprocal lattice vector is reciprocal of its interplanar spacing.
17. The reciprocal lattice vectors are given by the following equation:

$$\vec{c}^* = \frac{2\pi(\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{a}^* = \frac{2\pi(\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{b}^* = \frac{2\pi(\vec{c} \times \vec{a})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

18. Reciprocal lattice for BCC is given by the following equation:

$$\vec{a}^* = \frac{2\pi \cdot (\vec{B} \times \vec{C})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{j} + \hat{k})$$

$$\vec{b}^* = \frac{2\pi \cdot (\vec{C} \times \vec{A})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{k} + \hat{i})$$

$$\vec{c}^* = \frac{2\pi \cdot (\vec{A} \times \vec{B})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{i} + \hat{j})$$

19. Reciprocal lattice for FCC is given by the following equation:

$$\vec{a}^* = \frac{2\pi(\vec{B} \times \vec{C})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{b}^* = \frac{2\pi(\vec{C} \times \vec{A})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{i} - \hat{j} + \hat{k})$$

$$\vec{c}^* = \frac{2\pi(\vec{A} \times \vec{B})}{\vec{A} \cdot (\vec{B} \times \vec{C})} = \frac{2\pi}{a} (\hat{i} + \hat{j} - \hat{k})$$

20. The primitive cell in reciprocal lattice represents the Brillouin zone. The family of straight lines is given by
[type Figure (44)]

21. The Brillouin's zones for BCC is given by

$$h = \pm 1 \text{ and } k = 0 = l, \text{ then } \pm k_3 \pm k_2 = -\frac{2\pi}{a}$$

$$h = 0, k = \pm 0, \text{ and } l = 0, \text{ then } \pm k_1 \pm k_3 = -\frac{2\pi}{a}$$

$$h = 0, k = 0, \text{ and } l = \pm 1, \text{ then } \pm k_1 \pm k_2 = -\frac{2\pi}{a}$$

22. The Brillouin's zones for FCC is given by

$$h = \pm 1, k = 0, \text{ and } l = 0, \text{ then } \pm k_1 \pm k_2 \pm k_3 = 3\pi/a$$

$$h = 0, k = \pm 1, \text{ and } l = 0, \text{ then } \pm k_1 \pm k_2 \pm k_3 = 3\pi/a$$

$$h = 0, k = 0, \text{ and } l = \pm 1, \text{ then } \pm k_1 \pm k_2 \pm k_3 = 3\pi/a$$

23. The atomic scattering factor (f) is defined as amplitude of radiations that are scattered from the atom to the amplitude of radiations that are scattered from the electron. " f " denotes the total charge of an atom.

24. To obtain the total scattering, the amplitude of all the scattered wavelets by each atoms are added to get geometrical structure factor (S) and is given by the following equation:

$$S = \sum_i f_i e^{-2\pi i(u_i, h + v_i, k + w_i, l)}$$

Solid-State Physics

Keywords: phonons, lattice vibrations, acoustic and optical regime, Brillouin zones, Drude–Lorentz model, Ohm’s law, Wiedemann–Franz law, Sommerfeld theory, free electron gas, Bloch theorem, Kronig–Penney model

Learning Objectives

- ◆ To understand the vibrations of atoms in crystal lattice
- ◆ To learn about the difference between photon and phonon
- ◆ To obtain the dispersion relation in monoatomic lattice
- ◆ To obtain the Brillouin zones for monoatomic lattice
- ◆ To understand the origin of optical and acoustical branch for diatomic lattice
- ◆ To understand the free electron model, that is, Drude–Lorentz theory
- ◆ To derive and explain Ohm’s law, Wiedemann–Franz’s law, and conductivity phenomena based on free electron model
- ◆ To learn about one-dimensional analysis of free electrons using Sommerfeld’s quantum theory.
- ◆ To understand Fermi energy and total energy
- ◆ To know about Fermi velocity and density of states
- ◆ To learn about the variation of density of states with energy
- ◆ To understand the three-dimensional analysis of free electron gas
- ◆ To know about band theory of solids, that is, the charging potential experienced by electrons in each other’s vicinity
- ◆ To learn about Bloch function and Bloch theorem
- ◆ To know about Kronig–Penney model, that is, applying one-dimensional potential model to understand behavior of electrons
- ◆ To learn about area of potential barrier and its variation w.r.t. width
- ◆ To learn about variation of width of allowed bands w.r.t. energy values

Lattice dynamics deals with vibrations of atoms around the equilibrium position. Atoms always vibrate around their mean position even at absolute zero, although these vibrations may be negligible. As the temperature increases, the atoms displace from the equilibrium position. While talking about the crystal, it consists of regular arrangement of atoms/molecules. The neighboring atoms in the crystal have force of attraction or repulsion between them. Hence, the vibration spread among whole crystal lattice instead of being limited to any single atom. These vibrations are known as lattice

vibrations. Single atom vibrates like harmonic oscillator. The energy of harmonic oscillator is quantized and is given by the following equation:

$$E_n = \left(n + \frac{1}{2} \right) hf \quad (1)$$

Equation (1) signifies that the energy levels are discrete and not continuous. Different values of n correspond to different energy values:

$$\text{For } n = 0, E_n = \frac{1}{2} hf = \frac{1}{2} \hbar \omega \quad \left[\begin{array}{l} \omega = 2\pi f \\ f = \frac{\omega}{2\pi} \end{array} \right]$$

$\frac{1}{2} \hbar \omega$ is the zero point energy which indicates that even at absolute zero, the atom has $\frac{1}{2} \hbar \omega$ minimum energy which is in contrast to the Planck's hypothesis. According to Planck's hypothesis, $E_n = nhf$; hence for $n = 0$, $E = 0$. But the existence of zero point energy is verified. If we take two energy levels corresponding to n_1 , and n_2 , then the energy difference is given by the following equation:

$$E_2 - E_1 = (n_2 - n_1) hf \quad (2)$$

Similar analogy is given when crystal atoms absorb quantum of thermal energy. "Phonon" is the name given to this quantum of thermal energy in case of lattice vibrations. In other words, the interactions that take lattice vibrations into consideration always involve the interaction of phonons. Like photons, phonons also obey Bose-Einstein statistics. The difference between photon and phonon is that photons originate from elastic waves. Although photons belong to electromagnetic waves, phonons require material medium for their propagation. Phonons interact with particles in the lattice. Phonons also get in elastically scattered by long wavelength photons. We can demonstrate it as follows:

Let us suppose μ is the refractive index of medium, and c is the velocity of light in vacuum. We can give the velocity v , light photons to be

$$v = \frac{c}{\mu}$$

$$f = \frac{c}{\mu \lambda} \quad (3)$$

$$2\pi f = \frac{2\pi c}{\mu \lambda} \quad \left[k = \frac{2\pi}{\lambda} \right]$$

$$\omega = \frac{2\pi}{\lambda} \frac{c}{\mu} = \left(k \frac{c}{\mu} \right) \quad (4)$$

$$k = \frac{\mu w}{c} \quad (5)$$

k is the incident wavevector. The momentum of photon is given by $p = \frac{h}{\lambda} = \frac{h/2\pi}{\lambda/2\pi} = \hbar k$

$$\vec{p} = \hbar \vec{k} \quad (6)$$

We consider the interaction of photon with phonon and then photon gets scattered changing wavevector from $k \rightarrow k'$. The angular frequency of photon changes from $w \rightarrow w'$. If the phonon having angular frequency Ω and wavevector \vec{K} is created, then it follows the principle of conservation of momentum.

$$\hbar w = \hbar w' + \hbar \Omega$$

The principle of conservation of momentum gives (fig. 17.1)

$$\hbar \vec{k} = \hbar \vec{k}' + \hbar \vec{K} \quad (7)$$

$$\vec{k} = \vec{k}' + \vec{K}$$

$$\vec{K} = \vec{k} - \vec{k}' \quad (8)$$

To determine the magnitude of K , then from Eqn. (8)

$$K = (\vec{K} \cdot \vec{K})^{1/2} = [(\vec{k} - \vec{k}') \cdot (\vec{k} - \vec{k}')]^{1/2}$$

$$K = [\vec{k} \cdot \vec{k} + \vec{k}' \cdot \vec{k}' - 2\vec{k} \cdot \vec{k}']^{1/2}$$

$$K = [k^2 + k'^2 - 2k k' \cos \phi]^{1/2}$$

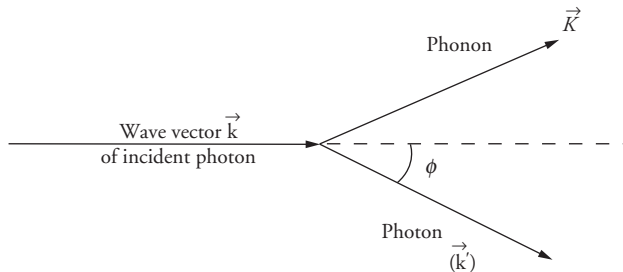


Figure 17.1 Schematic of interaction between photon and phonon.

If we take the magnitude of $\vec{k} \approx \vec{k}'$, then

$$K = [2k^2 (1 - \cos \phi)]^{1/2} = \left[4k^2 \sin^2 \frac{\phi}{2} \right]^{1/2} = 2k \sin \frac{\phi}{2}$$

$$K = 2k \sin \frac{\phi}{2} \quad (9)$$

ϕ is angle between the scattered and incident photon. Let v_p be the velocity of photons inside the crystal, then

$$v_p = \frac{\text{Angular frequency}}{\text{Wavevector}} = \frac{\Omega}{K}$$

$$\Omega = v_p K = 2v_p k \sin \frac{\phi}{2} = \frac{2v_p w \mu}{c} \sin \frac{\phi}{2} \quad (10)$$

17.1 One-Dimensional Monoatomic Lattice

Consider infinite chain of atoms on a straight line with interatomic spacing a . All the atoms are identical having same mass m . The following assumptions are made:

- (i) Atom is considered to be like a sphere. Each atom is connected to each other with a spring (spring constant = β).
- (ii) Atoms follow Hooke's law, that is, the force between the nearest neighbor atoms depends directly on the extension and contraction between them.
- (iii) The interaction extends only between nearest neighbors.
- (iv) The spring between atoms is considered to be mass less.

During equilibrium position, the atoms are present at their equilibrium position. But during motion, the atoms get displaced from their equilibrium position. If x_1, x_2, x_{n+1} are the displacement of 1st, 2nd, and $(n+1)$ th atom from respective equilibrium positions, then the force on n th atom due to $(n-1)$ th atom is $\beta(x_n - x_{n-1})$ as shown in fig 17.2. Similarly, force on n th atom due to $(n+1)$ th atom is given by $\beta(x_{n+1} - x_n)$. These forces are opposite to each other and the net force is given by

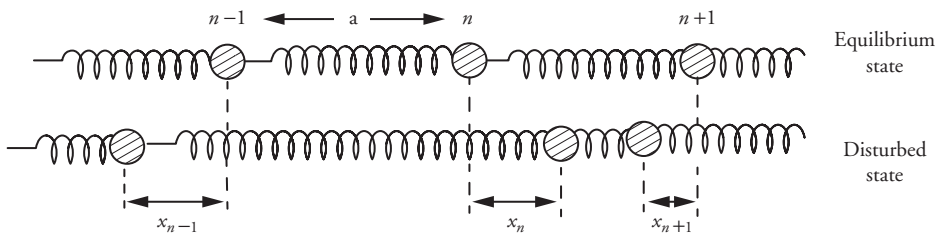


Figure 17.2 Equilibrium and disturbed state of monoatomic lattice.

$$F_n = \beta(x_{n+1} - x_n) - \beta(x_n - x_{n-1})$$

$$m \frac{d^2 x_n}{dt^2} = \beta(x_{n+1} - x_n) - \beta(x_n - x_{n-1}) \quad [\text{Newton's second law}]$$

$$m \frac{d^2 x_n}{dt^2} = \beta[x_{n+1} + x_{n-1} - 2x_n] \quad (11)$$

Let the solution of Eqn. (11) be given by wave represented by

$$x_n = Ae^{i(\omega t - kna)} \quad (12)$$

$k = 2\pi/\lambda$ (wavevector), ω is angular frequency of wave and na is distance of n th atom from origin. For $(n-1)$ and $(n+1)$ th atom, the solution is given by the following equation:

$$x_{n-1} = Ae^{i(\omega t - k(n-1)a)}, \quad x_{n+1} = Ae^{i(\omega t - k(n+1)a)} \quad (13)$$

Using Eqs (12) and (13) in Eqn. (11), we will obtain

$$-m\omega^2 = \beta(e^{-ika} + e^{ika} - 2) \quad \left[\frac{e^{ix} + e^{-ix}}{2} = \cos x \right]$$

$$-m\omega^2 = \beta[2 \cos ka - 2]$$

$$\omega^2 = \frac{4\beta}{m} \sin^2 \frac{ka}{2}$$

$$\omega = \pm \sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2} \quad (14)$$

But ω can only be positive quantity, hence

$$\omega = \sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2} \quad (15)$$

Equation (15) is called dispersion relation. Further, these dispersion relations could be discussed as follows.

The medium is dispersive whenever velocity is nonlinear function of wavelength or wave number. For nondispersive media, w and k are linearly dependent on each other.

$$w = 2\pi f = \frac{2\pi}{\lambda} \lambda f = kv$$

$$w \propto k \quad (16)$$

Variation of w vs. k is shown in Figure 17.3, which could be explained as follows:

(i) When frequency is small, $k \rightarrow 0$

$$\text{then, } \sin \frac{ka}{2} \approx \frac{ka}{2}$$

Equation (15) can be written as follows:

$$w = \sqrt{\beta/m} ka \quad (17)$$

The phase and group velocity are given by v_p and v_g , respectively, and can be computed as follows:

$$v_p = \frac{w}{k} = \left(\sqrt{\beta/m} \cdot \right) a \quad (18a)$$

$$v_g = \frac{dw}{dk} = \left(\sqrt{\beta/m} \cdot \right) a \quad (18b)$$

From Eqn. 18(a)–(b), the phase velocity becomes equal to group velocity. Moreover, both are independent of k . Hence for long wavelength, the atomic nature of medium is not of much importance. In other words, the medium behaves as a homogenous elastic medium. Discreteness of medium has less effect on large wavelengths. This could also be attributed to the fact that large number of atoms participate in all displacement. This is represented by straight dotted lines in Figure 17.3.

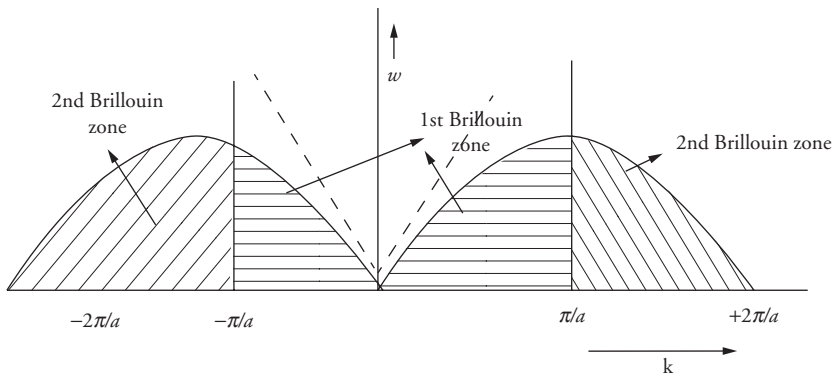


Figure 17.3 Plot of w vs. k .

(ii) For higher frequency, the k does not tend to zero.
then

$$v_p = \frac{w}{k} = \frac{2}{k} \sqrt{\frac{\beta}{m}} \sin \frac{ka}{2} \quad (19a)$$

$$v_g = \frac{dw}{dk} = \frac{d}{dk} \left[\sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2} \right] = a \sqrt{\frac{\beta}{m}} \cos \frac{ka}{2} \quad (19b)$$

Hence, from Eqn. 19(a)–(b), it is clear that phase and group velocity depend on k . When the frequency is high, the medium behaves as dispersive medium.

(iii) When frequency $w = \sqrt{\frac{4\beta}{m}}$, this represents maximum value of frequency.

$$\text{i.e.} \quad \sin \frac{ka}{2} = 1$$

$$\frac{ka}{2} = \pi/2$$

$$\lambda = 2a \quad (20)$$

then

$$v_p = \frac{2a}{\pi} \sqrt{\frac{\beta}{m}} \quad (21a)$$

and

$$v_g = 0 \quad (21b)$$

Equation (21b) represents that when $k \rightarrow \pi/2$, there is no transfer of energy. Waves act as stationary wave. Equation (20) represents the Bragg's condition of reflection [$2d \sin \theta = n\lambda$], first-order reflection is given by $\lambda = 2d$.

Brillouin Zones

We know

$$w = \sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2}$$

Only those waves can propagate, for which $|\sin \frac{ka}{2}| \leq 1$.

$$-1 \leq \sin \frac{ka}{2} \leq 1$$

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a} \quad (22)$$

Equation (22) indicates that waves propagate in positive and negative direction. The Brillouin zones are shown in Figure 17.3.

$$\left| \sin \frac{ka}{2} \right| \leq 1 \text{ is also satisfied, when } -\pi \leq \frac{ka}{2} \leq -\frac{\pi}{2} \text{ and } \frac{\pi}{2} \leq \frac{ka}{2} \leq \pi$$

$$-\frac{2\pi}{a} \leq k \leq -\frac{\pi}{a} \text{ and } \frac{\pi}{a} \leq k \leq \frac{2\pi}{a}$$

This represents second Brillouin zone.

17.2 Diatomic Lattice

Consider a diatomic lattice with two atoms per primitive cell, with m_1 and m_2 respective masses ($m_1 < m_2$). The interatomic distance between nearest neighbor is a . Let x_{2n} be the displacement of atom at $2n$ th position. Lighter atoms (with mass m_1) are placed at even-numbered positions and heavier atoms are placed at odd positions as shown in fig 17.4. All other assumptions are the same as that of monatomic lattice.

The force exerted on atoms could be written as follows:

$$F_{2n} = m_1 x_{2n} = \beta [x_{2n+1} + x_{2n-1} - 2x_{2n}] \tag{23a}$$

$$F_{2n+1} = m_2 x_{2n+1} = \beta [x_{2n+2} + x_{2n} - 2x_{2n+1}] \tag{23b}$$

For Eqn. (23a), the solution could be given by the following equation:

$$x_{2n} = A \exp[i(\omega t - 2kna)] \quad \text{and} \quad x_{2n+1} = B \exp[i(\omega t - (2n + 1)ka)] \tag{24}$$

Where A and B are the amplitude of lattice vibration set by atom m_1 and m_2 . Both atoms have different amplitudes, due to different masses.

Using Eqn. (24) in Eqn. 23(a)–(b), we get

$$-\omega^2 m_1 A = \beta B [\exp(ika) + \exp(-ika)] - 2\beta A$$

$$+(\omega^2 m_1 - 2\beta) A + 2\beta B \cos ka = 0 \tag{25}$$

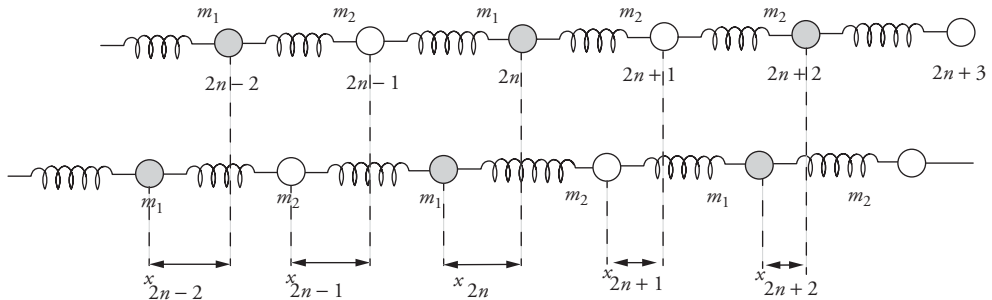


Figure 17.4 Diatomic lattice in equilibrium and disturbed state.

$$\text{and} \quad (w^2 m_2 - 2\beta)B + 2\beta A \cos ka = 0 \quad (26)$$

Using method of determinants, on Eqs (25)–(26),

$$\begin{vmatrix} (w^2 m_1 - 2\beta) & 2\beta \cos ka \\ 2\beta \cos ka & w^2 m_2 - 2\beta \end{vmatrix} = 0$$

$$\text{On} \quad m_1 m_2 w^2 - 2\beta(m_1 + m_2)w^2 + 4\beta^2 \sin^2 ka = 0 \quad (27)$$

The solution for w^2 is given by the following equation:

$$w^2 = \frac{2\beta(m_1 + m_2) + \sqrt{4\beta^2(m_1 + m_2)^2 - 16m_1 m_2 \beta^2 \sin^2 ka}}{2m_1 m_2}$$

$$w^2 = \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \pm \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}} \quad (28)$$

Equation (28) is the dispersion relation for the diatomic lattice w^2 has two values and both are allowed

$$\text{as } \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) > \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}}.$$

Therefore,

$$w_+^2 = \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) + \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}} \quad (29a)$$

and

$$w_-^2 = \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) - \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}} \quad (29b)$$

For long wavelengths, $ka \ll 1$. This implies $\sin ka$ is very small, and hence can be ignored and positive frequency is written as follows:

$$w_+ = \sqrt{2\beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right)} \quad (30)$$

and when $k \rightarrow \frac{\pi}{2a}$, $\sin ka \rightarrow 1$

$$w_+^2 = \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) + \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4}{m_1 m_2}}$$

$$w_+ = \sqrt{2\beta/m_1} \quad (31)$$

We should calculate the expression for w_- , for long wavelength $ka \ll 1$, then $\sin ka \approx ka$ (If we ignore $\sin ka$, then zero value of w_- is obtained), hence

$$w_-^2 = \beta \left[\frac{1}{m_1} + \frac{1}{m_2} \right] - \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \sqrt{1 - \frac{m_1 m_2}{(m_1 + m_2)^2} 4k^2 a^2}$$

$$w_-^2 = \frac{2\beta k^2 a^2}{m_1 + m_2} \quad \left[\begin{array}{l} \text{[using binomial theorem and} \\ \text{ignoring higher order term]} \end{array} \right]$$

$$w_- = ka \sqrt{\frac{2\beta}{m_1 + m_2}} \quad (32)$$

for $k \rightarrow \pi/2a$,

$$w_- = \sqrt{\frac{2\beta}{m_2}} \quad (33)$$

Figure 17.5 is obtained by plotting the solution of Eqs (30)–(33). It is clear that there exists a frequency gap b/w w_+ and w_- . This gap is termed as forbidden frequency gap. The width of this forbidden frequency gap depends upon the ratio of m_1 and m_2 . If $\frac{m_2}{m_1}$ is large, then the forbidden band is more wide and vice-versa.

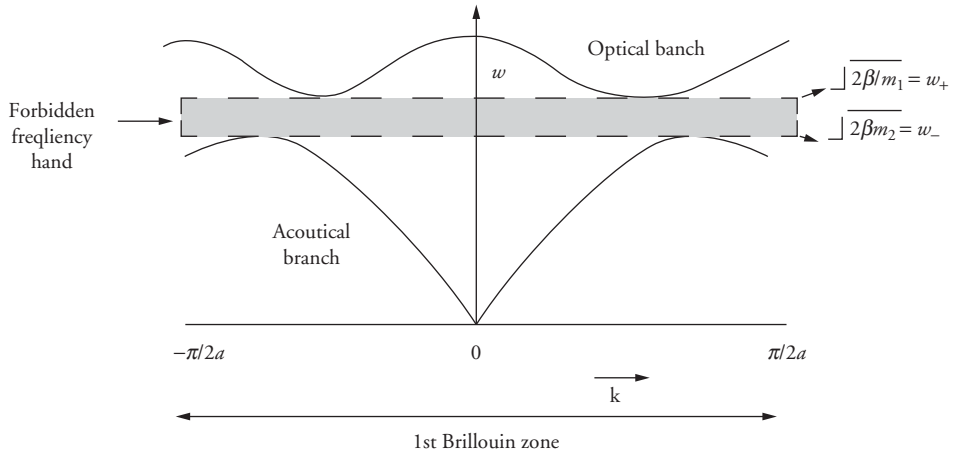


Figure 17.5 Optical and acoustical branch for diatomic lattice.

Following are the important conclusions obtained as outcome of lattice vibrations in diatomic lattice.

- (i) Two branches originate for frequencies: optical and acoustical branches.
- (ii) The graph between w_+ and k represents optical branch whereas graph between w_- and k represents acoustical branch.
- (iii) For optical branch,

When $k \rightarrow 0$ (longer wavelength), then eqn. (25) can be written as

$$(w^2 m_1 + 2\beta)A + (2\beta \cos ka)B = 0$$

as $k \rightarrow 0$, $ka \rightarrow 0$, and hence $\cos ka \rightarrow 1$

$$(w^2 m_1 - 2\beta)A + 2\beta B = 0 \quad (34a)$$

$$\text{Similarly,} \quad (w^2 m_2 - 2\beta)B + 2\beta A = 0 \quad (34b)$$

Eliminating w^2 from Eqs (34a) and (34b), we obtain

$$\frac{A}{B} = -\frac{m_2}{m_1} \quad (35)$$

Equations (35) signify that two atoms vibrate opposite to each other. Hence, the atoms vibrate perpendicular to direction of propagation of wave. These wavemotions are excited by transverse optical waves. Therefore, this branch is called optical branch.

For acoustical branch,

When $k \rightarrow 0$ (longer wavelength), then

$$\cos ka = 1 - \frac{k^2 a^2}{2}$$

and we obtain

$$\frac{A}{B} = 1 \quad (36)$$

Equation (36) signifies that all the atoms have same amplitude. Moreover, they vibrate in same direction. Hence, longitudinal waves are required to excite such wavemotion. Therefore, this wavemotion is called acoustical branch.

Note:

1. If $m_1 = m_2$, no forbidden gap exists and frequency for monatomic and diatomic lattices is same.
2. If $m_2 > m_1$, then acoustical branch gets almost flat and if $m_1 > m_2$, then optical branch is flat.
3. The 1st Brillouin zone extends from $-\pi/2a$ to $\pi/2a$.

17.3 Free Electron Model (Drude–Lorentz Theory)

D. Drude gave the free electron model in 1909. Free electrons are those electrons that are present in the outermost shell of atom. These electrons are free to move anywhere inside the metal kernel, but cannot come out of metal surface on their own. When some force is applied to these electrons, they

may come out of metal surface. Drude proposed that the free electrons are responsible for thermal and heat conduction of metal. Two basic assumptions are that there is no force of attraction b/w electrons, and the electrons move in constant uniform field. Hence, the electrons theory follows the same trend as that of kinetic theory of gases, Therefore, the name of the theory is called electron gas model or free electron theory or Drude–Lorentz theory.

This theory explains Ohm’s law, Wiedemann–Franz’s law, and many other phenomena’s. But certain concepts could not be explained using these theory, that is, nonlinear hall resistivities and higher order thermal conduction which were explained by Sommerfeld (he used quantum statistics).

17.4 Properties Explained By Free Electron Model

Electrons keep on moving in metal like molecules of gas. While in continuous motion, they keep on colliding with each other. Hence, when the electrons undergo these collisions, the direction and velocity of electron also get changed. As is clear from Maxwell–Boltzmann’s law, $v_{\text{rms}} = \sqrt{\frac{3k_B T}{m}}$. The root-mean-square value for electrons is $\approx 10^5$ m/s and k_B is Boltzmann constant.

As the electrons travel in zig-zag path, hence the average velocity of electrons is zero. But if electric field is applied across the ends of conductor, then the electrons gets accelerated in opposite direction to that of applied electric field. The average velocity with which the electrons drift opposite to applied electric field is called drift velocity. The average free path between two successive collisions is called mean free path and is given by λ . Further, the time between two successive collisions is given by relaxation time and is given by τ . We can define the following properties using free electron theory:

17.4.1 Ohm’s Law and Electrical Conductivity

If E is the electric field applied, then the electrons get accelerated and is given by the following equation:

$$a = \frac{d^2 x}{dt^2} = \frac{eE}{m} \quad (37)$$

The relation between relaxation time τ and mean free path λ is given by the following equation:

$$\tau = \frac{\lambda}{v} \quad (38)$$

where v is the velocity of electron.

Integrate Eqn. (37), we get,

$$\frac{dx}{dt} = \frac{eEt}{m} + c$$

For $t = 0$, $\frac{dx}{dt} = 0$ and hence $c = 0$

$$\frac{dx}{dt} = v = \frac{eEt}{m}$$

Hence, the distance travelled is given by the following relation:

$$\bar{x} = \int_0^{\tau} \left(\frac{eE}{m} t \right) dt = \frac{eE\tau^2}{2m} \quad (39a)$$

From Eqn. (39a), we can find out average velocity, i.e.

$$\bar{v} = \frac{(eE\tau^2/2m)}{\tau} = \frac{eE\tau}{2m} \quad (39b)$$

$$\bar{v} = \frac{eE\lambda}{2m\nu} \quad (39c)$$

According to kinetic theory of gases, $\frac{1}{2}mv^2 = \frac{3}{2}k_B T$,

$$\Rightarrow mv = \frac{3k_B T}{\nu} \quad (39d)$$

Substituting Eqn. (39d) in Eqn. (39c), we obtain

$$\bar{v} = \frac{eE\lambda}{2(3k_B T / \nu)} = \frac{eE\lambda\nu}{6k_B T} \quad (40)$$

For a conductor, the current is given by (cross section of conductor is A and n is the number of free electrons).

$$I = ne A \bar{v}$$

$$\frac{I}{A} = ne \bar{v} = \frac{ne^2 E \lambda \nu}{6k_B T}$$

$$J = \text{current density} = \frac{I}{A} = \frac{ne^2 E \lambda \nu}{6k_B T} \quad (41)$$

From Eqn. (41),

$$J = \frac{ne^2 E \lambda \nu}{6k_B T}$$

$$J = \left(\frac{ne^2 \lambda \nu}{6k_B T} \right) E$$

$$J = \sigma E \quad (42)$$

Where

$$\sigma = \frac{ne^2 \lambda v}{6k_B T} = \text{conductivity} \quad (43)$$

Equation (42) represents Ohm's law according to which the current density depends directly on electric field. Equation (43) signifies that conductivity depends on the number of free electrons (n).

17.4.2 Thermal Conductivity

Thermal conductivity is defined as the rate at which heat flows through a material that is maintained at temperature gradient. it can be explained in terms of following equation:

$$\frac{dQ}{dt} = -KA \frac{dT}{dx} \quad (44a)$$

$K \rightarrow$ Thermal conductivity

$\frac{dQ}{dt} \rightarrow$ rate of heat flow [perpendicular to cross-sectional area]

$\frac{dT}{dx} \rightarrow$ temperature gradient

$A \rightarrow$ cross-section area

According to the transport phenomena, the amount of heat Q passing through a cross section of strip/ area is given by the following equation:

$$\frac{dQ}{dt} = \frac{1}{3} nv \lambda \frac{dE}{dx} \quad (44b)$$

$\frac{dE}{dx} \rightarrow$ energy gradient

$v \rightarrow$ thermal velocity

$\lambda \rightarrow$ is mean free path.

Thermal velocity is given by

$$v = \sqrt{\frac{3k_B T}{m}}$$

From kinetic theory of gases,

$$E = \frac{3}{2} k_B T$$

$$\frac{dE}{dx} = \frac{3}{2} k_B \frac{dT}{dx} \quad (44c)$$

Substituting Eqn. (44c) in Eqn. (44b),

$$\frac{dQ}{dt} = \frac{1}{3} n \sqrt{\frac{3k_B T}{m}} \lambda \frac{3}{2} k_B \frac{dT}{dx}$$

$$\frac{dQ}{dt} = \frac{1}{6} n \lambda \frac{(3k_B)^{3/2}}{\sqrt{m}} \sqrt{T} \frac{dT}{dx} \quad (45)$$

Comparing Eqs (44a) and (45), we obtain

$$KA = \frac{1}{6} n \lambda \frac{(3k_B)^{3/2}}{\sqrt{m}} \sqrt{T} \quad (46)$$

$$K = \frac{n \lambda (3k_B)^{3/2} \sqrt{T}}{6A \sqrt{m}} \quad (47)$$

In Eqn. (44a) “–ve” sign signifies that energy flow takes place from higher to lower temperatures.

17.4.3 Wiedemann–Franz Law

The Wiedemann–Franz law states that the ratio of thermal and electrical conductivity of a metal for constant temperature is constant.

Dividing Eqs (47) and (43),

$$\frac{K}{\sigma} = \frac{n \lambda 3k_B \sqrt{\frac{3k_B T}{m}}}{6A} \bigg/ \frac{ne^2 \lambda v}{6k_B T}$$

$$= \frac{3k_B^2 T}{Ae^2}$$

For unit area,

$$\frac{K}{\sigma} = 3 \left(\frac{k_B}{e} \right)^2 T \quad (48)$$

Hence, $\frac{K}{\sigma}$ is constant, if T is kept constant. Eqn (48) called Wiedemann–Franz relation.

17.5 Merits And Demerits Of Drude–Lorentz Theory

Merits

It could explain Ohm’s law of electrical conductivity, thermal conductivity, and Wiedemann–Franz law.

Demerits

- (i) It could not explain the positive charge carriers in semiconductors.
- (ii) It could not explain the preference of certain structures by metals.

- (iii) At low temperatures, it fails to explain the long mean free paths.
- (iv) It could not explain the paramagnetic susceptibility of conduction electrons.

17.6 Sommerfeld's Quantum Theory [One-Dimensional Analysis Of Free Electrons]

Many points could not be explained by Drude–Lorentz theory. While considering classical theory, electrons were considered to be distinguishable particles. But Sommerfeld gave the quantum mechanical explanation of free electron gas. He used Pauli exclusion principle and Fermi–Dirac statistics, that is, no two electrons can have same quantum numbers. Figure 17.6 shown an electron enclosed in one-dimensional box.

The electron can move freely inside the box, but the walls are perfectly rigid and potential limit is up to infinity. Hence, it is almost impossible for the electron to come out of the box without doing infinite work. Here, the potential could be divided as follows:

$$V = 0, \text{ for } 0 < x < a \quad (49a)$$

$$V = \infty, \text{ for } x \geq a \text{ and } x \leq 0 \quad (49b)$$

Applying Schrodinger wave equation on energy E of electron, we get

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \varphi(x) = 0 \quad (50)$$

Using boundary condition Eqn. (49a) in Eqn. (50), we get [For $0 < x < a$]

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{2mE}{\hbar^2} \varphi = 0$$

$$\frac{\partial^2 \varphi}{\partial x^2} + k^2 \varphi = 0 \quad (51a)$$

where

$$k^2 = \frac{2mE}{\hbar^2} \quad (51b)$$

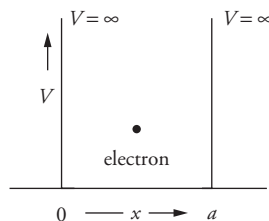


Figure 17.6 Electron inside one dimensional box

$$\varphi = A \sin kx + B \cos kx \quad (52a)$$

Let Eqn. (52a) be the general solution for Eqn. (51a). A and B are the arbitrary constants.

Applying boundary condition, $\varphi = 0$, at $x = 0$ and a .

For $x = 0$, we obtain $B = 0$ from Eqn. (52a)

Hence, Eqn. (52a) becomes

$$\varphi = A \sin kx \quad (52b)$$

Using the second boundary condition, that is, $\varphi = 0$, at $x = a$

$$\phi = A \sin ka = 0$$

$$\Rightarrow A \sin ka = 0$$

$$\Rightarrow ka = n\pi$$

$$\Rightarrow k = \frac{n\pi}{a} \quad (53)$$

Using Eqn. (53) in Eqn. (52b), we obtain

$$\varphi = A \sin \frac{n\pi x}{a} \quad (54)$$

Here $n = 1, 2, 3, \dots$, no zero or negative values are acceptable for Eqn. (54). When $n = 0$, it means electron is at rest which is not possible.

We can obtain the value of A by normalization, as follows:

$$\int_0^a |\varphi(x)|^2 dx = 1$$

$$\int_0^a A^2 \sin^2 \left(\frac{n\pi x}{a} \right) dx = 1$$

Upon solving it, we get

$$A = \sqrt{\frac{2}{a}} \quad (55)$$

Using Eqn. (55) in Eqn. (54), we get

$$\varphi = \sqrt{\frac{2}{a}} \sin \left(\frac{n\pi x}{a} \right) \quad (56)$$

From Eqs (51b) and (53), we get

$$\frac{2mE}{\hbar^2} = \left(\frac{n\pi}{a} \right)^2$$

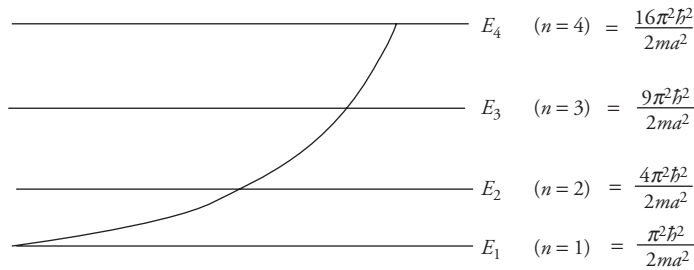


Figure 17.7 Discrete energy-level diagram for electron inside infinite potential well / one dimensional box.

$$\Rightarrow \quad E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (57)$$

The n takes values of 1, 2, 3, ...; and hence, electron can take only discrete values. Figure 17.7 shows the energy-level diagram. From Eqn. (57), it is clear that energy $\propto n^2$. Hence, energy follows parabolic function. Further, Sommerfeld theory used different terms like Fermi energy, total energy, and Fermi velocity which are discussed below.

Arnold Johannes Wilhelm Sommerfeld was a German physicist. He is well known for his findings and contributions in atomic and quantum physics. He gave the second quantum number, that is, azimuthal quantum number and the fourth quantum number, that is, spin quantum number. Along with these quantum numbers, he gave the fine-structure constant. He was born on December 5, 1868. Sommerfeld did his studies at Albertina University, Königsberg, East Prussia. He received his PhD in 1891 at the age of 23. After receiving his doctorate, Sommerfeld passed the national exam in 1892. Then he started working in military service with the reserve regiment of Königsberg. Even after completing his obligatory military service in 1893, he worked as a volunteer for military service. Sommerfeld was appointed as the Director of the new Theoretical Physics Institute at the University of Munich in 1906. Sommerfeld applied FD statistics to the free electron model in metals (Drude model). His model was able to solve many of the problem that could not be explained by the free electron theory. He was the only scientist who was nominated 81 times for the Nobel Prize but never received the award. In 1951, Sommerfeld died after an accident, which left the scientific community speechless.



A.J.W. SOMMERFELD

17.6.1 Fermi Energy

Let us distribute N electrons in orbitals. According to Pauli exclusion principle; no two electrons can have all the quantum numbers to be the same. Every orbit can accommodate two electrons, that is, one with spin up and the other with spin down. The lower orbitals are filled first and then the higher orbit. In other words, at absolute zero temperature, the electrons occupy certain energy levels known as Fermi levels and the energy corresponding to the Fermi level is called Fermi energy (E_F).

Let us consider N electrons (even number of electrons) and n_F be the principle quantum number of Fermi state, then

$$N = 2n_F \quad (58)$$

Hence, according to Sommerfeld theory, the energy is given by the following equation:

$$E_F = \frac{n_F^2 \pi^2 \hbar^2}{2ma^2} \quad (59)$$

$$E_F = \frac{N^2 \pi^2 \hbar^2}{8ma^2} \quad (60)$$

Equation (60) represents the Fermi energy corresponding to Fermi level,

17.6.2 Total Energy

The total energy is the sum of energies of all N electrons. As each level occupies two electrons, N electrons are occupied in $\frac{N}{2}$ levels. Total energy is given by the following equation:

$$E_T = 2 \sum_{n=1}^{N/2} E_n = \frac{\pi^2 \hbar^2}{ma^2} \sum_{n=1}^{N/2} n^2$$

$$E_T = \frac{\pi^2 \hbar^2}{ma^2} \left[\frac{1}{6} \left(\frac{N}{2} \right) \left[2 \left(\frac{N}{2} \right)^2 \right] \right]$$

$$E_T = \frac{1}{3} \frac{N^3 \pi^2 \hbar^2}{8ma^2} \quad (61a)$$

$$\left[\sum_{n=1}^x n^2 = 1^2 + 2^2 + \dots + (x-1)^2 = \frac{1}{6} x(2x^2 + 3x + 1) \approx \frac{1}{6} x(2x^2) \right]$$

Here $x = \frac{N}{2}$

$$E_T = \frac{1}{3} NE_F \quad (61b)$$

The average energy is given by the following equation:

$$\bar{E} = \frac{E_T}{N} = \frac{E_F}{3}$$

$$\bar{E} = \frac{E_F}{3} \quad (61c)$$

Hence, the average kinetic energy of electron is equal to $\frac{1}{3}$ rd of Fermi energy.

17.6.3 Fermi Velocity and Density of States

From Sommerfeld theory, it is quite evident that the energy of electrons at 0 K is not zero for uppermost levels. The velocity that Fermi electrons possess is called Fermi velocity. Fermi electrons are electrons that have energy equal to E_F .

Therefore, in equilibrium,
KE of Fermi electrons = E_F

$$\frac{1}{2}mv_F^2 = \frac{N^2\pi^2\hbar^2}{8ma^2}$$

$$v_F = \frac{Nh}{4ma} \quad (62)$$

Equation (62) gives the Fermi velocity.

The density of states represents the quantum states per unit energy range and is denoted by $D(E)$.

$$D(E) = \frac{dn}{dE} \quad (63)$$

Here dn represents number of quantum states in the energy range between E and $E + dE$.

As specified, there are two electrons present in each quantum state, hence

$$D(E) = 2 \frac{dn}{dE} \quad (64a)$$

Now, we have to evaluate $\frac{dn}{dE}$ as follows:

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$\frac{dE}{dn} = \frac{\hbar^2\pi^2 n}{ma^2} \quad (64b)$$

Substituting Eqn. (64b) in Eqn. (64a), we obtain

$$D(E) = \frac{2ma^2}{\hbar^2\pi^2 n} \quad (64c)$$

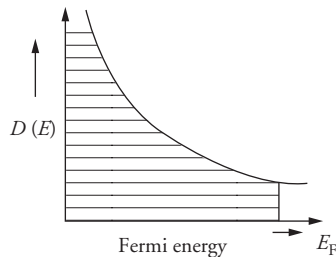


Figure 17.8 Variation of density of states with Fermi energy.

For computing $D(E)$ as a function of energy, we need to compute $\left(\frac{1}{n}\right)$ from eqn (57) and then substitute it in Eqn. (64c):

$$D(E) = \frac{2ma^2}{\hbar^2 \pi^2} \left[\frac{\pi \hbar}{a\sqrt{2mE}} \right]$$

$$D(E) = \frac{2ma^2}{\hbar^2 \pi^2} \left[\frac{\pi \hbar}{a\sqrt{2mE}} \right]$$

$$\left[E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n^2 = \frac{2mEa^2}{\pi^2 \hbar^2}, \quad \frac{1}{n} = \frac{\pi \hbar}{a\sqrt{2mE}} \right]$$

$$D(E) = \frac{a}{\pi \hbar} \sqrt{\frac{2m}{E}} \quad (65)$$

The variation of density of states with energy is shown in Figure 17.8. The figure clearly indicates that the energy states up to Fermi level are filled.

17.7 Free Electron Gas in Three Dimensions

We have given one-dimensional treatment to electron gas. Now, we assume the electrons gas in three-dimensional box.

It is assumed that the potential inside the box is zero and that outside the box is infinite. Then the Schrodinger wave equation is given by the following equation:

$$\frac{-\hbar^2}{2m} \nabla^2 \varphi(\vec{r}) = E \varphi(\vec{r})$$

$$\frac{+\hbar^2}{2m} \nabla^2 \varphi(\vec{r}) + E \varphi(\vec{r}) = 0$$

$$\nabla^2 \varphi(\vec{r}) + \frac{2mE}{\hbar^2} \varphi(\vec{r}) = 0$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi(\vec{r}) + \frac{2mE}{\hbar^2} \varphi(\vec{r}) = 0 \quad (66)$$

The solution for Eqn. (66) is given by the following equation:

$$\varphi(\vec{r}) = A \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right) \quad (67)$$

In Eqn. (67), the side of cubical box is assumed to be a . A is an arbitrary constant, whose value can be obtained after normalization.

$$\begin{aligned}
\iiint_v \varphi^*(\vec{r}) \varphi(\vec{r}) dv &= 1 \\
\iiint_v A^2 \sin^2\left(\frac{n_x \pi x}{a}\right) \sin^2\left(\frac{n_y \pi y}{a}\right) \sin^2\left(\frac{n_z \pi z}{a}\right) dx dy dz &= 1 \\
A^2 \int_0^a \sin^2 \frac{n_x \pi x}{a} dx \int_0^a \sin^2 \frac{n_y \pi y}{a} dy \int_0^a \sin^2 \frac{n_z \pi z}{a} dz &= 1 \\
A^2 \left(\frac{a}{2}\right) \left(\frac{a}{2}\right) \left(\frac{a}{2}\right) &= 1 \\
A^2 &= \frac{8}{a^3} \\
A &= \sqrt{\frac{8}{a^3}} \tag{68}
\end{aligned}$$

Hence, using Eqn. (68) in Eqn. (67), we obtain

$$\varphi(\vec{r}) = \sqrt{\frac{8}{a^3}} \sin k_x x \sin k_y y \sin k_z z \tag{69a}$$

where $k_x = \frac{n_x \pi}{a}$, $k_y = \frac{n_y \pi}{a}$, and $k_z = \frac{n_z \pi}{a}$

Such that

$$\begin{aligned}
k^2 &= k_x^2 + k_y^2 + k_z^2 = \frac{\pi^2}{a^2} (n_x^2 + n_y^2 + n_z^2) \\
k^2 &= \frac{\pi^2}{a^2} n^2 \tag{69b}
\end{aligned}$$

where
From Eqn. (66),

$$n^2 = n_x^2 + n_y^2 + n_z^2 \tag{69c}$$

$$k = \frac{2mE}{\hbar^2}$$

$$E = \frac{\hbar^2}{2m} [k_x^2 + k_y^2 + k_z^2]$$

$$E = \frac{\pi^2 n^2 \hbar^2}{2ma^2} \tag{70}$$

In Eqn. (70),

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

From Eqn. (70), we obtain that energy eigenvalues are quantized and possess discrete values.

17.8 Band Theory of Solids

Many properties such as heat capacity, conductivity phenomena, and susceptibility could be explained using free electron theory, yet many issues need to be addressed. Free electron theory could not explain the difference between conductors, semiconductors, and insulators. This theory also predicted negative Hall coefficients for the metals, whereas some metals such as beryllium and zinc possess positive Hall coefficients. The free electron theory predicts that conductivity is directly proportional to electron concentration. But despite this fact, some monovalent metals possess positive Hall coefficients. The free electron theory predicts that conductivity is directly proportional to electron concentration. But despite this fact, some monovalent metals possess high conductivity than the divalent and trivalent metals.

In free electron theory, the electron is supposed to move inside constant or zero potential that implies zero force on electron. Anyhow, electron always experiences force when it passes near some neighboring ions. Hence, when the electron moves from one place to another, the electron no longer belongs to constant potential. In the subsequent sections, the electron wavefunction for electron is calculated when it is under the impact of changing potential.

17.8.1 Bloch Theorem

According to free electron theory, electron moves in constant potential V_0 such that the schrodinger equation is given by:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_0) \varphi = 0 \quad (71)$$

The solution for Eqn. (71) is as follows:

$$\varphi = \exp(\pm ikx) \quad (72a)$$

Consider one-dimensional Schrodinger wave equation, for an electron. Let a be the periodicity of lattice, such that

$$V(x) = V(x + a) \quad (72b)$$

Hence, Eqn. (71) is written as follows:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x)) \varphi = 0 \quad (72c)$$

Equation (72c) can be solved with the help of Bloch theorem.

The solution can be given in the following form:

$$\varphi(x) = e^{\pm ikx} U(x) \quad (72d)$$

and

$$U(x) = U(x + a) \quad (72e)$$

$\varphi(x)$ is the Bloch function, e^{ikx} represents wavefunction of free electron modulated by factor $U(x)$.

Let φ_1 and φ_2 be two independent and real solutions of Eqn. (72c). Then the solution for Eqn. (72c) is given by the sum of individual solutions, that is, φ_1 and φ_2 , that is,

$$\varphi(x) = A\varphi_1(x) + B\varphi_2(x) \quad (73)$$

A and B are the arbitrary constants, second-order differential equation has two solutions.

As per Eqn. (72e), we have taken the potential to be periodic, hence $\varphi_1(x+a)$ and $\varphi_2(x+a)$ should also represent the solutions of Eqn. (72c). Hence,

$$\varphi_1(x+a) = \alpha_1\varphi_1(x) + \alpha_2\varphi_2(x) \quad (74a)$$

$$\varphi_2(x+a) = \beta_1\varphi_1(x) + \beta_2\varphi_2(x) \quad (74b)$$

where α_1 , α_2 , β_1 and β_2 are constants.

In correlation to Eqn. (73), we can also write solution for $\varphi(x+a)$, that is,

$$\varphi(x+a) = A\varphi_1(x+a) + B\varphi_2(x+a)$$

$$\varphi(x+a) = A[\alpha_1\varphi_1(x) + \alpha_2\varphi_2(x)] + B[\beta_1\varphi_1(x) + \beta_2\varphi_2(x)]$$

Using Eqn. 74(a)–(b),

$$\varphi(x+a) = (A\alpha_1 + B\beta_1)\varphi_1(x) + (A\alpha_2 + B\beta_2)\varphi_2(x) \quad (74c)$$

$$\varphi(x+a) = \delta A\varphi_1(x) + \delta B\varphi_2(x) \quad (74d)$$

where

$$A\alpha_1 + B\beta_1 = \delta A \quad (75a)$$

$$A\alpha_2 + B\beta_2 = \delta B \quad (75b)$$

From Eqn. (74d),

$$\varphi(x+a) = \delta[A\varphi_1(x) + B\varphi_2(x)]$$

$$\varphi(x+a) = \delta\varphi(x) \quad (76)$$

From Eqs (75a) and (75b), we can write

$$(\alpha_1 - \delta)A + B\beta_1 = 0$$

$$\alpha_2 A + (\beta_2 - \delta)B = 0 \quad (77)$$

We can write Eqn. (77) in determinant form as follows:

$$\begin{vmatrix} \alpha_1 - \delta & \beta_1 \\ \alpha_2 & \beta_2 - \delta \end{vmatrix} = 0$$

$$(\alpha_1 - \delta)(\beta_2 - \delta) - \alpha_2\beta_1 = 0$$

$$\begin{aligned}\alpha_2\beta_1 + \alpha_1\beta_2 + \delta^2 - (\alpha_1 + \beta_2)\delta &= 0 \\ \delta^2 - (\alpha_1 + \beta_2)\delta + (\alpha_1\beta_2 - \alpha_2\beta_1) &= 0\end{aligned}\quad (78)$$

Equation (78) gives a factor $(\alpha_1\beta_2 - \alpha_2\beta_1)$ which is taken to be 1, and then Eqn. (78) becomes

$$\delta^2 - (\alpha_1 + \beta_2)\delta + 1 = 0 \quad (79)$$

We will prove that $\alpha_1\beta_2 - \alpha_2\beta_1 = 1$ as follows:

Differentiate Eqn. 74(a)–(b),

$$\varphi_1'(x+a) = \alpha_1\varphi_1'(x) + \alpha_2\varphi_2'(x) \quad (80a)$$

$$\varphi_2'(x+a) = \beta_1\varphi_1'(x) + \beta_2\varphi_2'(x) \quad (80b)$$

We can write Eqn. 74(a)–(b) and Eqn. 80(a)–(b) in matrix form:

$$\begin{vmatrix} \varphi_1(x+a) & \varphi_2(x+a) \\ \varphi_1'(x+a) & \varphi_2'(x+a) \end{vmatrix} = \begin{vmatrix} \varphi_1(x) & \varphi_2(x) \\ \varphi_1'(x) & \varphi_2'(x) \end{vmatrix} \begin{vmatrix} \alpha_1 & \beta_1 \\ \alpha_2 & \beta_2 \end{vmatrix} \quad (81)$$

Rewriting Eqn. (72c) in terms of φ_1 and φ_2 , we obtain

$$\frac{\partial^2 \varphi_1(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\varphi_1 = 0 \quad (82a)$$

$$\frac{\partial^2 \varphi_2(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\varphi_2 = 0 \quad (82b)$$

Multiplying Eqn. (82a) with φ_2 and Eqn. (82b) with φ_1 , and subtracting

$$\varphi_1(x) \frac{\partial^2 \varphi_2}{\partial x^2} - \varphi_2(x) \frac{\partial^2 \varphi_1}{\partial x^2} = 0$$

$$\frac{\partial}{\partial x} \left[\varphi_1(x) \frac{\partial \varphi_2}{\partial x} - \varphi_2(x) \frac{\partial \varphi_1}{\partial x} \right] = 0$$

Hence $\varphi_1(x) \frac{\partial \varphi_2}{\partial x} - \varphi_2(x) \frac{\partial \varphi_1}{\partial x} = \text{constant}$

$\Rightarrow \varphi_1(x)\varphi_2'(x) - \varphi_2(x)\varphi_1'(x) = \text{constant}$

$$\begin{vmatrix} \varphi_1(x) & \varphi_2(x) \\ \varphi_1'(x) & \varphi_2'(x) \end{vmatrix} = \text{constant} = \varphi(x) \quad (83)$$

From Eqs (81) and (83), we obtain

$$\begin{vmatrix} \varphi_1(x+a) & \varphi_2(x+a) \\ \varphi_1'(x+a) & \varphi_2'(x+a) \end{vmatrix} = (\alpha_1\beta_2 - \alpha_2\beta_1)\varphi(x)$$

$$\varphi(x+a) = (\alpha_1\beta_2 - \alpha_2\beta_1)\varphi(x) \quad (\text{using eqn. (76)})$$

$$(\alpha_1\beta_2 - \alpha_2\beta_1) = 1 \quad (84)$$

Equation (79) is quadratic equation, and hence has two solutions, that is, δ_1 and δ_2 are the two solutions. These values can be real or virtual depending on $(\alpha_1 + \beta_2)^2 - 4$. Consider the following cases:

(i) **Case I: For $(\alpha_1 + \beta_2)^2 < 4$**

Then two roots are given by the following equation:

$$\delta_1 = e^{ika} \quad \text{and} \quad \delta_2 = e^{-ika} \quad (85)$$

Corresponding wavefunction $\varphi_1(x+a)$ and $\varphi_2(x+a)$ could be written as follows:

$$\varphi_1(x+a) = \exp(ika)\varphi_1(x)$$

and

$$\varphi_2(x+a) = \exp(-ika)\varphi_2(x) \quad (86)$$

Generalized form could be written as follows:

$$\varphi(x+a) = \exp(\pm ika)\varphi(x) \quad (87)$$

Equation (87) also represents Bloch functions.

(ii) **Case II: For $(\alpha_1 + \beta_2)^2 > 4$**

Here, δ_1 and δ_2 represent real roots, given by the following equation:

$$\delta_1 = e^{+\sigma a} \quad \text{and} \quad \delta_2 = e^{-\sigma a} \quad (88)$$

[for real solutions, the product of roots = 1]

Hence, the solution for Schrodinger equation is

$$\varphi_1(x) = e^{\sigma a}U(x) \quad \text{and} \quad \varphi_2(x) = e^{-\sigma a}U(x) \quad (89)$$

σ is real, these wavefunction approach ∞ as x approaches infinity. Hence, the wavefunction is not acceptable and the energy band has forbidden and acceptable bands.

Felix Bloch was born on October 23, 1905 in Zurich, Switzerland. He attended the public primary school from 1912 to 1918. He joined Federal Institute of Technology in Zurich to study engineering but only after one year, he decided study physics at the same institution. He attended the courses given by Schrödinger, Debye, Scherrer, and Weyl. In 1928, he received his PhD in the quantum mechanics of electrons in crystals and developing the metallic conduction theory. He also worked with Heisenberg, Bohr, Pauli, Kramers, and Fermi. In 1934, he joined a position at Stanford University. In 1939, he performed an experiment at the Berkeley cyclotron in collaboration with L.W. Alvarez from which he obtained the magnetic moment of the neutron to an accuracy of about 1 percent. In 1940, he married Dr Lore Misch, who was a refugee from Germany and herself a physicist. In 1954, Bloch served as the first Director General of CERN in Geneva. He then returned to Stanford University where he continued working on nuclear magnetism and relaxation theory. In 1961, he was appointed as Max Stein Professor of Physics at Stanford University.



FELIX BLOCH

at Stanford University.

17.8.2 Kronig–Penney Model

Kronig and Penney assumed one-dimensional potential model for studying behavior of electrons. This model assumes the potential well to be in square shape. The period for the potential well is $a + b$. The potential energy of the electron is zero for region $0 < x < a$ and for $-b < x < 0$, its value is V_0 (as shown in fig. 17.9).

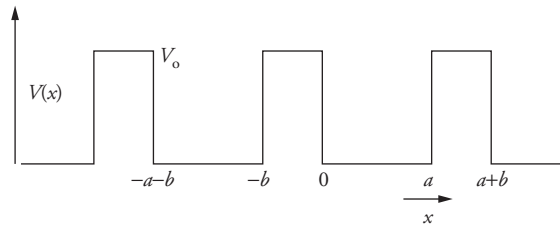


Figure 17.9 Kronig–Penney potential model.

The Schrodinger wave equation is given by the following:

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + \frac{2m}{\hbar^2} E \varphi(x) = 0 \quad \text{for} \quad 0 < x < a \quad (90a)$$

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_0) \varphi(x) = 0 \quad \text{for} \quad -b < x < 0 \quad (90b)$$

The basic assumption is that $E < V_0$ such that $E - V_0 < 0$.

Put
$$\frac{2mE}{\hbar^2} = k_1 \quad \text{and} \quad \frac{2m}{\hbar^2} (V_0 - E) = k_2 \quad (91)$$

Substituting Eqn. (91) in Eqn. 90(a)–(b), we obtain

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + k_1^2 \varphi(x) = 0 \quad (92a)$$

$$\frac{\partial^2 \varphi(x)}{\partial x^2} - k_2^2 \varphi(x) = 0 \quad (92b)$$

The solution of Eqn. 92(a)–(b) is given by Bloch function:

$$\varphi(x) = U(x) e^{ikx} \quad (93a)$$

where

$$U(x) = U(x + a + b) \quad (93b)$$

Differentiate Eqn. (93a),

$$\frac{\partial \varphi(x)}{\partial x} = ikU(x) e^{ikx} + e^{ika} \frac{\partial}{\partial x} U(x) \quad (94a)$$

Differentiating Eqn. (94a) w.r.t. x , we obtain

$$\frac{\partial^2 \varphi(x)}{\partial x^2} = e^{ikx} \left[\frac{\partial^2}{\partial x^2} U(x) + 2ik \frac{d}{dx} U(x) - k^2 U(x) \right] \quad (94b)$$

Use Eqs (94b) and (93a) in Eqn. 92(a)–(b):

$$\frac{\partial^2}{\partial x^2} U(x) + 2ik \frac{\partial}{\partial x} U(x) - (k_1^2 - k^2) U(x) = 0 \quad (95a)$$

and

$$\frac{\partial^2}{\partial x^2} U(x) + 2ik \frac{\partial}{\partial x} U(x) - (k_2^2 + k^2) U(x) = 0 \quad (95b)$$

The solutions for Eqn. 95(a)–(b) are given by the following equation:

$$\left. \begin{aligned} U_1 &= A e^{i(k_1 - k)x} + B e^{-i(k_1 + k)x} \\ U_2 &= C e^{(k_2 - ik)x} + D e^{-(k_2 + ik)x} \end{aligned} \right] \quad (96)$$

We have to use the boundary conditions, that is,

$$U_1 = U_2 \text{ at } x = 0$$

$$U_1(a) = U_2(-b)$$

$$\left(\frac{\partial U_1}{\partial x} \right)_{x=0} = \left(\frac{\partial U_2}{\partial x} \right)_{x=0} \quad \text{and} \quad \left(\frac{\partial U_1}{\partial x} \right)_a = \left(\frac{\partial U_2}{\partial x} \right)_{-b}$$

Using $U_1 = U_2$ at $x = 0$ in Eqn. (96), we obtain

$$A + B = C + D \quad (97a)$$

Using $U_1(a) = U_2(-b)$ in Eqn. (96), we obtain

$$Ae^{i(k_1-k)a} + Be^{-i(k_1+k)a} = Ce^{-(k_2-ik)b} + De^{(k_2+ik)b} \quad (97b)$$

Use the condition $\left(\frac{\partial U_1}{\partial x}\right)_{x=0} = \left(\frac{\partial U_2}{\partial x}\right)_{x=0}$ in Eqn. (96)

$$Ai(k_1 - k) - Bi(k_1 + k) = C(k_2 - ik) - D(k_2 + ik) \quad (97c)$$

Using $\left(\frac{\partial U_1}{\partial x}\right)_a = \left(\frac{\partial U_2}{\partial x}\right)_{-b}$ in Eqn. (96), we obtain

$$Ai(k_1 - k)e^{i(k_1-k)a} - Bi(k_1 + k)e^{-i(k_1+k)a} = C(k_2 - ik)e^{-(k_2-ik)b} - D(k_2 + ik)e^{(k_2+ik)b} \quad (97d)$$

Equations from 97(a)–(d) are written in determinant form as follows:

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ e^{i(k_1-k)a} & e^{-i(k_1+k)a} & e^{-i(k_2-ik)b} & e^{(k_2+ik)b} \\ i(k_1 - k) & -i(k_1 + k) & (k_2 - ik) & -(k_2 + ik) \\ i(k_1 - k)e^{i(k_1-k)a} & -i(k_1 + k)e^{-i(k_1+k)a} & (k_2 - ik)e^{-(k_2-ik)b} & -(k_2 + ik)e^{(k_2+ik)b} \end{vmatrix} = 0$$

Solving the determinate yields the following:

$$\frac{k_2^2 - k_1^2}{2k_1k_2} \sin hk_2b \sin k_1a + \cos hk_2b \cos k_1a = \cos k(a+b) \quad (98)$$

Kronig and Penney assumed that potential V_0 may tend to infinity and b can tend to zero, such that product V_0b remains constant. When b tends to zero, then $\sin hk_2b \rightarrow k_2b$ and $\cos hk_2b \rightarrow 1$, this eqn. (98) becomes

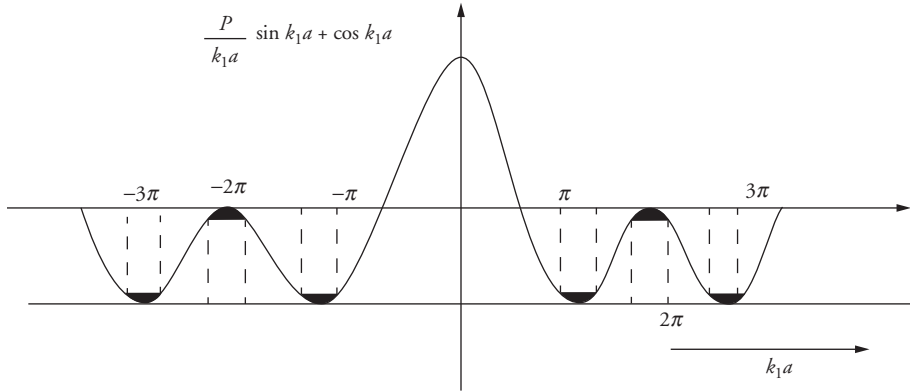


Figure 17.10 Variation of $\frac{P}{k_1 a} \sin k_1 a \cos k_1 a$ and $k_1 a$.

$$\left(\frac{k_2^2 - k_1^2}{2k_1 k_2} \right) k_2 b \sin k_1 a + \cos k_1 a = \cos ka \tag{99a}$$

as $k_2 > k_1$, hence $\frac{k_2^2 - k_1^2}{2k_1 k_2} = \frac{k_2^2}{2k_1 k_2}$

Hence, Eqn. (99a) becomes

$$\frac{k_2^2 b}{2k_1} \sin k_1 a + \cos k_1 a = \cos ka \tag{99b}$$

Let us introduce a new term P , such that

$$P = \frac{k_2^2 ab}{2} \tag{100}$$

$$P = \frac{2m}{\hbar^2} V_0 \frac{ab}{2} \quad [V_0 \gg E]$$

$$P = \frac{mV_0 ab}{\hbar^2} \tag{101a}$$

Equation (101a) measures area of potential barrier. If P decreases, it indicates that the electron is loosely bound to the potential well and vice versa. Put Eqn. (100) in Eqn. (99b), we get

$$\frac{P \sin k_1 a}{k_1 a} + \cos k_1 a = \cos ka \quad (101b)$$

Figure 17.10 shows the variation of $\frac{P}{k_1 a} \sin k_1 a + \cos k_1 a$ with respect to $k_1 a$. Following are important conclusion that could be drawn from this graph.

- (i) $\cos ka$ lies between -1 and $+1$. (Two horizontal lines represent the extreme for $\cos ka$. Hence, for $\cos ka = \pm 1$)

$$\Rightarrow ka = n\pi$$

$$\Rightarrow k = \frac{n\pi}{a}$$

Hence, there are allowed energy bands that are separated by forbidden energy gaps.

- (ii) The width of allowed bands varies directly as the energy values.

- (iii) As $\frac{2mE}{\hbar^2} = k_1^2$,

$$\Rightarrow E = \frac{k_1^2 \hbar^2}{2m} \quad (102a)$$

If P increases and tends to infinity, then the allowed region gets narrower and narrower; hence, Eqn. (101b) can have solution, only if $\sin k_1 a = 0$:

$$\Rightarrow k_1 a = n\pi \Rightarrow k_1 = \frac{n\pi}{a} \quad (102b)$$

Using Eqn. (102b) in Eqn. (102a), we obtain

$$\Rightarrow E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (103)$$

Equation (103) is the result for particle in box with constant potential.

- (iv) If $P \rightarrow 0$, then $\cos k_1 a = \cos ka$

$$\Rightarrow k_1 = k \quad (104a)$$

This gives
$$\Rightarrow E = \frac{\hbar^2 k^2}{2m} \quad (104b)$$

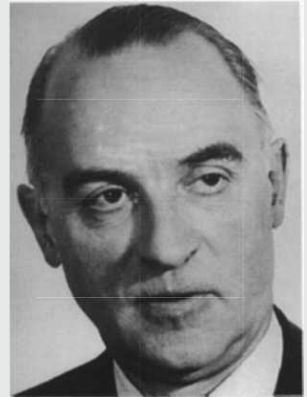
Equation (104b) gives the energy of free electron, when $P = 0$. This results is expected as an outcome.

Ralph Kronig was born in 1904 in Dresden, Germany, where he received his primary education. Then he went to Columbia University, New York, to pursue his studies and later on he became an assistant professor. He kept on visiting the theoretical centers in Germany and Copenhagen. He also worked with Pauli, Kramers, Bohr, and Heisenberg.

While doing his PhD at Columbia University, he gave the concept of electron spin, which was opposed by Werner Heisenberg and Wolfgang Pauli. Due to this criticism, Kronig could not publish his theory of electron spin. Although Ralph Kronig was the first one to give idea on electron spin, Uhlenbeck and Goudsmit are credited with the discovery.

It is believed by many of the scientists that Pauli could receive the Nobel Prize for his exclusion principle only due to particle spin theory of Kronig's. Kronig and Pauli were friends even though Pauli had opposed his ideas. Kronig exchanged his ideas on electron spin with Pauli before Pauli had published his paper explaining that two electrons occupying same orbital cannot have all the quantum numbers equal.

In 1939, Kronig was appointed as a professor of theoretical physics in the Netherlands. He also received Max Planck medal in 1962. Werner Heisenberg used Kronig ideas to develop his theories.



RALPH KRONIG

SUMMARY

This chapter deals with an understanding of phonons as quanta of lattice vibrations. Phonons obey BE statistics and require material medium for their propagation. One-dimensional mono and diatomic lattice have been discussed by making the assumption that atoms obey Hooke's law and the interaction extends only between nearest neighbors. For diatomic lattice, two branches originate for the frequencies, that is, optical and acoustic branch. When the masses of both the atoms are same, then no forbidden gap exists and monoatomic/diatomic lattices have the same frequency. Drude model/free electron model assumed that electron can move anywhere inside the metal kernel. This model could explain ohm's law, Wiedemann–Franz's law but failed to explain high order thermal conductivity, long mean free paths and paramagnetic susceptibility of conduction electrons. Hence, Sommerfeld gave quantum theory which assumed that electrons move freely inside a potential well. The energies have discrete values and are directly proportional to n^2 . The average kinetic energy of electron is $1/3$ of Fermi energy. According to Sommerfeld theory, the energy of electrons at 0 K is not zero. The three-dimensional analysis has been done for free electrons. On the basis of the free electron theory, the difference between conductors, semiconductors, and insulators could not be explained. According to band theory, the electron always experience force while passing across neighboring ions. Bloch function is given to find the solution for electron moving inside constant potential V_0 . Further, the behavior of free electron is studied, for a potential well to be in square-well shape. Kronig and Penney also assumed that V_0 may tend to infinity. A new term P is obtained which measures the area of potential barrier.

SOLVED PROBLEMS

Q.1: Obtain the phonon frequency (maximum) which is generated when visible light of wavelength $\lambda = 6000 \text{ \AA}$ is scattered. The sound velocity in medium is $5 \times 10^5 \text{ cm/sec}$ and the refractive index is 1.33.

$$\text{Ans:} \quad \Omega = v_p K = \frac{2v_p \omega \mu \sin \phi / 2}{c}$$

$$\text{Here} \quad \omega = 2\pi f = \frac{2\pi c}{\lambda}$$

$$\lambda = 6000 \text{ \AA}$$

$$v_p = 5 \times 10^5 \text{ cm/sec} = 5 \times 10^3 \text{ m/sec}$$

$$\mu = 1.33$$

For maximum phonon frequency $\phi = 180^\circ$,

$$\sin \frac{\phi}{2} = 1$$

$$\Omega_{\max} = \frac{2 \times 5 \times 10^3 \times 2\pi c}{c \lambda}$$

$$\Omega_{\max} = \frac{2 \times 5 \times 10^3 \times 2 \times 3.14}{6 \times 10^{-7}}$$

$$\Omega_{\max} = \frac{10^4 \times 6.28}{6 \times 10^{-7}}$$

$$\Omega_{\max} = 1.04 \times 10^{11} \text{ rad/sec}$$

Q.2: When light wave of wavelength 4500 Å is scattered from a crystal, obtain the fractional change of frequency of incident light. Given the refractive index of crystal is 1.5 and sound velocity is 5000 m/sec.

$$\text{Ans:} \quad \Omega = \frac{2\omega v_p \mu \sin \phi / 2}{c}$$

$$\text{Here, } \omega = 2\pi f = \frac{2\pi c}{\lambda}$$

For maximum frequency $\sin \frac{\phi}{2} = 1$,

$$\Omega_{\max} = \frac{2\omega v_p \mu}{c}$$

$$\Omega_{\max} = \frac{2 \times 2\pi c \times v_p \mu}{c \lambda}$$

$$\Omega_{\max} = \frac{4\pi v_p \mu}{\lambda}$$

$\mu = 1.5$, $\lambda = 4.5 \times 10^{-7}$ m, and $v_p = 5000$ m/s

$$\Omega_{\max} = \frac{4 \times 3.14 \times 1.5 \times 5000}{4.5 \times 10^{-7}}$$

$$\begin{aligned}\Omega_{\max} &= 209333 \times 10^7 \\ &= 2.09 \times 10^{11} \text{ rad/sec}\end{aligned}$$

Fractional change of frequency = $\frac{\omega - \omega'}{\omega}$

$$\frac{\omega - \omega'}{\omega} = \frac{2.09 \times 10^{11} \times 4.5 \times 10^{-7}}{2 \times 3.14 \times 3 \times 10^8} = 0.49 \times 10^{-4}$$

$$\frac{\omega - \omega'}{\omega} = 4.9 \times 10^{-5}$$

Q.3: The interatomic spacing for a lattice is given to be 2 \AA and velocity of sound is 4000 m/sec. Obtain the cut-off frequency for one-dimensional monoatomic chain. Also obtain phase velocity.

Ans: $v_p = \frac{2a}{\pi} \sqrt{\frac{\beta}{m}}$ and $v_g = 0$ for $\omega = \sqrt{\frac{4\beta}{m}}$

$$a = 2 \text{ \AA}$$

If S is the longitudinal stiffness and P represents mass/length, then

$$\Rightarrow S = \beta a$$

and

$$P = \frac{m}{a} \Rightarrow m = Pa$$

Hence,

$$v_p = \frac{2a}{\pi} \sqrt{\frac{S/a}{Pa}}$$

$$v_p = \frac{2}{\pi} \sqrt{\frac{S}{P}}$$

$$\sqrt{\frac{S}{P}} = \text{Velocity of sound} = 4000 \text{ m/sec}$$

$$v_p = \frac{2}{\pi} \times 4000 \text{ m/sec}$$

$$v_p = \frac{2}{3.14} \times 4000 = 2547.77 \text{ m/sec}$$

$$\omega_{\max} = \sqrt{\frac{4\beta}{m}} = 2\sqrt{\frac{\beta}{m}}$$

$$f_{\max} = \frac{\omega_{\max}}{2\pi} = \frac{1}{\pi} \sqrt{\frac{\beta}{m}}$$

Hence,

$$f_{\max} = \frac{1}{\pi} \sqrt{\frac{S/a}{Pa}}$$

$$f_{\max} = \frac{1}{\pi a} \sqrt{\frac{S}{P}}$$

$$f_{\max} = \frac{1}{3.14 \times 2 \times 10^{-10}} \times 4000$$

$$f_{\max} = \frac{4 \times 10^{13}}{6.28}$$

$$f_{\max} = 0.636 \times 10^{13}$$

$$f_{\max} = 6.36 \times 10^{12} \text{ Hz}$$

Q.4: Obtain the Fermi velocity of electrons for aluminum metal, if number density is $5.93 \times 10^{28} / \text{m}^3$ and inter atomic spacing (286 pm).

Ans:
$$v_F = \frac{N\hbar}{4ma}$$

$$\frac{N}{V} = 5.93 \times 10^{28} / \text{m}^3$$

$$a = 286 \text{ pm} \Rightarrow a = 2.86 \times 10^{-10} \text{ m}$$

$$v_F = \frac{5.93 \times 10^{28} \times 6.63 \times 10^{-34} \times V}{4 \times 9.1 \times 10^{-31} \times 2.86 \times 10^{-10}}$$

$$v_F = 0.377 \times 10^{28} \times 10^{-34} \times 10^{41} \times V$$

Here,

$$\begin{aligned} V &= (2.86 \times 10^{-10})^3 = 23.33 \times 10^{-30} \\ &= 2.33 \times 10^{-29} \text{ m}^3 \end{aligned}$$

$$v_F = 0.377 \times 10^{28} \times 10^{-34} \times 10^{41} \times 10^{-29} \times 2.33$$

$$v_F = 0.878 \times 10^6 = 8.78 \times 10^5 \text{ m/sec}$$

Q.5: The Fermi energy for silver and lithium is 5.51 and 4.72 eV, respectively. Obtain the Fermi velocity for these metals.

Ans: As we know

$$\frac{1}{2}mv_F^2 = E_F$$

Hence,
$$v_F = \sqrt{\frac{2E_F}{m}}$$

For silver,
$$E_F = 5.51 \text{ eV}$$

$$v_F = \sqrt{\frac{2 \times 5.51 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}}$$

$$v_F = \sqrt{1.937 \times 10^{12}}$$

$$v_F = 1.39 \times 10^6 \text{ m/sec}$$

For lithium, $E_F = 4.72 \text{ eV}$

Hence,

$$v_F = \sqrt{\frac{2 \times 4.72 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}}$$

$$v_F = \sqrt{1.659 \times 10^{12}}$$

$$v_F = 1.288 \times 10^6 \text{ m/sec}$$

Q.6: Show that the energy of electron becomes $E = \frac{\hbar^2 k^2}{2m}$, if the electron is free electron.

Ans: Using Kronig–Penney model,

$$P = \frac{mV_0 ab}{\hbar^2}$$

For free electron,

$$V_0 = 0$$

$$P = 0$$

$$\frac{P \sin k_1 a}{k_1 a} + \cos k_1 a = \cos ka$$

$$\cos k_1 a = \cos ka$$

$$k_1 = k$$

We know

$$k_1^2 = \frac{2mE}{\hbar^2}$$

Hence,

$$k^2 = \frac{2mE}{\hbar^2}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

OBJECTIVE QUESTIONS

1. The energy of harmonic oscillator is given by

(a) $\left(n + \frac{1}{2}\right)hf$ (b) nhf

(c) $\frac{n}{2}hf$ (d) 0

2. The zero point energy for harmonic oscillator is
- (a) $\left(n + \frac{1}{2}\right)hf$ (b) hf
 (c) $\frac{1}{2}hf$ (d) 0
3. The quantum of thermal energy in lattice vibrations is
- (a) photon (b) phonon
 (c) Cooper pair (d) Boron
4. Phonons do not require material medium for their propagation. (Yes/No)
5. The momentum of photon is given by
- (a) $\hbar\omega$ (b) $\hbar k$
 (c) hc (d) 0
6. The angular frequency of phonon is given by (Ω):
- (a) $2 - v_p \omega \mu$ (b) $2v_p \omega \mu \cos \phi/2$
 (c) $\frac{2v_p \omega \mu}{c} \sin \phi/2$ (d) $\frac{2v_p \omega \mu}{c} \tan \phi/2$
7. For one and two-dimensional monoatomic lattice, atoms should follow
- (a) Newton's law (b) Coulomb's law
 (c) Ampere's law (d) Hooke's law
8. For one-dimensional lattice, the angular frequency is given by
- (a) $\sqrt{\frac{2\beta}{m}} \cos \frac{ka}{2}$ (b) $\pm \sqrt{\frac{2\beta}{m}} \tan^2 \frac{ka}{2}$
 (c) $\pm \sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2}$ (d) $\pm \sqrt{\frac{m}{4\beta}} \sin \frac{ka}{2}$
9. For small frequencies, the angular frequency can be given by
- (a) $\sqrt{\frac{\beta}{m}} ka$ (b) $\sqrt{\frac{m}{\beta}} ka$
 (c) $\sqrt{\beta m} ka$ (d) $\sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2}$
10. For monoatomic lattice, the group and phase velocity, when $k \rightarrow 0$ is given by
- (a) $\sqrt{\frac{m}{\beta}}$ (b) $\sqrt{\frac{\beta}{m}} a$
 (c) 0 (d) $\sqrt{a/\beta}$

11. For monoatomic lattice, the group velocity at higher frequencies is given by

(a) $\sqrt{\frac{\beta}{m}} \cos \frac{ka}{2}$

(b) $\frac{2}{k} \sqrt{\frac{\beta}{m}} \sin \frac{ka}{2}$

(c) $\sqrt{\frac{\beta}{m}} \tan \frac{ka}{2}$

(d) $a \sqrt{\frac{\beta}{m}} \cos \frac{ka}{2}$

12. At higher frequencies, for monoatomic lattice, the phase velocity is given by

(a) $a \sqrt{\frac{\beta}{m}} \cos \frac{ka}{2}$

(b) $\frac{2}{k} \sqrt{\frac{\beta}{m}} \sin \frac{ka}{2}$

(c) $a \sqrt{\frac{\beta}{m}} \sin \frac{ka}{2}$

(d) $\frac{2}{k} \sqrt{\frac{\beta}{m}} \cos \frac{ka}{2}$

13. When frequency $\omega = \sqrt{\frac{4\beta}{m}}$, then the group velocity is

(a) $\frac{2a}{\pi} \sqrt{\frac{\beta}{m}}$

(b) $\frac{a}{\pi} \sqrt{\frac{m}{\beta}}$

(c) 0

(d) $a \sqrt{\frac{\beta}{m}}$

14. For frequency $\omega = \sqrt{\frac{4\beta}{m}}$, the phase velocity is given by

(a) $\frac{2a}{\pi} \sqrt{\frac{\beta}{m}}$

(b) $\frac{a}{\pi} \sqrt{\frac{m}{\beta}}$

(c) 0

(d) $a \sqrt{\frac{\beta}{m}}$

15. For monoatomic lattice, the first Brillouin zone lies between

(a) $-\frac{2\pi}{a} \leq k \leq \frac{2\pi}{a}$

(b) $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$

(c) $-\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$

(d) $-\frac{\pi}{3a} \leq k \leq \frac{\pi}{2a}$

16. The second Brillouin zone for monoatomic lattice lies between

(a) $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$

(b) $-\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$

(c) $-\frac{2\pi}{a} \leq k \leq -\frac{\pi}{a}$

(d) $-\frac{2\pi}{a} \leq k \leq \frac{2\pi}{a}$

17. The diatomic lattice, ω_+^2 is given by

$$(a) a\sqrt{\frac{\beta}{m}} \cos \frac{ka}{2}$$

$$(b) \frac{2}{k}\sqrt{\frac{\beta}{m}} \sin \frac{ka}{2}$$

$$(c) \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) - \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}}$$

$$(d) \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) + \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}}$$

18. For $F_{2n} = \beta[x_{2n+1} + x_{2n-1} - 2x_{2n}]$, the solution is given by

$$(a) x_{2n} = A \exp[i(\omega t - 2kna)]$$

$$(b) x_{2n} = A \exp[i(\omega t + 2kna)]$$

$$(c) x_{2n} = A \exp[i(\omega t - (2n+1)ka)]$$

$$(d) x_{2n} = A \exp[i(\omega t - (2n-1)ka)]$$

19. For diatomic lattice, ω_-^2 is given by

$$(a) \beta \left(\frac{1}{m_1} + \frac{1}{m_2} \right) + \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}}$$

$$(b) \frac{2}{k}\sqrt{\frac{\beta}{m}} \sin ka / 2$$

$$(c) a\sqrt{\frac{\beta}{m}} \cos ka / 2$$

$$(d) \beta \left[\frac{1}{m_1} + \frac{1}{m_2} \right] - \beta \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4 \sin^2 ka}{m_1 m_2}}$$

20. For diatomic lattice, when $k \rightarrow \pi/2a$, the ω_+ is given by

$$(a) ka\sqrt{\frac{2\beta}{m_1 + m_2}}$$

$$(b) \frac{2}{k}\sqrt{\frac{\beta}{m}} \sin \frac{ka}{2}$$

$$(c) \sqrt{\frac{2\beta}{m_1}}$$

$$(d) 0$$

21. For long wavelength regime, when $ka \ll 1$, then ω_- is given by

(a) $\sqrt{\frac{2\beta}{m_1}}$

(b) $ka\sqrt{\frac{2\beta}{m_1 + m_2}}$

(c) $\sqrt{\frac{2\beta}{m_2}}$

(d) $\sqrt{2\beta\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$

22. For $k \rightarrow \pi/2a$, ω_- is given by

(a) $\sqrt{\frac{2\beta}{m_2}}$

(b) $\sqrt{\frac{2\beta}{m_1}}$

(c) $\sqrt{\frac{\beta}{m}}$

(d) $\sqrt{\frac{\beta}{2m}}$

23. The optical branch is represented by graph between

(a) ω_- and k

(b) ω_+ and k

(c) ω_- and ω_+

(d) ω_-^2 and k

24. For optical branch, A/B is given by

(a) 1

(b) 2

(c) $-\frac{m_2}{m_1}$

(d) $\frac{m_1}{m_2}$

25. For acoustical branch, A/B is given by

(a) 1

(b) 2

(c) $-\frac{m_1}{m_2}$

(d) $-\frac{m_2}{m_1}$

26. For $m_1 = m_2$, which of the following is true?

(a) No forbidden gap exists

(b) Frequency of monoatomic and diatomic lattice are same

(c) Both (a) and (b)

(d) None of these

27. The r.m.s velocity of electrons is \approx

(a) 10^6 m/sec

(b) 10^4 m/sec

(c) 10^3 m/sec

(d) 10^5 m/sec

28. The conductivity, according to Drude's model is

- (a) $nv\lambda \frac{dE}{dx}$ (b) $\frac{ne^2\lambda v}{6k_B T}$
 (c) $\sqrt{\frac{3k_B T}{m}}$ (d) σE

29. The value of K (thermal conductivity) is

- (a) $\frac{3}{2}k_B T$ (b) $3\left(\frac{k_B}{e}\right)^2 T$
 (c) $\frac{n\lambda(3k_B)^{3/2}\sqrt{T}}{6A\sqrt{m}}$ (d) $n\lambda k_B T$

30. According to Wiedemann–Franz's law,

- (a) $K = \frac{n\lambda(3k_B)^{3/2}\sqrt{T}}{6A\sqrt{m}}$ (b) $\sigma = \frac{ne^2\lambda v}{6k_B T}$
 (c) $V = \sqrt{\frac{3k_B T}{m}}$ (d) $\frac{K}{\sigma} = 3\left(\frac{k_B}{e}\right)^2 T$

31. Which of the following is true for Drude–Lorentz model?

- (a) Could not explain positive charge carriers
 (b) Could not explain paramagnetic susceptibility.
 (c) Could not explain long mean free paths.
 (d) All of the above.

32. The normalization constant for one dimensional potential well is given by

- (a) $\sqrt{\frac{2}{a}}$ (b) $\frac{2}{a}$
 (c) $\sqrt{\frac{8}{a}}$ (d) $8/a$

33. The Fermi energy is given by

- (a) $\frac{\pi^2\hbar^2}{2ma^2}$ (b) $\frac{n^2\pi^2\hbar^2}{8ma^2}$
 (c) $\frac{N\hbar}{2\pi}$ (d) $1/2k_B T$

34. The average kinetic energy of electron is given by

- (a) $\frac{3}{5}E_F$ (b) $\frac{E_F}{2}$
 (c) $\frac{E_F}{3}$ (d) $\frac{E_F}{5}$

35. The Fermi velocity is given by

(a) $\frac{N\hbar}{4ma}$

(b) $\frac{N^2\hbar^2}{4ma}$

(c) $\frac{4ma}{N\hbar}$

(d) $N4ma$

36. The density of states is given by

(a) $\sqrt{\frac{2m}{E}}$

(b) $\pi\hbar\sqrt{\frac{2m}{E}}$

(c) $\frac{a}{\pi\hbar}\sqrt{\frac{2m}{E}}$

(d) $\frac{\pi}{\hbar}\sqrt{\frac{E}{2m}}$

37. In 3-D, the normalization constant is given by

(a) $\sqrt{\frac{8}{a}}$

(b) $\sqrt{\frac{8}{a^3}}$

(c) $\sqrt{\frac{2}{a}}$

(d) $\sqrt{\frac{2}{a}}$

38. According to Bloch theorem, $\phi(x+a)$ is

(a) $\phi(x+a) = \exp(\pm ika)\phi(x)$

(b) $\phi(x+a) = \log(ika)$

(c) $\phi(x+a) = \exp(\pm ika)$

(d) $\phi(x+a) = A\phi(x)$

39. The area of potential barrier is given as

(a) mV_0ab

(b) $\frac{\hbar^2}{mV_0ab}$

(c) $\frac{mV_0ab}{\hbar^2}$

(d) $\sin k a / k a$

40. The value of P is given by

(a) $\frac{\hbar^2}{mV_0ab}$

(b) $\sqrt{\frac{8}{a^3}}$

(c) mV_0ab

(d) $\frac{k_2^2 ab}{2}$

ANSWERS

- | | | | |
|---------|---------|---------|---------|
| 1. (a) | 11. (d) | 21. (b) | 31. (d) |
| 2. (c) | 12. (b) | 22. (a) | 32. (a) |
| 3. (b) | 13. (c) | 23. (b) | 33. (b) |
| 4. (No) | 14. (a) | 24. (c) | 34. (c) |
| 5. (b) | 15. (b) | 25. (a) | 35. (a) |
| 6. (c) | 16. (c) | 26. (c) | 36. (c) |
| 7. (d) | 17. (d) | 27. (d) | 37. (b) |
| 8. (c) | 18. (a) | 28. (b) | 38. (a) |
| 9. (a) | 19. (d) | 29. (c) | 39. (c) |
| 10. (b) | 20. (c) | 30. (d) | 40. (d) |

Micro-Assessment Questions

1. What is lattice dynamics?
2. What is zero point energy?
3. Define the Planck's hypothesis.
4. What is phonon?
5. Write down the dispersion relation for monoatomic lattice.
6. How does angular frequency vary with wavenumber for monoatomic lattice?
7. What are Brillouin zones?
8. What is the forbidden energy gap between the angular frequencies?
9. What is optical branch?
10. What is acoustic branch?
11. What are free electrons?
12. What is relaxation time?
13. What is thermal conductivity?
14. What is Weidemann–Franz law?
15. What is Fermi energy?
16. What do you understand by density of states?
17. How the density of states and energy vary?
18. Define P function for Kronig–Penney model.

Critical Thinking Questions

1. What is the difference between phonon and photon?
2. Define the momentum and wave vector for phonon.
3. How do phonon and photon interact with each other?
4. Give the assumptions made for one-dimensional monoatomic lattice.
5. Obtain the phase and group velocity for monoatomic lattice.
6. Give the first and second Brillouin zone for the monoatomic lattice.
7. What is the difference between the optical and acoustic branch?
8. Explain the effect on forbidden gap for diatomic lattice, when both the atoms are of same mass.
9. Give the postulates of Drude–Lorentz model.
10. Derive the Ohm's law and electrical conductivity using Drude–Lorentz model.
11. Obtain the thermal conductivity from Drude–Lorentz model.
12. Obtain the expression for Weidemann–Franz law.
13. List down the merits and demerits of Drude model.
14. Obtain the expression for Fermi energy using Sommerfeld model.
15. Show that the average kinetic energy of electrons is equal to $1/3$ of Fermi energy.
16. Define Fermi velocity and obtain its value in equilibrium condition.
17. Obtain the density of states for electrons and show that it depends inversely on square root of energy.
18. Give the postulates of band theory of solids.
19. Why is the free electron theory not being successful?
20. What was the assumption made for Kronig–Penney model?
21. Give the boundary functions for Kronig–Penney model.
22. Give the equation that measures the area of potential barrier. Give its significance.

Graded Questions

1. Obtain the dispersion relation for one-dimensional monoatomic lattice.
2. When the frequency is small for monoatomic lattice, show that the phase and group velocity are small.
3. Show that for high frequency in monoatomic lattice, the phase and group velocity depend upon the wavenumber.
4. Obtain the dispersion relation for diatomic lattice. Show that angular velocity has two values.
5. Obtain the angular velocity and Brillouin zones for the diatomic lattice.
6. Show that for the optical branch, the two atoms vibrate opposite to each other for diatomic lattice.
7. Show that for the acoustic branch, the two atoms are in phase with each other.
8. Explain in detail the properties explained by Drude–Lorentz model.
9. Obtain the energy of electron using Sommerfeld model.
10. Show that electron can take only discrete values of energy and energy is proportional to n^2 where n is principal quantum number.
11. Obtain the normalization constant for free electron gas in three dimensions.
12. State and explain the Bloch theorem.
13. Obtain the solution of Bloch equation. What are Bloch functions?
14. Explain in detail the Kronig–Penney model.

Remember and Understand

1. Lattice dynamics deals with the vibrations of atoms around the equilibrium position. Atoms vibrate around the mean position.
2. There always exists a zero-point energy for single-atom harmonic oscillators, which is in contradictory to the Planck's hypothesis.
3. Phonon is the quantum of thermal energy for lattice vibrations and obey BE statistics such as photons, but phonons originate from elastic waves.
4. For one-dimensional model, the atoms are considered like sphere connected to each other via springs. Atoms obey Hooke's law and the nearest neighbor atoms depends directly on the extension or contraction of atoms.
5. For diatomic lattice, two types of branches originate: optical and acoustic branch. For optical branch, the atoms vibrate opposite to each other; whereas for acoustic branch, the atoms are in phase of each other.
6. Free electrons are the atoms present in the outermost shells. Drude–Lorentz theory is also known as free electron theory which states that free electrons are responsible for thermal and heat conduction of metal.
7. Free electron theory could not explain the difference of conductors, insulators, and semiconductors. This theory also predicted the negative hall coefficients for metals. Band theory was able to explain the shortcomings of free electron theory as it assumed that the electron is moving under some force.

Characterization Techniques and Nanophysics

Keywords: transmission electron microscope, AFM, STM, SPM, nanophysics, buckyballs, fullerenes, surface/volume ratio, nanorods, nanoparticles, ball-milling, sol-gel method

Learning Objectives

- ◆ To study about transmission electron microscopy and the electron sources
- ◆ To understand the signals generated by X-ray beam
- ◆ To learn about the characteristics of electron beam
- ◆ To know about lens defect in TEM and imaging system as well as display system
- ◆ To know about electron detectors and specimen preparation
- ◆ To know about principle, working, and scanning modes of scanning probe microscopy (SPM)
- ◆ To understand the principle, working, and methodology of scanning tunneling microscopy
- ◆ To understand the principle and working of atomic force microscopy
- ◆ To know about AFM probes, contact mode, and noncontact mode
- ◆ To get insight of nanophysics and different nanostructures
- ◆ To learn about mechanical, optical, chemical, electrical, biological, and magnetic properties of nanoparticles
- ◆ To know about importance of surface area/volume ratio
- ◆ To understand the concept of quantum confinement
- ◆ To learn about nanomaterials and their synthesis techniques
- ◆ To know about buckyballs/fullerenes structure
- ◆ To understand carbon nanotubes and their structure
- ◆ To learn about chemical vapordeposition, laser vaporization techniques, and carbon arc discharge techniques
- ◆ To know about properties of CNTs

*This chapter is theoretical. Hence, there is no numerical problem/solved problem.

18.1 Introduction to Transmission Electron Microscope (TEM)

The electron microscope was made by Knoll and Ruska in 1930. TEM is transmission electron microscope; electrons are smaller than atoms that increase the resolving power. TEM generally operates at 300–400 kV (accelerating voltage) and are of many types (fig. 18.1 (a)). Before we proceed further, we should understand the properties of electrons. Electrons show both particle and wave-like characteristics. According to de-Broglie's hypothesis,

$$\lambda = \frac{h}{p} \quad (1)$$

In TEM, electron is accelerated through potential V , and hence electrons gain momentum as well as kinetic energy.

The potential energy of electron = eV

The kinetic energy of electron = $\frac{m_0 v^2}{2}$

$m_0 \rightarrow$ mass of e^-

$v \rightarrow$ velocity of e^-

At equilibrium,

$$PE = KE$$

$$eV = \frac{m_0 v^2}{2}$$

$$v^2 = \frac{2eV}{m_0} \Rightarrow v = \sqrt{\frac{2eV}{m_0}} \quad (2)$$

We know, momentum $p = m_0 v$

$$p = m_0 \sqrt{\frac{2eV}{m_0}} = \sqrt{2em_0 V} \quad (3)$$

Substituting Eqn. (3) in Eqn. (1),

$$\lambda = \frac{h}{\sqrt{2em_0 V}} \quad (4)$$

Hence, accelerating to Eqn. (4):

$$\text{Wavelength of electrons} \propto \frac{1}{\sqrt{\text{accelerating voltage}}} \quad (5)$$

Electrons are ionizing radiation that has the capability of removing tightly bound inner-shell electrons from the attractive field of nucleus. The advantages of using ionizing radiation are that it produces wide range of secondary signals (Figure 18.1(b)).

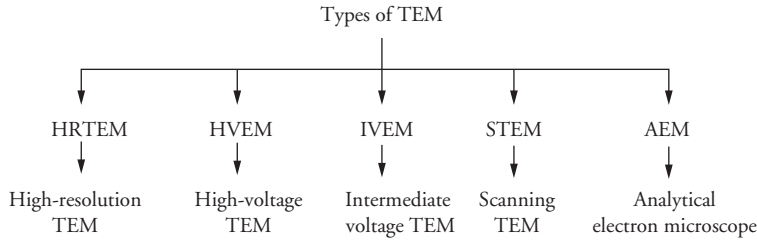


Figure 18.1(a) Types of TEM

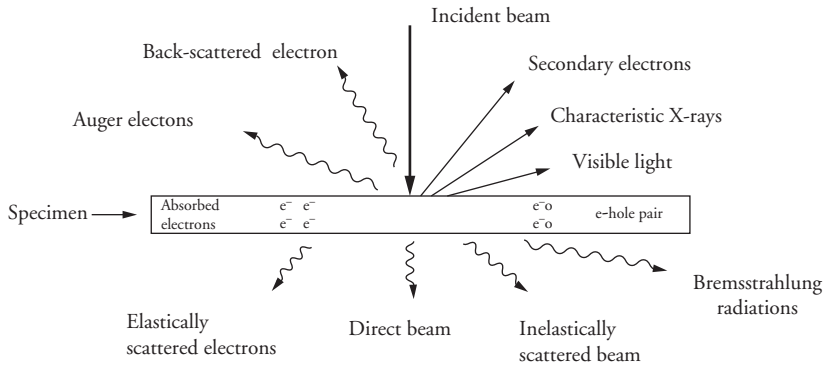
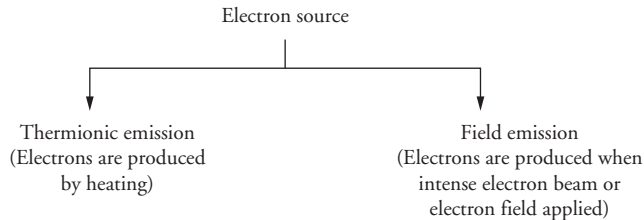


Figure 18.1(b) Signals generated by X-ray beam.

18.1.1 Electron Sources:

There are different types of electron sources as demonstrated below.



Two kinds of sources are used for TEM: thermionic source and field-emission source. These sources are part of electron gun.

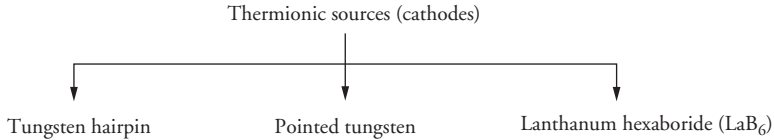
1. Thermionic Emission

When the material is heated to high temperature, then the electrons can overcome the natural barrier, which is termed as “work function” (W). Thermionic emission is based on Richardson law.

$$J = CT^2 e^{-W/k_B T} \tag{6}$$

- C → Richardson constant
- J → current density
- T → temperature (in Kelvin)
- k_B → Boltzmann’s constant

Thermionic sources are classified as follows:



Tungsten (W) has got high-melting temperature (3660 K) and LaB_6 has low work function. Pointed tungsten is fine thread having 0.1 mm diameter. When wire is bent into V shape, then it is called tungsten hairpin. LaB_6 are the rare-earth boride crystal not filaments are grown in $\langle 110 \rangle$ plane. Both tungsten and LaB_6 are used as cathode in triode gun. In addition to cathode, there is a grid called a Wehnelt cylinder and an anode at earth potential with a hole at its center. The cathode is attached to high-tension cable, (high voltage). This cable is also connected to W filament to supply a current to heat the filament (Figure 18.2).

As the filament current (I_F) increases, the temperature increases until the thermionic emission occurs. Subsequently, emission current (I_E) reaches a maximum such that I_F does not increase the current going into microscope. This condition is saturation current condition which is demonstrated in Figure 18.3.

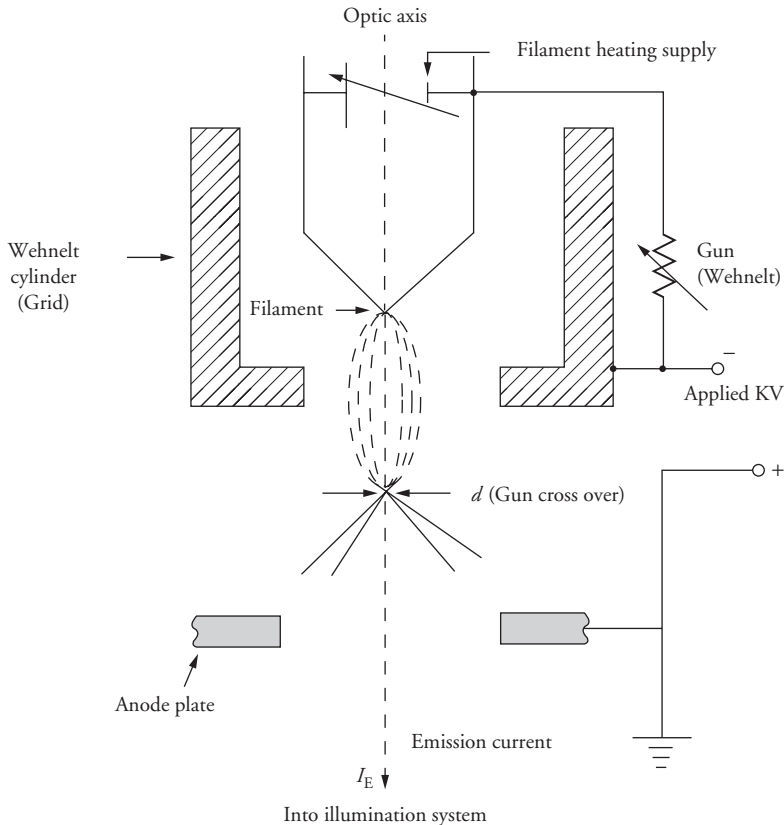


Figure 18.2 Electron gun.

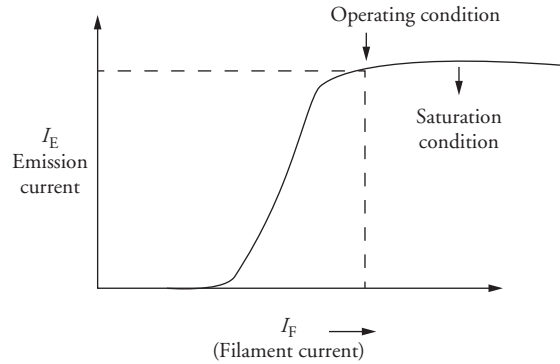


Figure 18.3 Variation of emission and filament current.

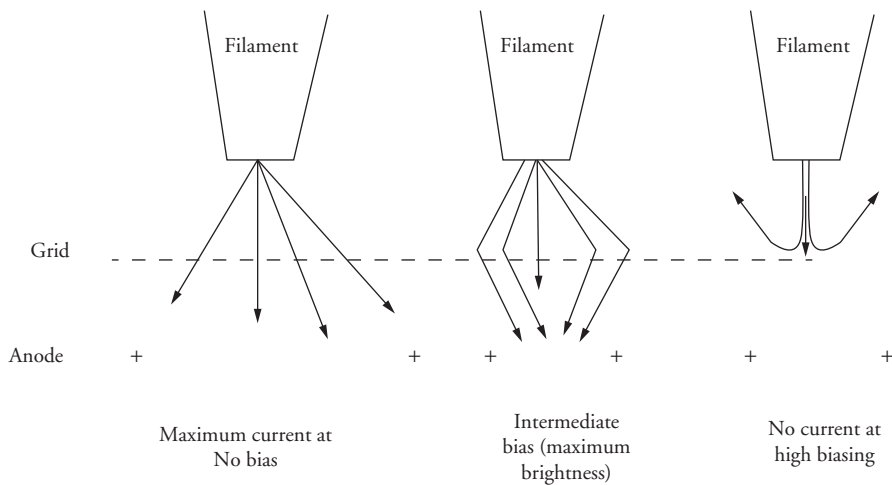


Figure 18.4 Effect of bias on the electron current.

All the thermionic sources should be operated at or just below saturation. Operating above saturation reduces film life. Operating below saturation reduces the current into specimen, thereby reducing the intensity of signals coming out of specimen.

In case of LaB_6 , it is preferable to operate little below saturation, because the electrons in halo are more coherent than those in central bright region. LaB_6 are more susceptible to thermal shocks and hence care should be taken while heating or cooling. Increasing the heating current should be done slowly, with 10–20 sec pause between each setting (Figure 18.4).

2. Field-emission Sources

We know the relation between electric field (E) and potential (V)

$$E = \frac{V}{r} \quad \text{(principle of FE sources)}$$

where r is the radius of spherical surface.

The principle of field emission sources is that the strength of an electric field E is high at sharp points (small r). Tungsten wire can be given a field radius of $<0.1 \mu m$. If 1 kV potential is applied, then

$$E = \frac{10^3 \text{ V}}{0.1 \times 10^{-6}} = 10^{10} \text{ V/m}$$

This lowers work function barrier, and the exhibits severe stress on the tip, hence the material has to be strong.

Field emission guns (FEG) are much simpler than thermionic guns. FEG is a cathode w.r.t. two anode as shown in fig. 18.5. First anode is positively charged by several kV w.r.t the tip and is called extraction voltage since it generates the intense electric field-extracting electrons by enabling them to tunnel out of the tip. Anode 2 accelerates the electrons upto 100 kV. The combined fields of both the anode posses the crossover properties of an electrostatic lens. Field emission requires pristine (pure) surface and even in ultrahigh vacuum conditions, surface contaminants build up on the tip. With time, the emission current falls and the extraction voltage has to be increased to compensate. But it is very necessary to clean the tip by “flashing.” This means reversing the potential to tip and “blowing off” a surface layer of atoms or to heat the tip at 5000 K. In most FEGs, flashing occurs automatically when the extraction voltage increases to a certain predetermined level (Figure 18.5). The comparison of all the electron sources is given in table 18.1.

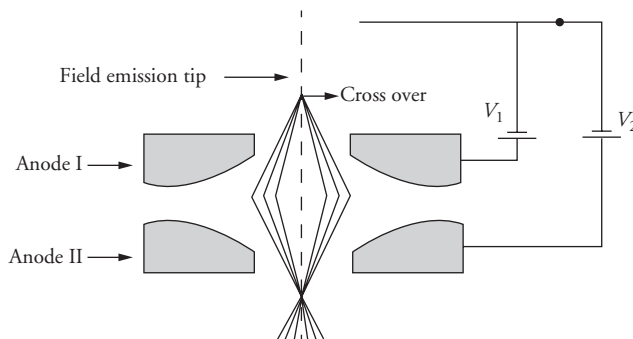


Figure 18.5 Crossover for field emission source.

Table 18.1 Comparison of guns

Property	Unit	Tungsten	LaB6	FE
Work function (ϕ)	eV	4.5	2.4	4.5
Richardson constant (C)	A/m^2k^2	–	4×10^5	6×10^5
Operating temperature	K	300	1700	2700
Current density	A/m^2	10^{10}	10^6	5×10^4
Crossover (d)	μm	<0.01	10	50
Brightness (B)	$A/m^2 \text{ Sr}$	10^{13}	5×10^{10}	10^9
Energy spread (AE)	eV	0.3	1.5	3
Emission current	%/hr	5	<1	<1
Vacuum	Pa	10^{-8}	10^{-4}	10^{-2}
Lifetime	hr	>1000	500	40 ~ 50

18.1.2 Characteristics of Electron Beam

1. Brightness

It is the current density/solid angle of the source. Electron sources differ considerably in size; and as a result, the electrons leave the source with a range of angles, so we cannot ignore the angular distribution compiling all the factors.

$$\text{Brightness} \quad \beta \propto \frac{I_E}{\pi \left(\frac{d}{2}\right)^2 \pi(\alpha)^2} \quad \left[\begin{array}{l} \frac{I_E}{\pi \left(\frac{d}{2}\right)^2} \rightarrow \text{emission current density} \\ d \rightarrow \text{beam diameter} \\ \alpha \rightarrow \text{divergence angle of beam} \end{array} \right]$$

Combining these,

$$\beta = \frac{4I_E}{(\pi d \alpha)^2} \quad (7)$$

The higher the value of β , more electrons can be put inside the beam and hence more information can be extracted.

2. Temporal Coherency and Energy Spread

Coherency indicates how well the electron waves are in step with one another. We know white light is incoherent because it consists of photons with a range of wavelengths and for coherency, monochromaticity is essential. Hence, temporal coherency refers to measure of how similar the “wave packets” are

$$\text{Coherence length } \lambda_c = \frac{v h}{\Delta E} \quad (8)$$

$v \rightarrow$ electron velocity

$\Delta E \rightarrow$ energy spread, which should be small.

3. Spatial Coherency and Source Size

Spatial coherency refers that the electrons were all emanating from the same point at the source. Spatial coherency is dependent on source size and small sources yield better coherency.

The effective source size d_c for coherent illumination is

$$d_c \ll \frac{\lambda}{2\alpha'} \quad (\alpha' - \text{angle subtended by source at the specimen}) \quad (9)$$

For better coherency, d_c should be small which can be obtained by using FE source. Spatial coherency is more important than temporal coherency. The threshold for beam damage of metals is less than 400 kV. Ceramics and polymers should be resolved at 100 kV.

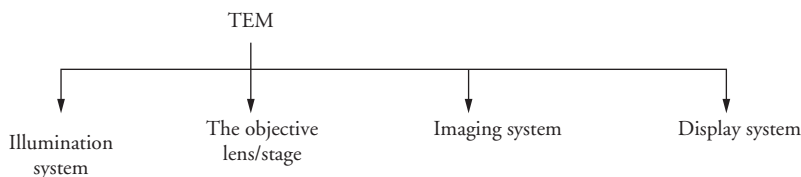
Max Knoll was a German electrical engineer born on July 17, 1897 in Wiesbaden. He studied in Munich and at the Technical University of Berlin. He obtained his doctorate in the Institute for high voltage technology. In 1927 he and his co-worker, Ernst Ruska, invented the electron microscope. In 1932, Knoll pursued work in the field of television design, and joined Telefunken in Berlin. Along with television designing, he was also a private lecturer in Berlin. Knoll joined as extraordinary professor in the University of after World War II. In 1948, he moved to the Princeton University, USA, to work at the department of Electrical Engineering. In 1956, he came back to Munich where he performed experiments on the generation of phosphenes at the Technische Hochschule. He got retired in 1966.



M.KNOLL

18.2 The Instrument

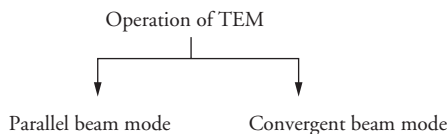
For studying the TEM, we need to know about its various components that constitutes its structure. TEM has four basic components as described below:



We will discuss them one by one.

18.2.1 Illumination System

This system takes the electrons from the gun and transfers them to specimen giving either a broad beam or focused beam. TEM generally operates on two modes: parallel-beam mode and convergent beam mode.



1. Parallel-beam Mode

In Figure 18.6(a) L_1 lens form demagnetized image of gun crossover. To produce an almost parallel L_2 lens is adjusted. In Figure 18.6(b), L_2 lens is focused to produce an image at the front focal plane of upper objective pole piece which in turn generates a broad parallel beam of electrons incident on the specimen. Parallel beam is essential to get the sharpest diffraction patterns as well as best image contrast. There is no need to change C_1 and can be kept constant.

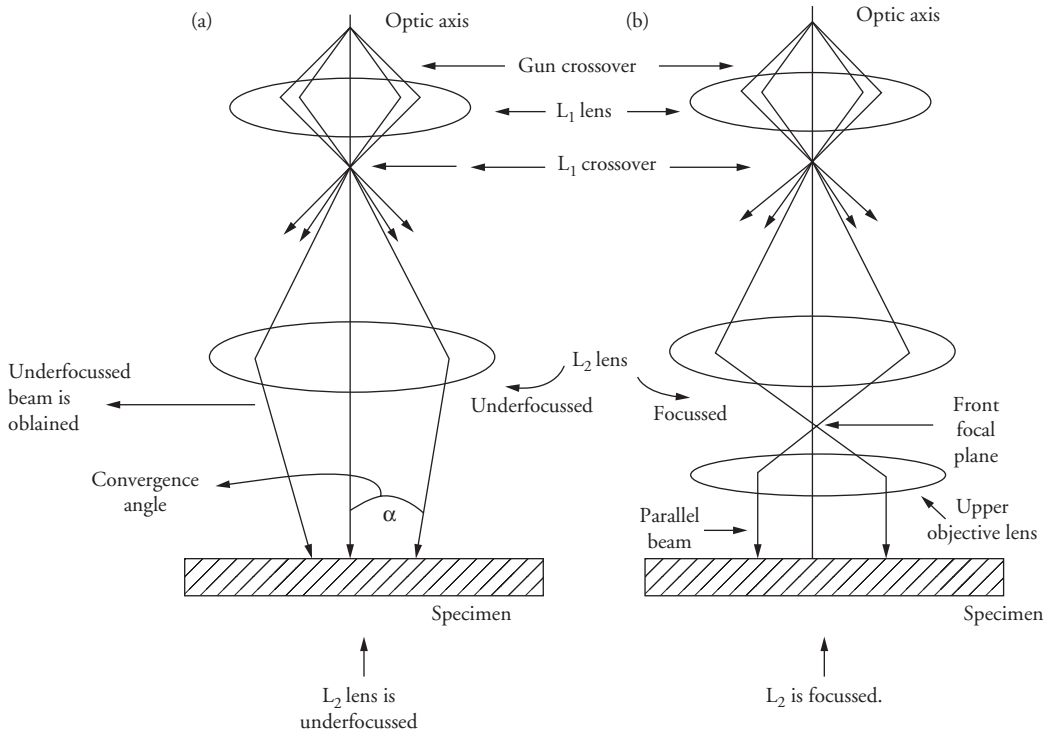


Figure 18.6 Parallel-beam mode.

2. Convergent beam Mode

If we minimize the area of the specimen that is being illuminated so we change L_2 lens. Sometimes, we deliberately require a focused convergent beam at the specimen. We then use convergent-beam mode. The convergence destroys the coherency and image contrast, and we cannot get the image of specimen immediately. Therefore, to see the image, we have to scan the beam, which forms the basis of STEM and AEM.

For getting convergent beam mode (Figure 18.7), we use a third L_3 lens also. The aperture of L_2 will control convergence angle (α). A smaller L_2 aperture gives a smaller α . Hence, the correct choice of L_2 aperture is important in convergent beam electron diffraction (CBED).

Next is regarding the alignment of illumination system. The beam can be tilted using scan coils and current through potentiometers is varied by using scan coils. These scan coils generate magnetic field to deflect the beam rather than to focus. To translate the beam, deflector scan coils are used. To tilt the beam, tilt scan coils are used between L_2 and L_3 . If the illumination system is correctly aligned, the gun crossover is on the optic axis and the electrons follow a straight line through the lenses and apertures until they hit the specimen.

L_2 aperture must be accurately centered on the optic axis of TEM. If the aperture is misaligned, the image of the beam on the screen moves off-axis and distorts as under focus or over focus L_2 .

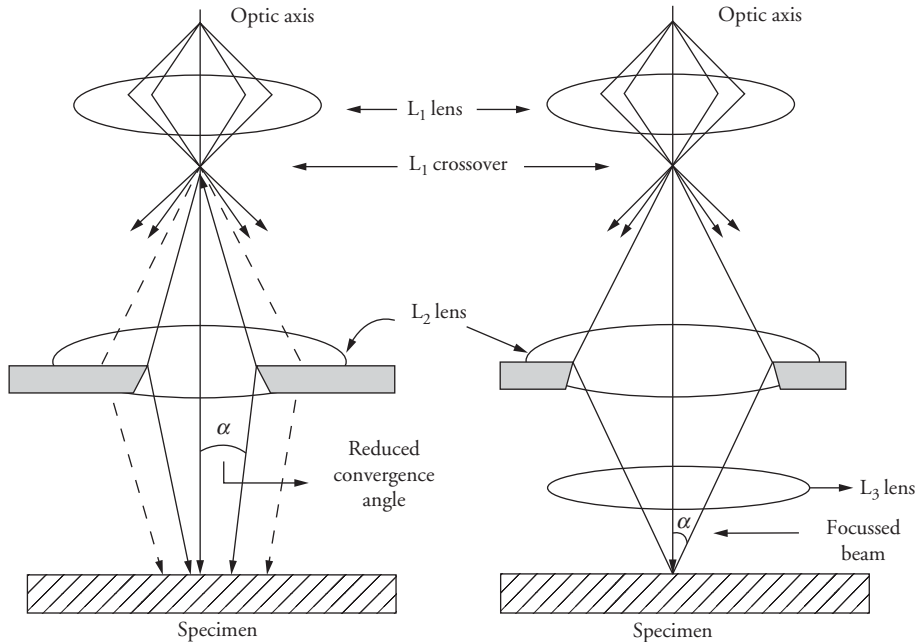


Figure 18.7 Convergent-beam mode.

NOTE: How to focus lens?

1. First, overfocus L_2 , so that the image of the beam is spread and outline of L_2 aperture is visible on the screen.
2. Then, use external drives to center the aperture on the screen.
3. Again adjust L_2 , so that image of beam is focused.
4. Center, the beam with deflector controls.
5. Underfocus the L_2 lens until you can again see aperture.
6. Repeat the whole operation iteratively until the image of the beam expands and contracts around the center of screen (Figure 18.8).

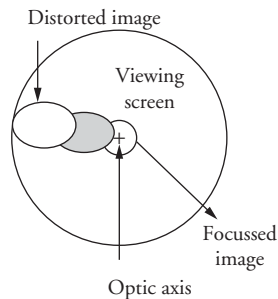


Figure 18.8 Focussed and unfocussed image.

Lens Defect in TEM

The illumination system lens suffers from the standard lens defects, such as aberrations and astigmatism. Lens defect should be paid much attention. If convergent beam mode is to be done (as in STEM and AES), then the following defects are to be taken into consideration.

1. Spherical Aberration

L_3 lens in convergent-beam mode is also known to be probe-forming lens, and it controls the minimum possible probe size (Image). L_3 should have short focal length. The spherical aberration limits the “minimum resolvable distance” to

$$r_{\min} = 0.91(L_s \lambda^3)^{1/4}$$

where $L_s \rightarrow$ spherical aberration coefficient for a particular lens. Hence, r_{\min} should be small so that L_s should be small.

The optimum probe size α [probe angle] convergence angle should be

$$\alpha_{\text{opt}} = .77 \left(\frac{\lambda}{L_s} \right)^{1/4}$$

2. Chromatic Aberration

This is related to the color of the electrons. The basic assumption is that electrons are monochromatic, but they are not. However, we can make high-tension supplies and the electron energy limits between smaller interval minimizing fluctuations. This aberration is highly energy dependent. The objective lens bends electrons of lower energy more strongly, and thus the electron from a point in the object once again form a disc image. The radius of the disk is given by

$$r_{\text{chr}} = L_c \frac{\Delta E}{E_0} \alpha$$

$L_c \rightarrow$ chromatic aberration coefficient

$\Delta E \rightarrow$ energy less of electrons

$E_0 \rightarrow$ initial beam energy

$\alpha \rightarrow$ semiangle/convergence angle

For reducing chromatic aberration, the specimen should be very thin so that after coming out of the specimen the electron beam energy spread should be small.

3. Astigmatism

Astigmatism occurs when the electrons sense a nonuniform magnetic field as they spiral around the optic axis. The soft-iron pole pieces cannot be perfectly cylindrical symmetrical. The soft iron may also have microstructural inhomogeneities that cause local variations in the magnetic field strength. Even if these difficulties are overcome, the apertures introduced into the lens may disturb the field if they are not precisely centered around the axis. Further, if the apertures are not clean, the contamination charges up and deflects beam. The distortion due to astigmatism is given by

$$r_{\text{ast}} = d \Delta x$$

$\Delta x \rightarrow$ maximum difference in focus induced by astigmatism

Astigmatism can be corrected using stigmators. Stigmators are small octuplets that introduce a compensating field to balance the inhomogeneities caused by astigmatism. If there is astigmatism, then image is elliptical and not circular (Figure 18.9).

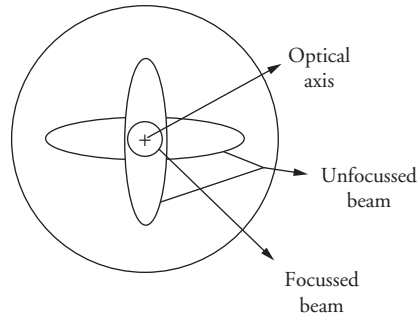


Figure 18.9 Demonstration of astigmatism.

Calibration of Illumination System

Following points must be considered while calibrating illumination system.

1. Maximum beam current should go with minimum beam size.
2. L_1 lens strength controls the probe size, As L_1 lens strength increases, the probe size decreases [probe size is measured in Full width half maximum (FWHM) (nm)] (Figure 18.10(a))
3. L_2 aperture size governs the convergence semi angle α . As L_2 aperture size is increased, the convergence angle also increases (Figure 18.10(b)).

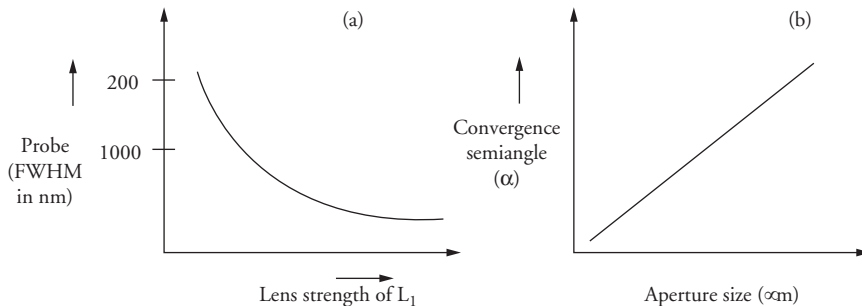


Figure 18.10 Variation of (a) Probe size with lens strength (b) Convergence angle with aperture size.

18.2.2 Objective Lens and Stage

The stage is used to clamp the specimen holder in correct position, so that objective lens can form images and diffraction patterns. In TEM, the positions of lens are fixed and we focus by changing the strength of the lenses. In most cases, the lenses which are used are magnetic, so that we change their strength by changing the magnetic field.

Magnification, $M = \frac{v}{u}$ and it should not be confused with resolution.

For magnetic lens (Figure 18.11), there is a cylindrically symmetrical core of soft magnetic material such as soft iron with a hole drilled in it. Soft iron pieces are known to be pole pieces. The distance

between the pole piece faces is called gap. The bore-to-gap ratio is important characteristic of lenses because it controls the focusing action of the lens. The second part of the lens is a coil of copper wire that surrounds each pole piece. When we pass a current through the coil, a magnetic field is created in the bore. This field is inhomogeneous along the length of lens, but axially symmetric. The lenses have to be cooled because they get resistively heated, and hence water recirculating system is essential part.

Strengthening the lens shorten the focal lengths (Figure 18.12). Therefore, a weaker lens f_1 produces higher magnification of object than the stronger lens (f_2). The image distance v changes, but u remains unchanged. We have to define a standard object plane for the main imaging lens of the microscope which is called eccentric plane. The specimen height should always be adjusted to sit in the eccentric plane because an image of an object in this plane will not move as the specimen is tilted. All other planes in the imaging system are defined w.r.t. eccentric plane. While inserting the specimen into TEM, it should be ensured that the object is in eccentric plane. To do this, tilt the specimen and adjust the height of specimen holder until the image of specimen remains stationary (± 30 on either side of zero).

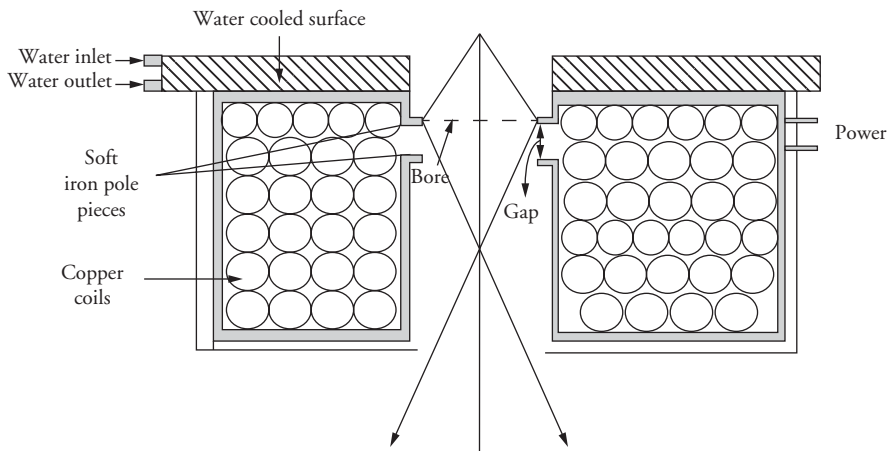


Figure 18.11 Magnetic lens.

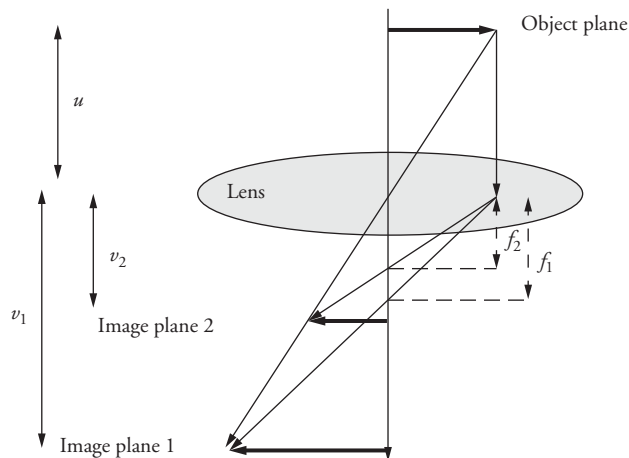


Figure 18.12 Weak lens producing high magnification and vice versa.

18.2.3 Imaging System

As shown in above ray diagram, the objective lens takes the electrons emerging from the specimen, disperses them to create diffraction pattern in back focal plane, and then recombines to form an image in image plane. There are two fundamental operations from the point of view of instrument. These are as follows:

- (i) Selected area electron diffraction (SAED)
- (ii) Bright-field and dark-field imaging

1. Selected Area Electron Diffraction

From Figure 18.13(a) (if no aperture is used), diffraction pattern contains electrons from whole of specimen that we illuminate. Such pattern is not very useful and the direct beam is so intense that it will damage viewing screen. Hence, we select a specific area of specimen to contribute to diffraction

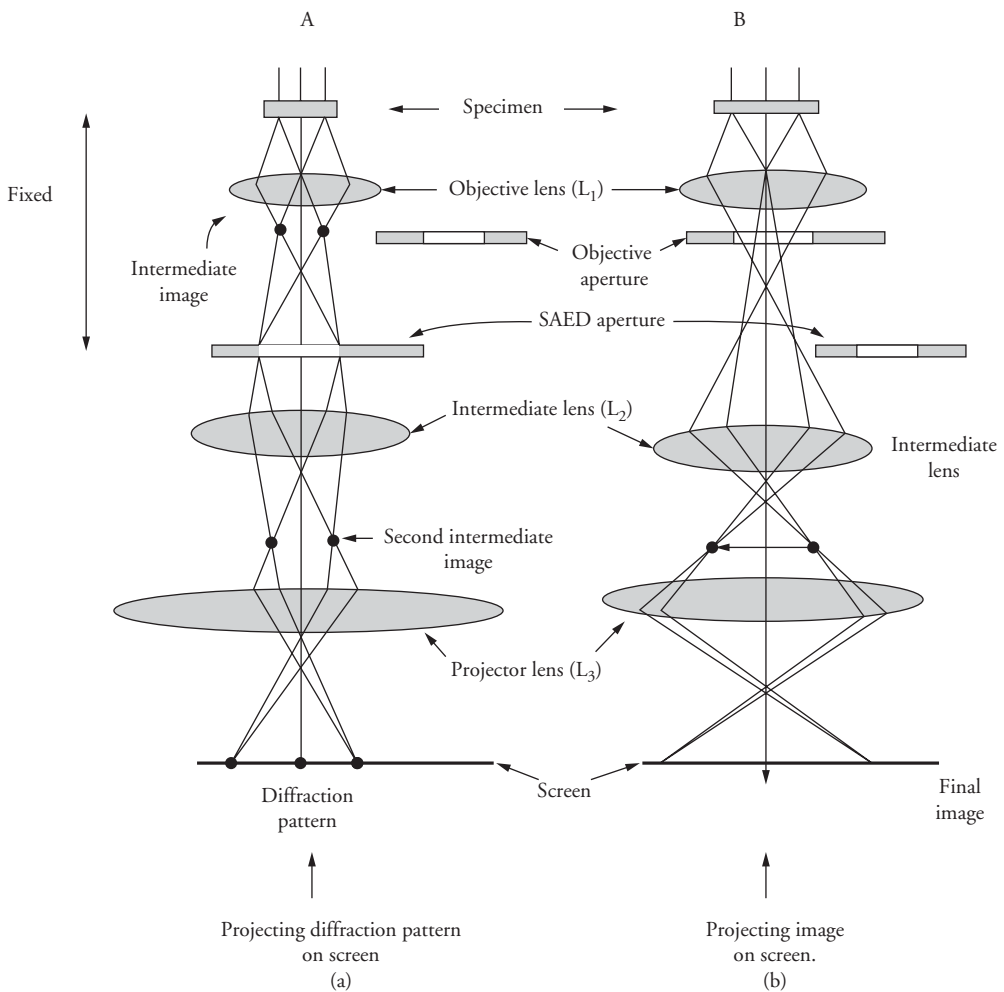


Figure 18.13 (a) Projecting diffraction pattern on screen and (b) projecting image on screen.

pattern. The pattern like Figure 18.13(a) (without aperture) is used in converged beam electron diffraction (CBED) as it uses L_2 and L_3 lens to converge the beam. Converging the beam destroys any coherence, and spots in the pattern are not sharply defined but spread into disks.

If we wish to obtain a diffraction pattern with parallel beam of electrons, the standard way is to select an aperture. The operation is called selected area electron diffraction (SAED pattern). We insert SAED aperture into the image plane of objective lens and center the aperture on the optic axis. By using aperture, any electron hitting the specimen outside the area will be excluded from contributing to the diffraction pattern. Basic principle of TEM operation is that when we want to look at diffraction pattern, we put an SAED aperture into the image plane of objective lens.

2. Bright Field and Dark Field

The SAED pattern contains a bright central spot that contains direct electrons and some scattered electrons. While forming images in TEM, an image is formed by moving central spot, or some/all of scattered electrons. External drives are used to move the aperture so that either the direct electrons or some scattered electrons go through it. When direct electrons form the image it is called bright-field image (Figure 18.14).

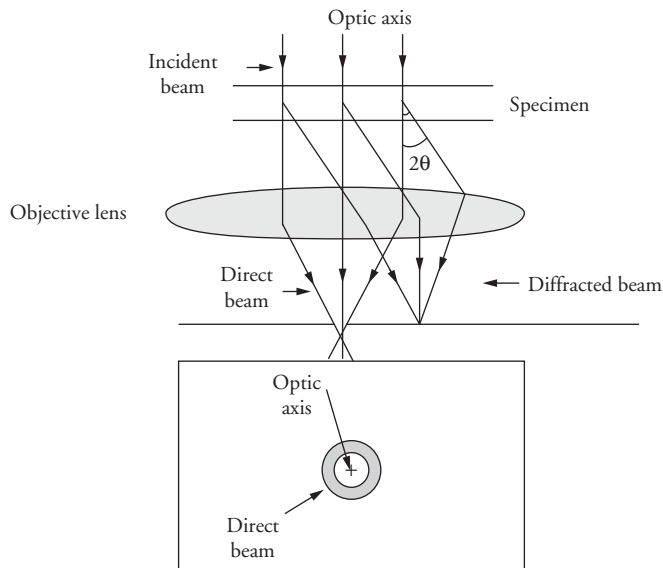


Figure 18.14 Bright field image.

If scattered electrons form an image then it is called dark-field image (Figure 18.15).

Conclusively following points must be taken into consideration:

1. If we want to have diffraction pattern, then SAED aperture should be inserted.
2. If we want to look for image, then SAED aperture has to be removed and objective aperture should be inserted.

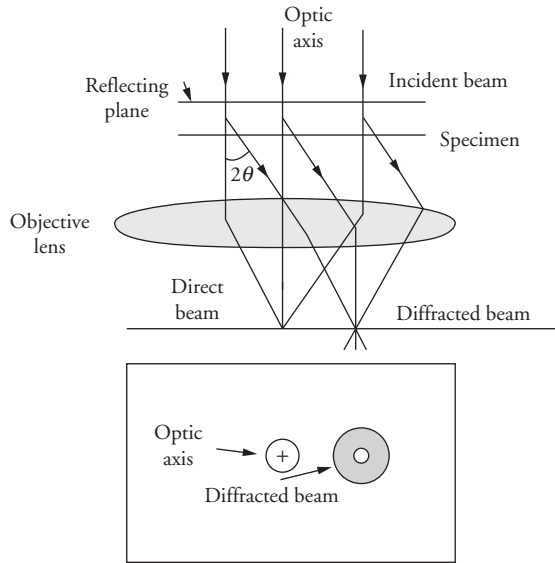


Figure 18.15 Dark-field image.

18.2.4 Display System

TEM images can be seen with the help of charge-coupled devices (CCD). In order to compare the properties of detection and recording devices, we often use “detection quantum efficiency”(DQE).

$$DQE = \left(\frac{S_{out}}{N_{out}} \right)^2 / \left(\frac{S_{in}}{N_{in}} \right)^2$$

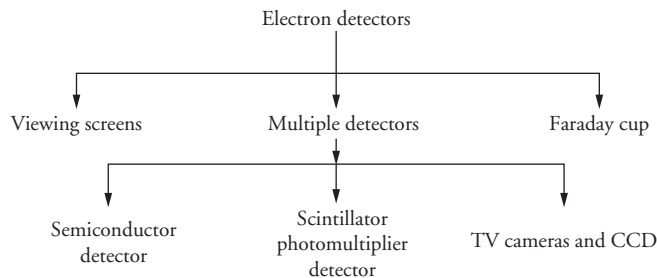
where $\frac{S_{out}}{N_{out}} \rightarrow$ Output signal to noise ratio.

and $\frac{S_{in}}{N_{in}} \rightarrow$ Input signal to noise ratio

For, perfect detector DQE = 1; otherwise, DQE < 1.

18.2.5 Electron Detectors

Electron detectors can be classified as following:



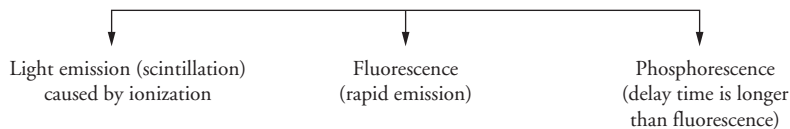
1. Viewing screen

It is coated with a material such as ZnS (grain size is ~50 μm). The greatest source of screen damage is intense direct beam that comes through thin specimens and constitutes the central spot in diffraction patterns. The burning of screen is minimized by (i) going to diffraction mode using SAED,

(ii) Going to diffraction mode with L_2 under focused, and (iii) if the spot appears exceptionally intense, then insert the beam stop.

2. Multiple Detectors

Electrons display screen emits light falling on it in one of the following ways:

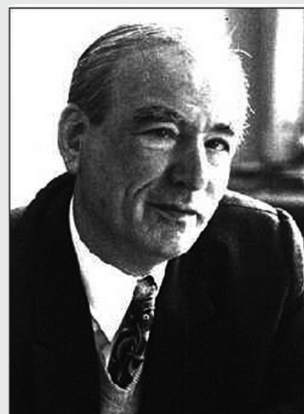


- (i) **Semiconductor detectors:** They are easy to fabricate, cheap to replace, and can be cut into any shape. They are sensitive to electrons with sufficient energy (>5 keV). Hence, they are mostly used for back-scattered imaging. These detectors have large dark current (The current registered when no signal is incident on the detector.) This introduces noise in the imaging and hence, its DQE is poor. They are insensitive to low-energy electrons such as secondary electrons.
- (ii) **Scintillator–photomultiplier detector:** We use yttrium–aluminum garnet (YAG) as scintillating materials. These materials have decay time of order of nanoseconds rather than of microseconds. Once the incoming electron signal is cemented to visible light, the light from the scintillate is amplified by a photomultiplier (PM) system. The gain of this system is very high, and hence high DQE ≈ 0.9 . The noise level is also low, but it is not as robust as semiconductor detector. Scintillate can also be coated with aluminium to prevent visible light from generating noise.
- (iii) **TV cameras and CCD:** Charge coupled devices (CCD) are devices that store charge generated by light or electron beams. CCD consists of thousands or millions of pixels that are electrically isolated from each other by creating potential wells, so that they can accumulate charge in proportion to incident electron beam intensity. They have DQE > 0.5 .

3. Faraday Cup

Faraday cup is like a black-hole for electrons. It is a detector that simply measures total electron current in the beam. Once the electrons enter the Faraday cup, they cannot leave except by flowing to ground through an attached pico-ammeter that measures the electron current.

E. Ruska was born on December 25, 1906, in Heidelberg. He graduated from grammar school in Heidelberg. He studied at the Technical College in Berlin. Thereafter, he started working with high voltage and vacuum technology at the Institute of High Voltage under the guidance of Dr Max Knoll. Along with his other coworkers, he worked on the development of a high-performance cathode ray oscilloscope. While working with Dr Knoll, they constructed the first electron microscope in 1931. In 1934, he got his doctoral thesis on the properties of electron lenses with short focal lengths. He also worked with Dr Bodo von Borries on the development of high-resolution electron microscopes. In 1945, he helped in reconstituting the Institute of Electron Optics in Berlin-Siemensstadt, which was disbanded due to bombing, so that the electron microscopes can be built again. The "Elmiskop 1" was discovered in 1954, which is in use over 1,200 institutions. He also worked at the German Academy of Sciences in Berlin-Buch. In 1957, he was made the Director of the Institute for Electron Microscopy. He retired on December 31, 1974, and died on May 25, 1988.



E.RUSKA

18.3 Specimen Preparation

Following precautimary points must be taken care of while preparing sample for TEM.

1. Have the “antidote” at hand.
2. Make up enough of the solution for one polishing session.
3. Never use mouth pipette for measuring any component.
4. Do not prepare cyanide solutions. The only metal where it excels is gold.
5. Perchloric acid in ethanol/methanol are used as universal polish, with density below 1.48. Always add acid to the solvent, never solvent to acid.
6. Avoid using nitric acid in combination with ethanol, as they form explosive mixtures. But methanol can be used in place of ethanol.
7. Use dilute solutions of hydrofluoric and cover the skin as it penetrates and dissolves the bone.

18.3.1 Preparing Self-Supporting Disk

A self-supporting specimen is one where the whole specimen consists of one material. Other specimens are supported on a grid or a copper (Cu) washer with a single slot. However, if X-ray analysis is performed on a specimen, then grid may contribute to signals. If we have to make a disk of sample, then it should be ≈ 3 mm in thickness. The rim of specimen must be relatively thick and total area of material at center should be thin.

It involves the following steps:

1. Thin Slice from Bulk Sample

For ductile materials such as metals, we should use chemical saw or wafering saw to get a thin slice <200 μm . Brittle materials such as ceramics can be cleaved with razor blade or diamond cutter, but the sample can be damaged. For such samples, we can use ultramicrotome.

2. Cutting the Disk

For obtaining a circular disc, we can use mechanical punch for metals. For brittle materials, one should be using spark erosion, ultrasonic drilling, and a grinding drill. In each case, the cutting tool is a hollow tube with inner diameter of 3 mm spark erosion is used for conducting samples and introduces least amount of mechanical damage.

3. Prethinning of the Disk

The aim of the process is to thin the center of the disk while minimizing damage to the surface. This stage is also referred to as dimpling. Mechanical dimples are used to grind and polish the disk to a fined radius of curvature in the center. If we are going for mechanical polishing, then always gradually decrease the grit size and conclude with the finest available. The better the polished surface, the better the final specimen.

4. Final Thinning of the Disk

(a) Electropolishing

It can only be used for mechanically and electrically conducting samples such as metals and alloys. There is a certain applied voltage at which the current due to anodic dissolution of the specimen creates a polished surface. This constitutes the basic principle for electropolishing (Figure 18.16).

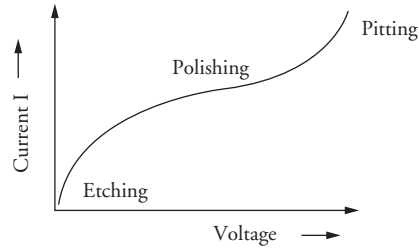


Figure 18.16 Electropolishing curve.

Two types of electropolishing are as follows:

- (i) Jet electropolishing
- (ii) Twin-jet electropolishing

Jet electropolishing allows a single jet of gravity-fed electrolyte to thin a disk supported on positively charged gauze, and the disk has to be related periodically as shown in Figure 18.17(a). Twin-jet electropolishing thins the sample from both sides, and the sample is held between teflon holders (Figure 18.17(b)).

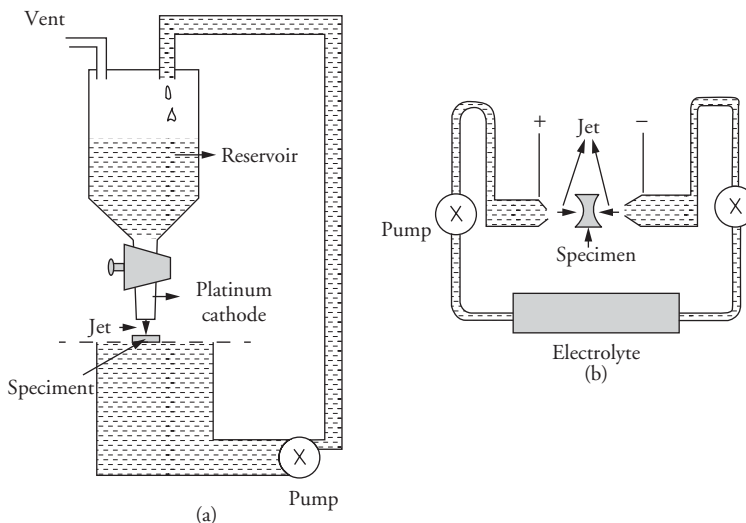


Figure 18.17 (a) Jet electropolishing (b) Twin-jet electropolishing.

(b) Ion Milling

It involves bombarding delicate thin TEM specimen with energetic ions or neutral atoms and sputtering material from film at an accelerating voltage of 4–6 keV. Ion gas is known as plasma and mostly argon or helium is used (Figure 18.18).

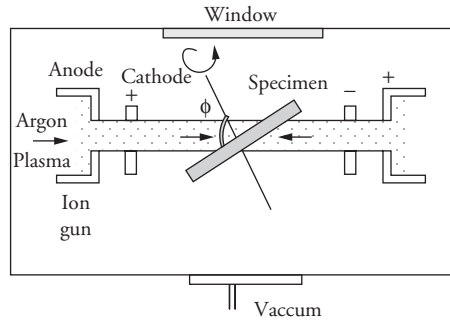
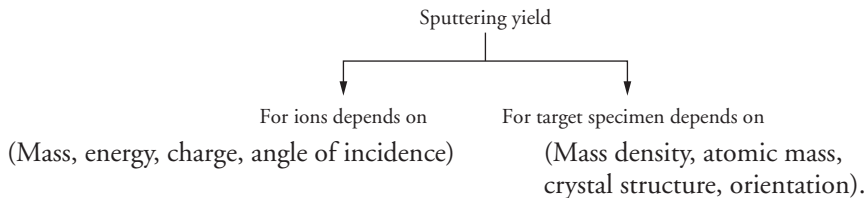


Figure 18.18 Ion beam thinning.

The ion beam can penetrate the sample up to some extent. Hence, the ion beam is aligned at an angle of $15^\circ - 25^\circ$ to the surface. If we use aligning angle $< 5^\circ$, then the deposition of ion beam in a region close to the specimen occurs. A lower beam energy also causes less damage; but in both the cases, the milling time is increased.

We define sputtering yield to be the number of atoms ejected/incident ion, which depends on mass of incoming ion and the sample ion milled, i.e



Argon is used mainly due to its inert nature and hence no contamination or corrosion to the device. Most of the thinning parameters are fixed, except for ion energy, angle of incidence. One should start with rapid thinning (heavy ions, high incidence angle) and slow the thinning rates as perforation approaches (Figure 18.19). Cooling of the specimens is required as the ion beam might heat it to 200°C or even higher. The creation of vacancies through ion damage can cause diffusion changes.

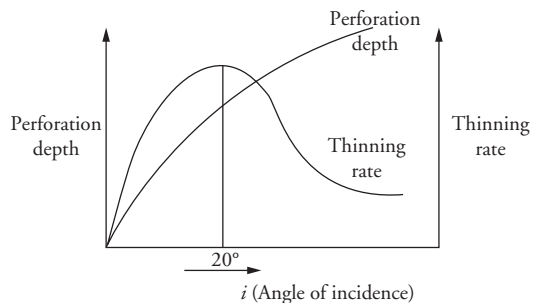


Figure 18.19 Variation of thinning rate and perforation depth with incident angle.

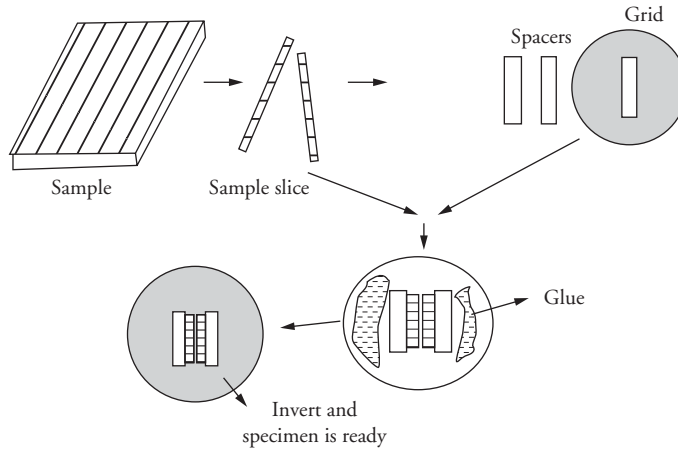


Figure 18.20 Specimen preparation.

The graph shown in Figure 18.19 highlights following points:

1. High incidence angles promote implantation, which is undesirable.
2. The rate of thinning reaches a maximum at $\sim 20^\circ$ after which the beam penetrates rather than sputtering the sample surface.
3. The specimen should also be rotated; otherwise, we tend to get surface structures/ grooves which are running in certain directions.

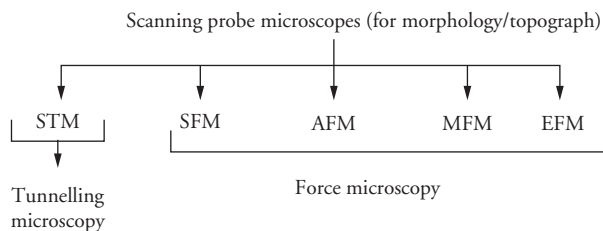
Figure 18.20 shows to put the samples on grids/washers, that is,

1. The specimen is cut into thin slices normal to interfaces.
2. They are glued together between spacers (that could be Si, glass).
3. The sandwich structure is then inverted and ion-milled to perforation.

18.4 Scanning Probe Microscopy (SPM)

Scanning probe microscopes (SPMs) provides direct relation between the structure and material properties (ductility, strength, reactivity, etc.). It indicates the relation between surface features and materials property.

Scanning probe microscopes can be classified as follows:



18.4.1 Operating Principle of SPM (Instrumentation)

In a scanning probe microscope Figure 18.21, the sample surface is scanned by sharp probe at a distance of less than few nanometers. For scanning, either the tip moves against the fixed sample or

vice versa. The moving element is mounted on piezoceramic scanner. The tip and sample are brought closer so that probing interactions can be measured with an appropriate detector. The detector signal is used for feedback control to adjust the tip–sample distance during the scanner. The functions of components of SPM are discussed below:

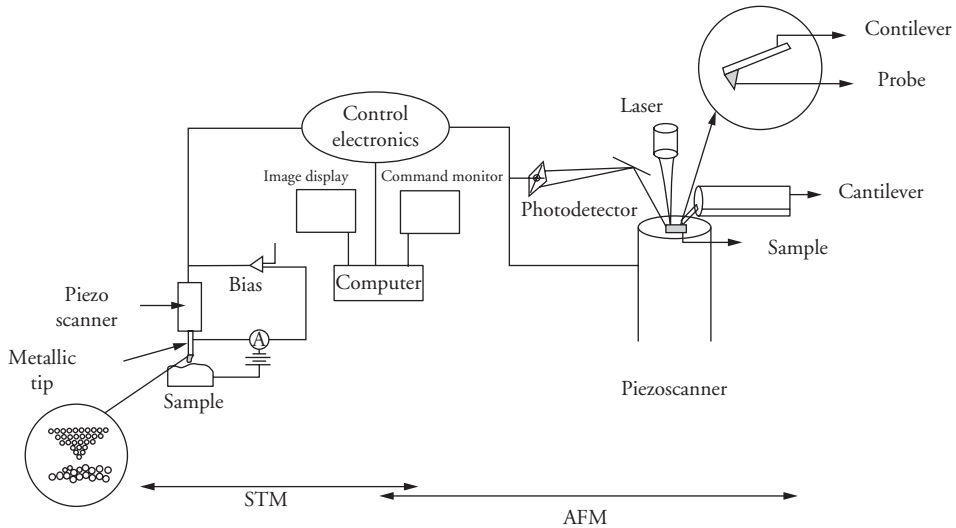


Figure 18.21 Schematic of scanning probe microscope.

1. Scanner

The driving motion is performed by piezoceramic drives (hollow tube scanner), which have property of changing dimensions under applied voltage. They can move the tip or sample in all three mutually perpendicular directions. The detection of atomic-scale images requires a short-tube scanner and long-tube scanner for covering large areas ($100 \times 100 \mu\text{m}$). At low voltages, the nonlinear response is given by long-tube scanner and can be corrected by computer software.

2. Tip–sample Approach

The tip should be positioned close enough to the sample surface to measure the strength of local–probing interactions between tip and the sample. The damage of the sample by a tip–sample contact, the approach is delicate. Tip and sample are put close to each other manually by rotating the high-precision mechanical screws. Stepper monitor brings the tip to the sample closer at atomic separations. Then, the lateral scanning is activated. The scanning tip can crash into the sample surface due to surface roughness and imperfect tip–sample alignment, unless the scanning is performed with feedback mechanism. Different type of feedback gain parameters (linear or logarithmic) can be used to generate the response of scanner.

18.4.2 Scanning Modes and Parameters

The lateral motion proceeds independently, whereas the vertical motion of the tip is adjusted according to the chosen feedback gain. Conventionally, x and y are taken to be fast and slow scanning directions (Figure 18.22). Scanning from left to right is taken to be “trace” scan and right to left is “retrace” scan.

The tip moves from one border to another performing trace and retrace motions alternatively covering square area along the slow scanning direction (y).

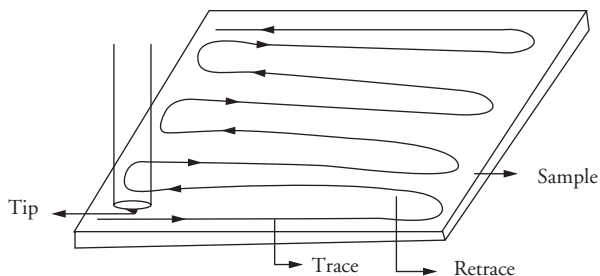


Figure 18.22 Trace and retrace directions.

Generally, three models are applied for SPM: constant height mode, constant current mode, and barrier height mode. In constant height mode, feedback mechanism is turned off, and the interactions at constant tip height are observed. In constant current mode, feedback is activated. In barrier height mode, both feedback and tip-sample distance are variables.

In commercial scanning probe microscope, each line scan consists of 512 points and scanning proceeds with scanning frequency in 1–60 Hz range. Imaging of areas larger than $1 \times 1 \mu\text{m}$ is performed with scanning frequency is 1–4 Hz range. For scanning flat areas of the order $40 \times 40 \text{ nm}$, the atomic and molecular size images are collected (8–60 Hz). Ideally, the position of sample is fixed in space and tip scans an area from one border to another. However, at ambient temperatures, the sample position drifts during the scanning and causes an image distortion. The thermal drift is large just after the sample has been installed and diminishes with time when the equilibrium between stage and sample has been achieved. Carry out small area scanning with high scanning rate to avoid damage of sample surface. The probability of damage increases if tip spends more time at a given location.

18.4.3 Images and Filtering

Trace image typically consisting of 512×512 pixels and can be generated by collecting data for trace scans when the data is collected in retrace direction, then retrace image is obtained. The contrast in imaging refers to spatial variation of z -height of the tip. Bright spots correspond to elevated surface regions and places with stronger probing interactions and vice versa.

For increasing the quality of imaging, one can filter raw images by means of fast Fourier transform procedure. The filtering highlights periodic features of images but can result in lose of nonperiodic features due to local defects. A plane-fit adjustment is necessary when the sample surface under observation is not exactly perpendicular to the scanner z -axis. Zooming, low pass, erasing scan times flattening, etc., are done with software.

Vibrational noise must be avoided to detect surface features. Hence, the microscope head should be placed on the platform supported by rubber cords that have low natural frequency ($\sim 1 \text{ Hz}$). Interference of lab vibrational noises and acoustic noise should also be isolated. Suspension with springs, stacked plate systems, and pneumatic systems can be used for reducing vibrational noise.

18.5 Scanning Tunneling Microscope (STM)

It allows us to determine the structure of surface with a spatial resolution on angstrom scale. Since a tunneling current is employed in STM, the application of this method is mostly limited to metals and semiconductors. The real-space visualization of surfaces on atomic scale can be obtained by STM.

18.5.1 Principle

Whenever a sharp conducting tip is brought very near to a metallic or semiconducting surface, then the bias between the two surfaces can allow electrons to tunnel through the vacuum between them. For low voltages, this tunneling current is a function of local density of states (LDOS) at the Fermi level (E_F) of the sample. Whenever a probe passes over the surface then the variations in current are translated to an image.

18.5.2 Methodology and Tunneling

Tunneling is possible only if there is an empty level of same energy on the other side of barrier for electron to tunnel onto. That is, why tunneling current is dependent upon $\rho(r, E_F)$ (density of available or filled states in sample). Conclusively, the current (I) due to applied voltage (V) depends on the number of free states to tunnel into on the other side of barrier. The higher the density of available states, the greater the tunneling current. The bias voltage V_{bias} determines which levels of the sample electronic states will participate in tip–sample electron transfer. For two metal surfaces near each other, the height of barrier can roughly be estimated by average work function of sample and tip.

$$\omega = \frac{1}{2} [\omega_{\text{sample}} + \omega_{\text{tip}}]$$

Only electronic states very near the Fermi level (within eV) are excited when the bias voltage is small. The excited electrons can tunnel across the carrier and hence, tunneling occurs mainly due to electrons whose energies lie near the Fermi level.

The bias voltage V_{bias} values are typically in 0.001–5 V range. When V_{bias} is positive, then electrons flow from tip to the sample and vice versa (Figure 18.23). The common tunneling current is 0.1–40 nA. Tip sample distance should be upto 0.01 Å. According to classical physics an electron cannot penetrate into or across a potential barrier if its energy E is smaller than potential V within the barrier (barrier width d).

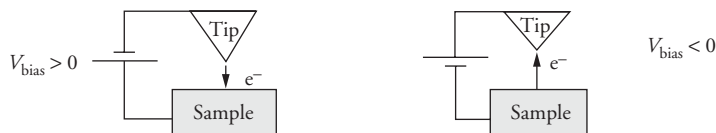


Figure 18.23 Electron transfer in STM.

Suppose that tip and sample are both metals and form a metal–insulator–metal junction. The gap between tip and sample provides insulating barrier (e.g. air, vacuum). When the bias voltage (V_{bias}) between the electrodes is zero, their Fermi level becomes equal and no tunneling current is observed. When V_{bias} is positive (i.e. tip is grounded), the energy levels of sample are lowered by eV_{bias} , so that electrons in the occupied level of tip tunnel to unoccupied levels of sample. When bias is negative (i.e. tip is grounded), the energy levels of the sample are raised by eV_{bias} , and the electrons in the occupied levels of the sample tunnel to unoccupied level of tip (Figure 18.24).

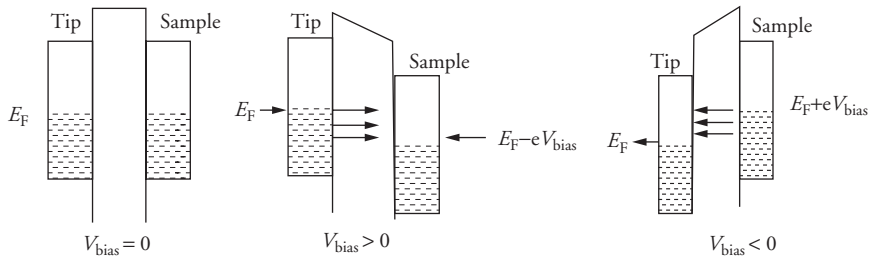


Figure 18.24 Energy bands with metal-insulator-metal junction.

18.5.3 STM Tips

Monoatomic sharp apex tips are ideal tips for STM which can be prepared and characterized by means of a field-ion microscope. Tips are also prepared by mechanically cutting/electrochemical etching of wires [tungsten, Au, Pt/Ir, Rh/Ir]. Only the outermost atom or few atoms of the tip are expected to participate in the electron transfer. Pt/Ir tips are preferred over tungsten (W) for ambient conditions because W is easily oxidized in air. The tungsten tips are mostly used in ultrahigh vacuum, as oxidation is less likely to happen. Electrochemically etched W or Pt/Ir tips have well-defined sharp microscopic profile. For current detection in a scanning tunneling microscope a combination of logarithmic and standard amplifiers is used because.

18.5.4 Construction of STM

The schematic of STM is shown in Figure 18.25. Tube scanner is a cylinder made out of piezoceramics and is covered inside/outside with metal acting as electrodes (Figure 18.26).

The tunneling current is converted into a voltage by a current amplifier. To get a linear response with respect to tunneling gap, the signal is processed by a logarithmic amplifier. The output of

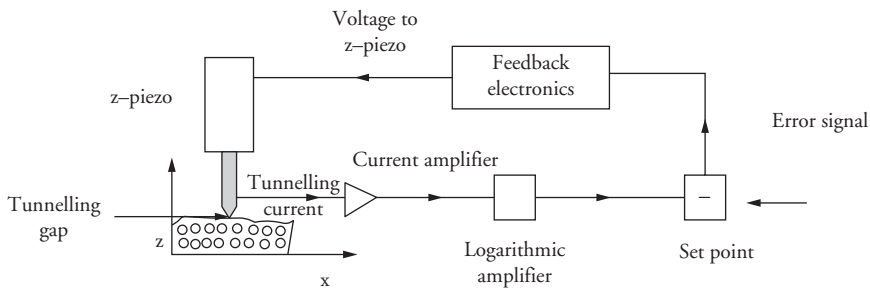


Figure 18.25 Schematic of STM.

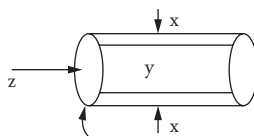


Figure 18.26 Tube scanner.

logarithmic amplifier is compared with predetermined voltage (reference current). The error signal is passed to feedback electronics that applies a voltage to the piezo to keep the difference between the current set point and tunneling current small.

Hence the required circuit is feedback circuit (for measuring constant current), a feedback circuit has to be build up to control z -piezo. Data acquisition cards are required to read voltage and control the system through computer. Data acquisition software is required to control mode and scanning and also to acquire the required data. Data analysis software is required to analyse the acquired data.

18.6 Advantages of SPM

1. The resolution is not limited by diffraction, but by the size of probe-sample interaction volume. It can measure small local differences in height (135 pm step on < 100 > silicon).
2. Interaction can modify sample to create small structures.
3. Unlike electron microscopes, specimens do not require a partial vacuum, but can be observed at Standard Temperature and Pressure.
4. Organic molecules that are insulating can be imaged when they are adsorbed on conducting substrate.

18.7 Disadvantages of SPM

1. Detailed shape of tip is difficult to examine. Noticeable effect is observed if specimen varies greatly in height over lateral distances of 10 nm or less.
2. Scanning techniques are generally slower in acquiring data, due to scanning process.
3. The maximum image size is generally smaller.
4. It is not useful for buried solid/solid or liquid-liquid interfaces.

18.8 Atomic Force Microscopy (AFM)

Atomic force microscopy (AFM) consists of optical block and base (Figure 18.27). The base has stepper motor; the alignment screws and the scanner. The sample is mounted on top of scanner. The optical block consists of viewing window at the top mirrors diode layers and positional split-diode photodetector. The cantilever holder is fixed on the top of alignment screws, and the tip is positioned over the samples.

Principle: Force curve plots the distance of scanner movement vs. cantilever deflection and are used to measure the vertical force of tip on the surface (Figure 18.28). In contact mode, it can be used to examine the attractive, repulsive, and adhesive interactions between the tip and the sample. The curve begins with the tip not touching sample, so that cantilever is undeflected and scanner retracted. When the tip comes close to the sample, the cantilever is deflected from its equilibrium position in response to the force experienced by the tip. It bends toward the sample when the force is attractive and away from it when the force is repulsive. The van der Waals' (VDW) attraction bends the cantilever toward the sample when the sample approaches the tip in the non-touching regime.

When the sample is moved further, then the attraction force gradient exceeds the spring constant of cantilever $\left[k = \frac{F}{m} \right]$ at some point and the tip comes onto sample surface, thereby making contact

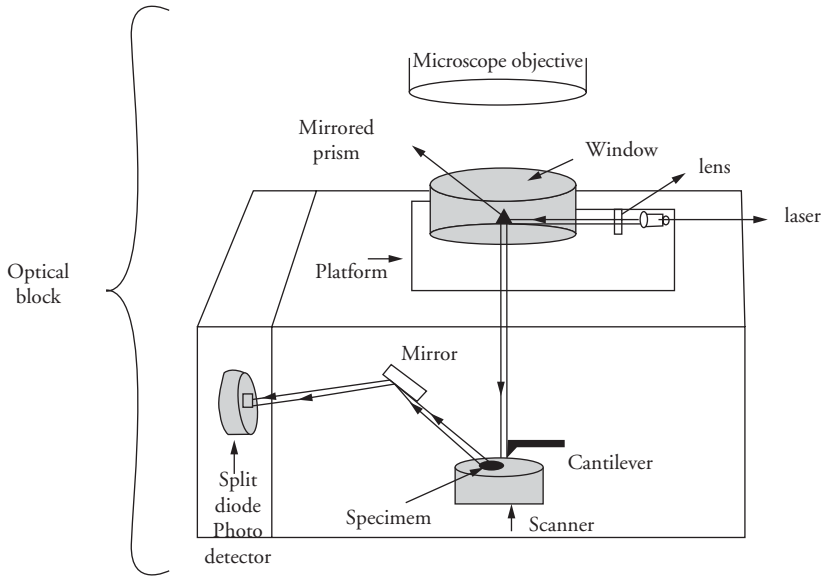


Figure 18.27 Schematic of AFM.

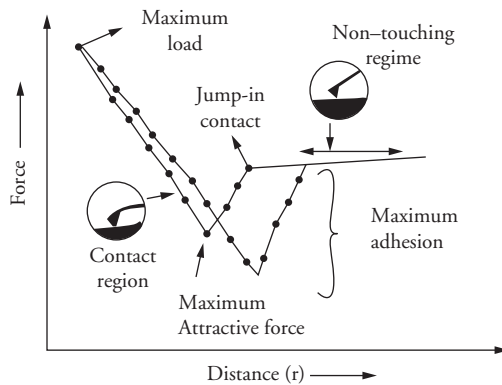


Figure 18.28 Force vs distance curve in AFM.

with the sample. As the sample further moves toward the tip, the cantilever is deflected (touching regime). In addition to the bending of cantilever, the tip and sample may undergo elastic (reversible) or plastic (irreversible) deformations (Figure 18.29).

The cantilever moves again with the sample when the sample is retracted from the tip in touching regime. This may result in deflection toward the sample before the tip breaks contact with sample due to adhesive and capillary forces. The capillary forces arise from the contamination liquid layer covering the sample surface. At the jump-out point (transition from touching to non-touching regime), the tip loses contact with sample surface, and the force vs. distance curve returns to the nontouching line. The difference between the minimum point of retrieval and the nontouching time is called pull-out force. In attractive force regime, the curve exhibits hysteresis, and the behavior of probe is influenced by long-range forces.

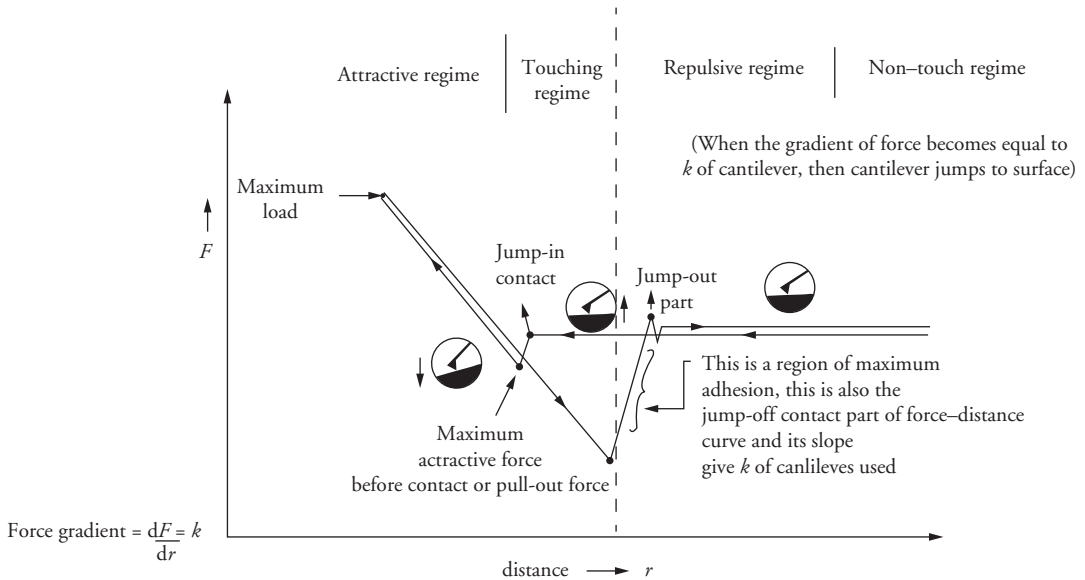


Figure 18.29 Magnified image for Figure 18.28.

Two forces that influence probe interaction with sample are as follows:

1. Short-range Forces

These forces are strongly repulsive at short distance and slightly attractive at long distance. This leads to sharp force vs. distance curve and endows the basis for high-resolution surface imaging in contact mode AFM. During scanning in contact-mode AFM, the tip moves laterally and the cantilever experiences vertical (normal) as well as lateral friction forces. The frictional forces are proportional to the load and scanning speed.

2. Long-range Forces

VanderWaal's (VDW) forces act between the bodies separated beyond the chemical bonding distance. VDW forces are important because depending on the shape of tip, the atoms at the tip apex experience strong repulsion and deformation due to VDW attractions. The VDW interactions between silica probe and metal surface immersed in various liquids is of the order of $1-10^4$ nN. Immersion of tip/sample system in high polar liquids is found to reduce VDW forces. For biological applications of AFM, it should be noted that in water many surfaces are charged. The surface charging is attracted to dissociation of surface groups on from adsorption of ions onto the surface. The surface charges attract other counterions, and form a double-layer near the surface.

Two other subsidiary forces due to short or long range interaction are as follows:

(a) Adhesive Forces

It is a consequence of long-range and short-range interaction. AFM measures the variation in local adhesion of the surface by studying the hysteresis of the force vs. distance curves.

(b) Capillary Forces

The tip apex is sometime coated by liquid contamination on the surface, hence forming a capillary between tip and sample. This gives rise to capillary force ($10-100$ nN). The capillary force increases pull-out force, and hence leads to additional load on the sample. Capillary forces should be negligible.

18.8.1 AFM Probes

The probes used for AFM measurements are cantilever integrated Si_3N_4 or silicon tip. The cantilevers are prepared with different lengths, thickness, and shapes. Their elastic constants vary in 0.01–50 N/m, range. The spring constant (k) of a cantilever is given by the following equation

$$k = \frac{Et^3b}{4L^3}$$

E → elasticity modulus

b → width of cantilever

t → thickness of cantilever

L → length of cantilever

The famous probe consist of Si_3N_4 triangular cantilever (200 μm length, 0.18 N/m) with integrated pyramids (2.9 μm height, $r < 20$ nm). Rectangular cantilevers ($k = 20$ N/m, Si) are used with integrated. Trans tip (10 μm height, $r < 10$ nm, Si).

The following points must be taken into account while designing cantilever.

1. The spring constant should be as small as possible to measure small forces.
2. Thermal excitations set the lower limit on spring constant.
3. The cantilever's resonance frequency should be higher than building and acoustic frequency

(~ kHz). Resonance frequency $\propto \sqrt{\frac{k}{m}}$.

4. Mass should be small for higher resonance frequencies.
5. The cantilever tip should be robust for contact applications.
6. Cantilever design depends on modes of operation and deflection system.

Silicon nitride probes are typically made using semiconductor photolithography techniques. Using it, a square opening is etched on SiO_2 film. The chemical etching of part of Si (100) wafer exposed through the square opening self-terminates at Si (111) planes leading to pyramidal pit. After removing SiO_2 protection layer, Si_3N_4 is deposited on wafer to form the shape of cantilever using lithographic method. All remaining silicon is etched away, and back of cantilever is coated with gold in order to reflect the laser beam. These probes are used for contact modes. Silicon probes are fabricated from single crystal silicon. Silicon tips are often conical in geometry with high aspect ratio. These are much sharper than Si_3N_4 but are easily broken. Silicon probes can dissipate charge much better than Si_3N_4 . They possess higher spring constant and higher resonant frequency. They are best suited for contact applications.

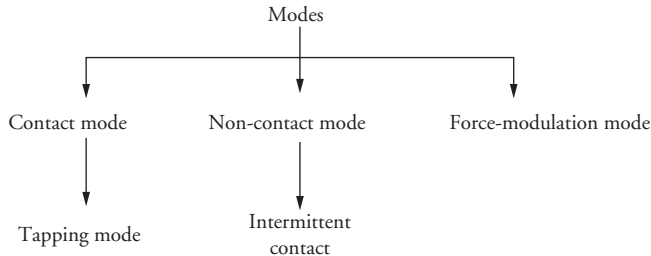
18.8.2 Selecting a Tip for Probe

Following points must be taken care of before selecting a tip for probe.

1. Tip radius should be minimum (2–60 nm radio).
2. Tips should image at much higher resolution than predicted by the geometries as most tips have defects on their surface. These defects interfere with the resolution.
3. If the sample is very flat, then the smaller radii of curvature of defect may image the surface.
4. For best resolution, sharp tips should be used but sharp tips are less durable and very expensive also.

18.8.3 Modes

The modes of operation for AFM are classified below, and we will be discussing them one by one.



1. Contact Mode (Tapping Mode)

In tapping mode, the tip is vertically oscillated at its resonant frequency. The sample approaches vibrating tip, lowering the vibrational amplitude. The tip makes soft physical contact with sample as it scans the surface. The changes in cantilever deflection are monitored with photodiode. Topography changes may occur due to constant force between tip and sample causing cantilever deflection (Figure 18.30). Topographic data are generated by two modes:

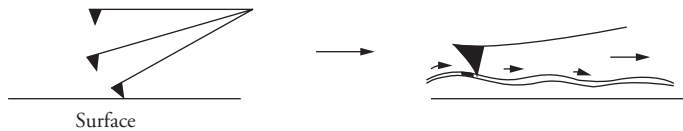


Figure 18.30 Contact mode.

- Constant height mode:** In this mode, the spatial variation of cantilever deflection is used to generate data. It is applicable for changing surfaces (speed is essential) or when cantilever deflections are small (atomically flat surface).
- Constant force mode:** In this mode, scanner motion generates image as scanner is moved up and down to keep cantilever deflection constant. This is preferred mode because feedback circuits limits the response time of circuit.

For the tip to penetrate contamination overlayer, application of rigid cantilever (Resonant frequency 300–400 kHz) and high operating amplitudes (10–100 nm) is required.

2. Noncontact Mode

In noncontact mode, the bottom-most point of each cycle is in attractive region of force–distance curve (Figure 18.31). Since long-range attractive forces do not exhibit sharp force vs. distance behavior, the spatial variation of Vander Waals' forces is very weak in noncontact mode and the operation must be carried out in ultrahigh vacuum by using mode techniques with frequency shift detection, long-range attractive forces are insensitive to a small change in tip–sample separation and hence the information for subnanometer scale cannot be collected.

In noncontact mode following points must be noted:

1. An oscillator drives the tip up and down. Furthermore the tip do not touch the surface, rather it oscillates upon the adsorbed fluid on the surface. This is also called intermittent contact and the bottom-most point is in repulsive region.
2. This mode studies soft and elastic samples because total force between tip and sample is very low (10–12 N). As the tip comes near the sample, the system detects variation in resonant frequency/vibration amplitude.

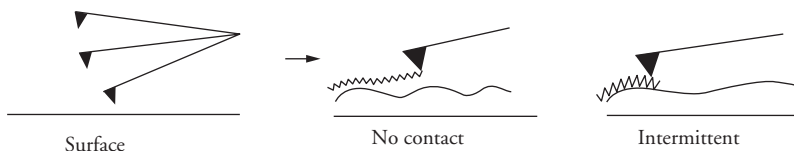


Figure 18.31 Non-contact mode.

3. Cantilever must be stiff as the force is low in non-contact regime so that they are not pulled into contact with sample surface. Moreover, more stiff cantilevers have high force constant.

(c) Force-Modulation Mode

In this mode, the tip does not leave contact with the surface at all during the oscillation cycle. This technique uses a much smaller amplitude of vibrating cantilever to prevent tip/sample disconnection. By measuring amplitude and phase shift of cantilever, one can detect spatial variation of elasticity of surface. In this technique, force is applied directly on the tip rather than modulating the cantilever. The frequency range is 10 Hz ~ 20 kHz ; sometimes, the tip is coated with magnetic material and external magnetic field is applied to produce modulation on tip surface. Force up to 1 nN is used in this technique.

18.8.4 Applications of STM/AFM

1. Surface Roughness measurement with spatial variations in the submicron range.
2. With STM, one can profile conducting samples and insulators coated with metallic over layer.
3. However tip/sample force interaction might introduce undefined changes to tip and sample geometry. Therefore, development of low current STM instrumentation is important. Therefore, AFM has broader applicability due to small, better controlled forces and rapid improvements in force sensors.

18.9 Nanophysics

Nanoscience is branch of physics that deals with the study of phenomena related to the object of size 1–100 nm (at least along one dimension). The applications features and characteristics of nanoparticles are different from that of macroscopic particles. Although classical description could not be applied to the nanoparticle, quantum mechanical approach is quite valid. It is a revolutionary field due to its technological and industrial applications. When we talk about nanotechnology, then it involves the study, synthesis, and processing of the structure at nanometer scale. Quantum

confinement and Gibbs–Thomson effects fall in this category. Basically, quantum confinement deals with the interaction of nanoparticles with bulk material resulting in electromagnetic as well as optical properties. Some structures such as carbon nanotubes follow lowering of melting point that is due to Gibbs–Thomson effect.

Many techniques are used to produce nanoparticles such as tip top down, lithography, etching, focused ion beam machining, and vapor deposition. For the study and observation of individual nanoparticles, following three techniques are vastly exploited. Hence, before we proceed for properties and other important aspect of nanotechnology, we should study the characterization techniques elaborately, that is, transmission electron microscopy, atomic force microscopy scanning probe microscopy, and scanning tunneling microscopy which are discussed in previous sections.

18.9.1 Different Types of Nanostructures

Nanoscience is an interdisciplinary field that involves the phenomena of chemistry, biology, physics, and materials. At the same time, nanotechnology describes the vast technology that could find potential applications in almost every aspect of science.

Nanostructures are indispensable part of nanotechnology. The objects whose size lies in between 0.1 nm and 1 μm are nanostructures. If we consider three-dimensional objects, then only one dimension may be satisfying the condition of nanostructure and other dimensions could be very large. Some of these nanostructures are described below:

1. Nanoparticles

Those particles whose dimensions are ≤ 100 nm are called nanoparticles. When some materials are converted to nanoparticles, many material properties get modified due to increased surface to volume ratio (discussed later). Some ultrafine particles exhibit size between 1 and 100 nm. Nanoparticles are of vast technological use for the scientific community. Further, if one dimension of material is in nanorange while other are still large, then the structure of material is said to be quantum well. If two dimensions of material get reduced to nanodimension, then the material structure is said to be quantum wire. When all three dimensions get reduced to nanosize, then it is said to be quantum dot. (Figure 18.32)

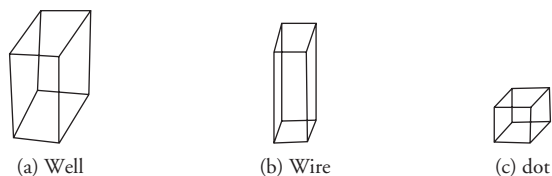


Figure 18.32 Various nanostructures.

2. Nanorods

These have at least two dimensions in the nanoscale range. These structures are produced from chemical synthesis. Most of the metals and semiconductors could be used to make nanorod. Diamond nanorods are produced, which is nanocrystalline form of carbon. This material is considered among one of hardest substance. Nanorods have wide range of applications such as display technologies, thin film-based computers, etc. The pixels involved for improving picture quality of television are also made up of nanorods.

18.10 Properties of Nanoparticles

Following are the important properties of nanoparticles.

1. Mechanical Properties

Nanostructured materials exhibit very high mechanical properties. When 2 nm Al_2O_3 is made to precipitate into thin films of pure nickel, then the yield strength increases from 0.15 to 5 GPa. Further, steel is known to be stronger than carbon. But when it comes to nanocylinders of carbon, it exhibits 100 times more strength than the steel.

2. Optical Properties

At nanoscale level, the color as well as transparency of the material changes. Most common examples are of gold silicon and zinc oxide. The nanoscale zinc oxide is transparent while in bulk and is white in color, whereas bulk gold is yellow in color and bulk silicon is dark gray in color. The main reason for change of optical properties of nanoparticles is the change in degree of freedom of electron motion. As the size of nanoparticles is very small; hence, they are not free to move and react differently with the light photons that result in different optical properties than the bulk material.

3. Chemical Properties

The surface area for nanoparticles is higher than the bulk material; hence, nanoparticles are more reactive. Especially, when the nanoparticles act as catalysts, then the chemical reaction activity increases. Moreover, nanoparticles exhibit higher average energy than the bulk atoms.

4. Electrical Properties

For nanoparticles, especially carbon nanotubes (CNTs), the conductivity is highly dependent upon the dimensions specially the cross-section area. We know that graphite that is allotropic form of carbon is a good conductor of electricity, but carbon nanotube can be conducting or semiconducting.

5. Biological Properties

Many revolutionary regimes have been explored using biotechnology and nanotechnology. The field of nanodrug delivery has been of wide applications. This field of medicine used nanoparticles for delivering target-oriented drug for this purpose; the cytocompatibility of nanoparticle is indispensable criteria.

6. Magnetic Properties

Nanoparticles exhibit higher magnetic interactions due to higher surface to volume ratio. Magnetic particles contain magnetic particles such as cobalt and iron, etc. Nanocomposite materials are also extensively investigated due to their various technological applications. These nanocomposite have high remanence. Magneto-restrictive materials also allow a wide variety of applications due to deformation of material on applying magnetic field. In the nanosize domain, magnetic nanoclusters couple their spins and combine to produce a single giant particle. This further gives rises to super-paramagnetism, that is, free rotation of giant ferromagnetic parameter at room temperature.

18.11 Surface Area/Volume Ratio

Nanomaterials have large surface area. If we consider a nanosphere of radius r , then its volume is $\frac{4}{3}\pi r^3$ and $4\pi r^2$ is the surface area.

Therefore,

$$\frac{\text{Surface area}}{\text{Volume}} = \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = \frac{3}{r} \quad (1)$$

When r decreases, then surface area increases. Due to increase in surface area, the nanoparticle becomes more reactive. As r approaches zero, surface-area-to-volume approaches infinity. There is critical radius r at which the surface to volume ratio is 3:2. The particles that are smaller than critical radius are called embryos and the particles with radius greater than critical radius are called nuclei.

18.12 Quantum Confinement/Electron Confinement

In bulk, the solid atoms exhibit splitting of energy levels and they form bands. Individual atoms exhibit discrete energy level. Quantum confinement effect is observed when the size of nanoparticle approaches magnitude of wavelength of electron. In the nanosize regime, nanoparticles exhibit different properties from the bulk materials. For the nanosize particles, the band gap decreases. The nanoparticle behaves when it is confined inside a box of confining dimensions. When the confining dimensions are comparable to wavelength of electron, then the energy of particle is fixed; or in other words, the energy spectrum is continuous. When the dimensions decrease and reach in nanoscale limit, then the energy levels turn to be discrete. That critical measurement where the energy levels turn to be discrete from continuous is called Bohr radius. Hence, electrons and holes are confined to Bohr radius. The band gap changes and hence the properties of nanomaterial change accordingly. For silicon and germanium, the confinement limit extends up to 6–7 nm.

18.13 Nanomaterials and Their Synthesis

Nanomaterials are the materials that have at least one dimension <100 nm. They have variety of applications. Nanomaterials are strong, ductile, water-resistant, chemically active, corrosion-resistant, and very hard. In the form of thin films or surface coatings, they are one dimensional in nature. Nanowires and nanotubes are two dimensional in nature. Quantum dots and colloids, etc., are three dimensional in nature. Nanometer-sized grains of nanocrystalline material fall in this category. The nanomaterials can be synthesized by using the following techniques.

18.13.1 Top-Down Approach

In this technique, the structures are miniaturized to nanoscale region. The most common technique adopted in top-down approach involves ball-milling and sol-gel processes as discussed below.

1. Ball-Milling

In this process, the materials are ground to yield fine particle with nanosize. For making such particles, mill is used as shown in Figure 18.33. Some of the materials yield highly nanocrystalline particles. During the process of ball-milling, the energy is imparted to samples due to collisions. The colliding balls trap the powder in between them and the compaction of particles start taking place. During the process of compaction of particles within the balls, the particles slide over each other such that they undergo fracture and deformation. This produces particles of irregular dimensions. Further, during next stages, particles undergo plastic and elastic deformation. Then, the particles undergo more

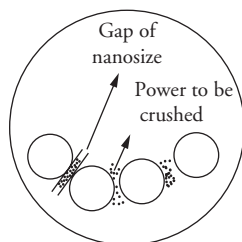


Figure 18.33 Ball-milling to obtain nanosized particle.

fragmentation, which reduces the particle size. Although ball-milling is the most commonly used technique to produce nanoparticles, it may cause contamination. The milling process may take up to 150 h to obtain uniform powder. Hence, ball-milling is a combination of many subprocesses, that is, grinding, deformation, mixing, and homogenization. Ball-milling processes have some demerits too, that is, ball-milling process may cause atomic defects. Further, the shape of nanoparticles may not be regular. Sometimes, the mixture obtained after ball-milling may have some amorphous powder in it.

2. Sol-Gel Synthesis

Sol-gel process deals high-purity nanoparticles. For sol-gel synthesis, suitable precursors such as acetates, carbonates, etc., are taken and mixed with deionized water. The chemical solution acting as precursor is known as sol, and the diphasic system consisting the solid and liquid phase is known as gel. When the gels are formed after mixing precursors and deionized water, then the gels are dried and they shrink. Hence, after drying, we get oxide polymer. This polymeric unit is usually three dimensional in nature, having interconnected porosity. Compared to the process of ball-milling, we get homogenized, uniform, and isotropic nanoparticles. The sol-gel process can be done at low temperatures and it produces large quantity of nanoparticles. Hence, the complete process of sol gel involves, mixing (to obtain sol), gelation, drying, polymerization (densification). Hence, sol-gel process has the following merits:

1. It can synthesize almost any material, along with that, it can cosynthesize two or more materials.
2. It can produce homogenous and uniform nanoparticles.
3. It can produce ultrapure nanoparticles.
4. Sol-gel process involves microscopic synthesis and polymerization.
5. It can produce large quantity at very economic level.

18.14 Bucky Balls and Fullerenes

We were familiar with two pure forms of carbon, that is, graphite and diamond were commonly known allotropes. Then, Richard Smalley, Robert Curl, and Harold Kroto discovered buckyballs or fullerene structures. Basically, fullerenes are a hollow cluster of 60 carbon atoms that are arranged in shape of soccer ball.

Carbon and graphite possess different structural arrangements hence different properties. Bucky balls possess very high stability. Different buckyballs with different number of carbon atoms have been discovered, for example C_{60} and C_{80} , etc. C_{60} buckyball possess the truncated polyhedrons shape,

that is, 12 pentagons surrounded by 5 hexagons. Buckyballs are quite resistant to the deformation. In other words, its characteristics are elastic in nature, that is, it regains its original shape when the external force is removed. Among other allotropes of carbons, buckyballs are comparatively soluble in water. The inside of fullerenes is hollow from inside; hence, they can accommodate some atom inside them. They have been of importance due to the following reasons:

1. They are used in field of medicine. They can act as drug carrier, and hence are very useful diagnostic tool.
2. In STM technique, the probe tip sometimes spoils and scratches the surface. Scientists are thinking of replacing the tip of probe with buckyball.
3. They are also considered potential candidates for lubrication and superconductivity. Further, they are also considered to activate many reactions by acting as catalysts.

R. Buckminster Fuller was born on July 12, 1895 in Milton, Massachusetts. His grandfather was the literary critic Margaret Fuller. Fuller had poor vision during his youth due to which he was out of the army in World War I, but the navy accepted him. In 1913, he graduated from Milton Academy. Then, he went to Harvard University where he was expelled in his first year as he was indisciplined. Then, his mother sent him for mechanic job in a cotton factory run by a distant relative in Sherbrooke, Quebec, Canada. The chief engineer was impressed by Fuller's ability and convinced him to keep a notebook of his design sketches. In 1914, Harvard University reinstated Fuller and then again expelled him officially in 1915 for bunking classes. In 1917, he married Anne Hewlett.



R.B. FULLER

18.15 Carbon Nanotubes

These are cylindrical structure of carbon atoms. In other words, it is cylindrical fullerene where carbon atoms are covalently attached to each other. The ends of CNTs can be open or closed and their length to diameter ratio can be greater than 1,000,000. Graphene is a two-dimensional allotrope of carbon, and CNT can be obtained by rolling the sheet of grapheme. CNT can be classified as single-walled CNT(SWCNT) or multiwalled CNT(MWCNT). Single-walled CNT can be obtained by rolling grapheme sheet, but multiwalled CNT is obtained by the coaxial assembly of SWCNT cylinders, that is, SWCNT cylinders, one within another. The separation between coaxial cylinders is of the order of interlayer distance between natural graphite. The following sections give more insight of CNTS.

18.15.1 Structure of CNTs

High-resolution techniques are required (discussed in early sections) to describe and explore the structure of CNT. The three nanotubes are commonly known, that is, zig-zag, chiral, and simple nanotubes. The shape of CNT depends on the way graphene sheet is rolled up. One of the structures is shown in Figure 18.34.

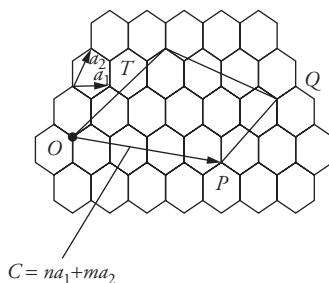


Figure 18.34 Chiral vector for CNT.

From Figure 18.34, it is clear that a_1 , and a_2 are the unit vectors of honeycomb structure. The points O and P are connected by vector C . By drawing normal to C , we obtain lines PQ and OT . When PQ and OT are superimposed, then properly capped nanotube is obtained. n and m decide the structure of CNT as follows:

- (i) If $n = m \rightarrow$ then the CNTs are called armchair.
- (ii) If $m = 0 \rightarrow$ then the CNTs are zig zag.
- (iii) If $n \neq m$, then the CNTs are called chiral.

18.15.2 Synthesis Techniques for CNTs

Three techniques that are widely used to study the structure of CNTs are given as follows:

- (i) **Chemical vapor deposition:** In this method, pure carbon fibers are produced by vapor decomposition of hydrocarbon. A substrate layer of metal particles (Ni, Fe, Co, etc.) is prepared. MWCNTs require inert gas atmosphere at temperature of 300–800°C. SWCNT are produced at high temperature with mixture of four and inert gas such as argon. The inlet is provided which supplies carbon containing gases such as acetylene and ethylene. Upon heating in furnace, the thin film of carbon gets deposited on the substrate containing metal particles. This technique produces bulk quantities of CNTs.
- (ii) **Laser vaporization technique:** Upon focusing laser on graphite, the carbon atoms become free, which are further used for fabricating CNTs. For laser vaporization technique, graphite is kept in quartz tube and the furnace is kept at 1200°C. During the process, inert gas such as argon or helium is used. Copper collector is used at one end, which is cooled by water. On the other end, laser is used, when laser is incident on graphite, then carbon is liberated and moves toward cold region (copper collector). When they move toward cold region, they condense and form CNTs (≈ 10 – 20 nm in diameter).
- (iii) **Carbon arc discharge:** This technique uses two graphite electrodes, in inert atmosphere of helium. Direct current is passed through these electrodes. Graphite anode is consumed and the carbon gets deposited on the cathode. Two shells of carbon are deposited on cathode, that is, outer hard gray shell and inner soft black shell and the inner shell forms MWCNTs. For SWCNT, small amount of metal particles such as Fe, Co, Ni, etc., are incorporated inside the electrode.

18.15.3 Properties of CNTs

1. They are very strong and have high Young's modulus than steel.
2. They have covalent bonds, hence they keep on vibrating.
3. MWCNT's inner shell slide without friction. Hence, this constitutes perfect rotational bearing.
4. The thermal conductivity is very high due to good vibrational properties of CNTs
5. They have minimum defects, hence high electrical conductivity.

SUMMARY

This chapter deals with the characterization techniques such as transmission electron microscopy, scanning probe microscopy, scanning tunneling microscopy, and atomic force microscopy. Transmission electron microscopy is used to determine the lattice fringing and planar structure of materials scanning probe microscopy provides direct relation between structure and material properties. STM allows us to determine the structure of surfaces with a spatial resolution on angstrom scale. It also provides real-space visualization of surfaces on atomic scale. Nanophysics deals with the phenomena related to the objects of size 1–100 nm. Nanostructures are of different types. When one dimension of material is in nanorange, while others are still large, then the material structure is quantum well. If two dimensions of materials get reduced to nanodimension, then the material is a quantum wire. When the three dimensions are reduced to nanoise, then it is quantum dot. Nanostructures are more strong than material itself. Nanomaterials have large surface area. The surface-area-to-volume ratio is $3/r$. The critical radius r at which the surface to volume ratio is 3:2. Quantum confinement is observed when the size of nanoparticles approaches the magnitude of wavelength of electron. Nanomaterials are synthesized using top-down approach, ball-milling, and sol-gel synthesis. Apart from diamond and graphite, carbon possesses buckyball structures. Basically, fullerene/buckyball structures have 60 carbon atom arranged in shape of soccer ball. Buckyballs are used in the field of medicine and they act as drug carrier. Carbon nanotubes are cylindrical structures of carbon atoms. Graphene is 2-D allotrope of carbon and CNT can be obtained by rolling grapheme sheet.

OBJECTIVE QUESTIONS

1. Which of the following is signal generated by X-rays?
 - (a) Back-scattered beam
 - (b) Secondary electrons and Bremsstrahlung radiations
 - (c) Anger electrons and characteristic X-rays
 - (d) All of the above
2. In thermionic sources,
 - (a) electrons are produced by heating.
 - (b) electrons are produced by electric-field.
 - (c) electrons are produced by light.
 - (d) electrons are produced by X-rays.
3. In field-emission sources, electrons are produced by
 - (a) heating
 - (b) electric field
 - (c) light
 - (d) X-rays

4. According to Richardson's law,

(a) $J = CT^2$
 (c) $J = CT^2 e^{-\phi/k_B T}$

(b) $J = CT^2 e^{\phi/k_B T}$
 (d) $J = e^{\phi/k_B T}$

5. Tungsten has high melting temperature of 3660 K (Yes/No).

6. LaB_6 crystals are grown in

- (a) $\langle 111 \rangle$ plane
 (c) $\langle 311 \rangle$ plane

- (b) $\langle 112 \rangle$ plane
 (d) $\langle 110 \rangle$ plane

7. Which of the following is used for triode gun?

- (a) Tungsten
 (c) Both (a) and (b)

- (b) LaB_6
 (d) None of these

8. Which of the following is true?

- (a) For LaB_6 filaments, it is preferable to operate below saturation.
 (b) LaB_6 is susceptible to thermal stress.
 (c) LaB_6 has low work function.
 (d) All of the above.

9. The field radius for tungsten wire is

- (a) $0.2 \mu\text{m}$
 (c) $< 0.1 \mu\text{m}$

- (b) $0.5 \mu\text{m}$
 (d) $0.3 \mu\text{m}$

10. The tip in FEG guns is cleaned by

- (a) flashing
 (c) annealing

- (b) owenching
 (d) all of these

11. Operating temperature in field emission guns is

- (a) 2700 K
 (c) 1700 K

- (b) 300 K
 (d) 2000 K

12. The life-time of tungsten pin is

- (a) 100 h
 (c) 500 h

- (b) 40 - 50 h
 (d) > 1000 h

13. The energy spread for field-emission gun is

- (a) 0.3 eV
 (c) 5 eV

- (b) 3 eV
 (d) 10 eV

14. The brightness of electron beam is given by

(a) $B = \frac{I_E}{\pi d \alpha}$

(b) $B = \frac{\pi d \alpha}{I_E}$

(c) $B = \frac{4 I_E}{(\pi d \alpha)^2}$

(d) $B = \frac{(\pi d \alpha)^2}{4 I_E}$

15. The coherence length for energy spread is

- (a) $\frac{v\hbar}{\Delta E}$ (b) $\frac{\Delta E}{v\hbar}$
 (c) $\frac{v}{\Delta E}$ (d) $v\hbar\Delta E$

16. The effective source size d_c for coherent illumination is

- (a) $\frac{\lambda}{\alpha}$ (b) $\frac{\lambda}{2\alpha}$
 (c) $\frac{\lambda}{3\alpha}$ (d) λ

17. The operation of TEM can occur in parallel beam mode or convergent beam mode. (True/False)

18. Which defect does not hinder the working of parallel-beam formation?

- (a) Spherical aberration (b) Chromatic aberration
 (c) Astigmatism (d) All of these

19. The minimum resolvable distance for spherical aberrations

- (a) $r_{\min} = \frac{\lambda}{L_s}$ (b) $r_{\min} = 0.91(L_s\lambda^3)^{1/4}$
 (c) $r_{\min} = (L_s)^{1/4}$ (d) $r_{\min} = (L_s\lambda)^{1/4}$

20. The optimum probe size for TEM is

- (a) $(\lambda L_s^3)^{1/4}$ (b) $\left(\frac{\lambda}{L_s}\right)^3$
 (c) $0.77\left(\frac{\lambda}{L_s}\right)^{1/4}$ (d) $0.77(\lambda L_s)^{1/4}$

21. The radius of chromatic disk is given by

- (a) $r_{\text{chr}} = \frac{\Delta E}{E_0}$ (b) $r_{\text{chr}} = L_c \frac{\Delta E}{E_0} \alpha$
 (c) $r_{\text{chr}} = \frac{E_0}{\Delta E} \alpha$ (d) $r_{\text{chr}} = 0.91(L_2\lambda^3)^{1/4}$

22. For reducing chromatic aberration, the specimen should be very thick. (True/False)

23. The distortion due to astigmatism is given by

- (a) $\alpha \Delta f$ (b) $\frac{\alpha}{\Delta f}$
 (c) $\frac{\Delta f}{\alpha}$ (d) $(\alpha \Delta f)^2$

24. In case of astigmatism, the image is

- (a) circular (b) cylindrical
(c) elliptical (d) conical

25. TEM operation requires _____ lens.

- (a) optical (b) magnetic
(c) colored (d) all of these

26. Which of the following constitute the imaging system?

- (a) Selected area diffraction (b) Bright-field imaging
(c) Dark-field imaging (d) All of the above

27. The detection quantum efficiency is given by

- (a) $\left[\frac{\left(\frac{S_{out}}{N_{out}} \right)}{\left(\frac{S_{in}}{N_{in}} \right)} \right]^2$ (b) $\left[\frac{\left(\frac{S_{in}}{N_{in}} \right)}{\left(\frac{S_{out}}{N_{out}} \right)} \right]^2$
(c) $\left[\frac{S_{in}}{S_{out}} \right]^2$ (d) $\left[\frac{N_{in}}{N_{out}} \right]^2$

28. For perfect detector, DQE is

- (a) <1 (b) 2
(c) 1 (d) 0

29. Phosphorescence is

- (a) light emission (b) delayed light emission
(c) rapid emission (d) none of these

30. Semiconductor detectors are sensitive to electrons of energy

- (a) 2 keV (b) >5 keV
(c) 0.5 keV (d) 3 keV

31. Semiconductor detectors have poor DQE. (True/False)

32. YAG (Yttrium aluminum Garnet) cannot be used as a scintillating material. (True/False)

33. What is DQE of scintillator detector?

- (a) 0.5 (b) 1
(c) 0.1 (d) 0.9

34. Electro polishing can be done for
- (a) ceramic samples
 - (b) glass samples
 - (c) alloys
 - (d) insulators
35. In twin-jet electropolishing, the sample is held between
- (a) metal holders
 - (b) ceramic holders
 - (c) alloy holders
 - (d) teflon holders
36. For ion-milling _____ accelerating voltage is used.
- (a) 10 keV
 - (b) 4–6 keV
 - (c) 2 keV
 - (d) 15 keV
37. For measurable tip and sample interaction, the tip and sample should be
- (a) placed close
 - (b) kept at a distance $\sim 0.5 \mu\text{m}$
 - (c) kept at a distance $\sim 0.8 \mu\text{m}$
 - (d) kept at a distance $\sim 10 \mu\text{m}$
38. For Schottky emission, the up-sample separation is
- (a) 100 nm
 - (b) 0.5–1 nm
 - (c) 1–2 nm
 - (d) 10 μm
39. The common tunneling current is
- (a) 100 A
 - (b) 0.5–1 mA
 - (c) 0.1–40 nA
 - (d) 100 nA
40. The typical values of bias voltage are
- (a) 10 V
 - (b) 0.001–5 V
 - (c) 5–8 V
 - (d) 100 V
41. The SPM can measure differences in height up to
- (a) 200 pm
 - (b) 135 pm
 - (c) 250 pm
 - (d) 100 pm
42. In optical deflection technique, the noise is almost
- (a) 150 pm D.C.
 - (b) 200 pm D.C.
 - (c) 100 pm D.C.
 - (d) 500 pm D.C.
43. Which of the following is true?
- (a) Piezoresistivity yields 10 pm AC noise.
 - (b) Piezoresistivity is suitable for low temperatures.
 - (c) Piezoresistivity gives low DC force resolution.
 - (d) All of the above

44. The spring constant for AFM probe is given to be

$$(a) \quad k = \frac{E t^3 \omega}{4 L^3}$$

$$(b) \quad k = \frac{4 L^3}{E t^3 \omega}$$

$$(c) \quad k = \frac{4 L^3 E}{t^3 \omega}$$

$$(d) \quad k = \frac{t^3 \omega 4 L^3}{E}$$

45. The Si_3N_4 triangular cantilever has

(a) tetrahedral tip

(b) pyramidal tip

(c) spherical tip

(d) rectangular tip

46. Tapping and intermittent made are noncontact modes. (True/False)

47. For noncontact mode, the force between tip and sample is

(a) 50 N

(b) 20 – 30 N

(c) 10 – 12 N

(d) 1 N

48. The nanophysics deals with objects of dimension:

(a) 1 – 10 nm

(b) 1 – 10 μm

(c) 1 – 100 nm

(d) > 200 nm

49. Nanostructures have dimensions between

(a) 0.1 and 1 μm

(b) 1 and 100 nm

(c) > 100 nm

(d) < 1 nm

50. Carbon nanocylinders are 100 times weaker than the steel. (True/False)

51. Optical properties of nanoparticles are due to change in degree of freedom of electron motion (True/False).

52. The nanoparticles are more reactive than the bulk material because

(a) they act as catalysts.

(b) their surface area is more than bulk materials.

(c) both (a) and (b)

(d) none of these

53. The surface area/volume ratio for nanoparticles varies as

$$(a) \quad \frac{1}{r^2}$$

$$(b) \quad \frac{3}{r}$$

$$(c) \quad \frac{5}{r^3}$$

$$(d) \quad r$$

54. C_{60} buckyball possesses
(a) tetrahedral shape (b) octahedral shape
(c) spherical shape (d) truncated polyhedron.
55. For arm-chair CNTs,
(a) $n = m$ (b) $n = 0$
(c) $m = 0$ (d) $n \neq m$
56. For chiral CNTs,
(a) $n = m$ (b) $n = 0$
(c) $m = 0$ (d) $n \neq m$
57. During chemical vapor deposition technique, the temperature should be
(a) $800 - 1000^\circ\text{C}$ (b) $1500 - 2000\text{\AA}$
(c) $300 - 800^\circ\text{C}$ (d) $1000 - 1500\text{\AA}$
58. During laser vaporization technique, the temperature should be
(a) 1200°C (b) 1500°C
(c) 2000°C (d) 2200°C

Answers

- | | | | |
|------------|-------------|-------------|---------|
| 1. (d) | 18. (a) | 35. (d) | 52. (c) |
| 2. (a) | 19. (b) | 36. (b) | 53. (b) |
| 3. (b) | 20. (c) | 37. (a) | 54. (d) |
| 4. (c) | 21. (b) | 38. (a) | 55. (a) |
| 5. (Yes) | 22. (False) | 39. (a) | 56. (d) |
| 6. (d) | 23. (a) | 40. (b) | 57. (c) |
| 7. (c) | 24. (c) | 41. (b) | 58. (a) |
| 8. (d) | 25. (b) | 42. (c) | |
| 9. (c) | 26. (d) | 43. (d) | |
| 10. (a) | 27. (a) | 44. (a) | |
| 11. (b) | 28. (c) | 45. (b) | |
| 12. (b) | 29. (b) | 46. (True) | |
| 13. (a) | 30. (b) | 47. (c) | |
| 14. (c) | 31. (True) | 48. (c) | |
| 15. (a) | 32. (False) | 49. (a) | |
| 16. (b) | 33. (d) | 50. (False) | |
| 17. (True) | 34. (c) | 51. (True) | |

Micro-Assessment Questions

1. What is electron microscopy?
2. What are electron sources for TEM?
3. What is the brightness for electron gun?
4. What is the temporal coherence and energy spread of electron beam?
5. What is the lens defect for TEM?
6. What do you understand by spherical aberration?
7. What is chromatic aberration?
8. What is astigmatism?
9. What is the display system for TEM?
10. What is electropolishing?
11. What is spring constant for AFM?
12. What is contact mode of AFM?
13. What is noncontact mode for AFM?
14. What is the resolution mode for AFM?
15. Explain the term “nanaoscience.”
16. What are nanoparticles?
17. What is topdown technique?

Critical Thinking Questions

1. Give the principle of TEM.
2. Write down the principle of AFM.
3. What do you understand by thermionic emission?
4. List the various thermionic sources.
5. Show schematically the signals produced by X-ray beam.
6. Why are lanthanum hexaboride filaments used in electron gun?
7. Show the schematic representation of electron gun.
8. Explain in detail the field emission sources.
9. Explain the characteristics for electron beams.
10. Explain the spatial coherency and source size for the beam.
11. What is the operating voltage for TEM?
12. Give the operation of TEM in terms of parallel and convergent beam mode.
13. Explain the focusing of lens.
14. What is the difference between spherical and chromatic aberration?
15. How can information system be calibrated?
16. Explain the objective lens for TEM. Why is it known as magnetic lens?
17. What is selected area diffraction pattern? Explain in detail.
18. What is the bright and dark field for TEM?
19. Explain the process of ion-milling.
20. Give the operating principle of SPM.
21. What is tip-sample approach?
22. What are different scanning parameters and modes for SPM?

23. Give the properties for STM tips.
24. Explain the effect of bias voltage on STM working.
25. What are the various modes of operation for STM?
26. List the advantages and disadvantages of SPM.
27. What is atomic force microscopy?
28. Describe the AFM probes in detail with their properties.
29. What is the criterion of selection of a tip for probe?
30. List the various resolution issues for AFM.
31. What is pixelization for AFM?
32. What is the difference between nanoparticles and nanorods?
33. Define surface area/volume ratio for nanoparticles.
34. Explain the quantum confinement.
35. What is the principle behind sol-gel synthesis?
36. How does ball-milling reduce particle size?
37. What are buckyballs/fullerene structures?
38. List the various properties of CNTs.

Graded Question

1. Give the detailed construction of transmission electron microscope.
2. Give the detailed working of atomic force microscopy.
3. Give the detail, the various types of defects in the lens system for TEM.
4. What are the various detectors used in TEM system? Explain in detail.
5. Explain the specimen preparation for the TEM investigation.
6. Give the operation and working of SPM.
7. Give the principle and methodology for STM.
8. Explain the electron transfer process and tunneling for STM.
9. Describe the construction of STM.
10. Explain the detailed principle of AFM.
11. List the various forces that influence probe interaction with sample.
12. What are the various modes of operation of AFM?
13. List the different types of nanostructures.
14. Give in detail the various properties of nanoparticles.
15. What are the various techniques, which are used to synthesize the nanomaterials?
16. What are carbon nanotubes? Give the structure of CNTs in detail.
17. Write down the synthesis techniques for CNTs.

Remember and Understand

1. In TEM, electrons are accelerated through potential V , and hence electrons can gain momentum as well as kinetic energy.
2. There are two types of electron sources, that is, thermionic emission and field emission. In thermionic emission, the electrons are produced by heating; whereas in field emission, the electrons are produced by intense electron beam.

3. There are two modes of operation for TEM: parallel beam mode and convergent beam mode.
4. To look at the diffraction pattern obtained from TEM, we use SAED aperture into the image plane of objective lens. To look at the image, SAED aperture is removed and objective aperture is introduced.
5. Scanning probe microscopy gives the relation between the structure and material properties. The sample surface is scanned with the sharp probe at a distance of less than few nanometers. For scanning, either the tip moves against the fixed sample or vice versa.
6. Scanning tunneling microscopy allows determining the structure of surface with spatial resolution on angstrom scale. It gives real-space visualization of surface on atomic scale.
7. STM tips must be monoatomically sharp apex, which could be prepared by field ion microscope. Tips are also prepared by mechanical cutting and electrochemical etching of wires.
8. Nanoscience deals with the study of phenomena related to the objects of size 1–100 nm. The properties of nanoparticles are different from that of macroscopic particles.
9. The particles with dimension less than 100 nm are called as nanoparticles. Nanorods have at least two dimensions in nanoscale range.
10. Nanoparticles have very high mechanical strength. The color as well as the transparency of material changes at nanoscale region. The surface area for nanoparticles is higher than the bulk material, hence they are more reactive.
11. Quantum confinement effect is observed when the size of nanoparticle approaches magnitude of wavelength of electron. In the nanoparticle regime, nanoparticles exhibit different properties from bulk materials.
12. Ball-milling and sol-gel synthesis are the most common techniques used for the synthesis of nanoparticles. In ball-milling, the materials are ground to yield fine particles. Sol-gel method gives high-purity nanoparticles. For sol-gel synthesis, suitable precursors are used.
13. Fullerenes are hollow clusters of 60 carbon atoms, which are arranged in shape of soccer ball. C_{60} buckyballs possess the truncated polyhedron shape.
14. Carbon nanotubes are cylindrical structures. It is cylindrical fullerene where the carbon atoms are covalently attached to each other. CNTs are classified as single-walled and multiwalled CNT.

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