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**APPLIED PHYSICS FOR COMPUTER SCIENCE AND
ENGINEERING**
A SHORT NOTES - FIRST EDITION

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Part I

MODULE 1 : LASER AND OPTICAL FIBERS

Chapter 1

LASER

1.1 Introduction

LASER is an acronym for Light Amplification by Stimulated Emission of Radiation. The first LASER was built by Theodore H Maiman in the year 1960. Thus it finds various applications starting from industries to communication.

1.2 Characteristics of a LASER beam

The LASER beam has the following four characteristics.

1. LASER beam is highly monochromatic.
2. LASER beam is highly coherent.
3. LASER beam is highly directional.
4. LASER is a high intensity beam of light.

1.3 Interaction of radiation with matter

The interaction between radiation and matter occurs through the following three processes.

1. Induced absorption
2. Spontaneous emission
3. Stimulated emission

1.3.1 Induced Absorption

When a photon of right energy is incident on the atom then the photon is absorbed. This process is induced by the photon and hence it is called Induced Absorption.

Consider an atom in a lower energy states E_1 , it will excite to higher energy states E_2 by absorbing the incident photon of energy $E = h\nu = E_2 - E_1$. Here E_1 energy of the lower energy state, E_2 is the energy of the higher energy state, h is the Planck's constant ν is the frequency of photon.

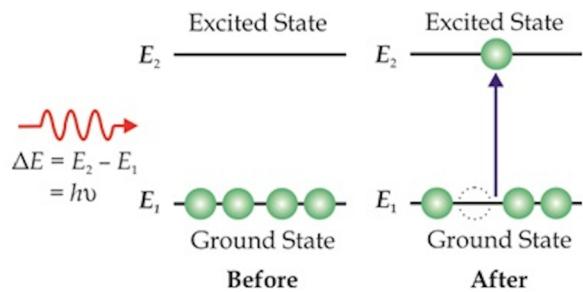


Figure 1.1: Induced absorption

1.3.2 Spontaneous Emission

Spontaneous emission is the process of emission of photon, when an atom transits from higher energy level to lower energy level without the influence of any external energy.

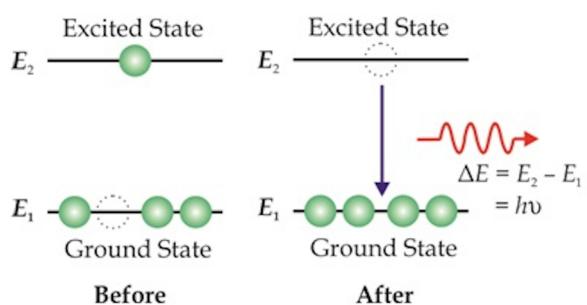


Figure 1.2: Spontaneous emission

An electron in the higher energy state of an atom makes a transition to lower energy state without the action of any external agency. the energy of the photon emitted is given by $E = h\nu = E_2 - E_1$. In this process the emitted photons need not travel in the same direction. Thus the light beam is not directional.

1.3.3 Stimulated Emission

When a photon of suitable energy interacts with an atom in the higher energy state then the atom is stimulated (Forced) to make transition from higher energy state to a lower energy state with the emission of a photon. Both the incident photon and the emitted photons are coherent and travel in the same direction. Thus the process is called stimulated emission.

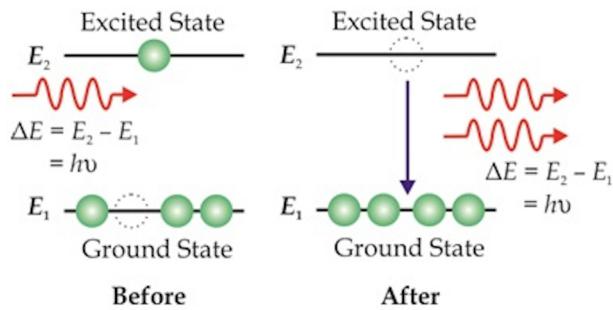


Figure 1.3: Stimulated emission

When a photon of energy $h\nu = E_2 - E_1$ interacts with an atom in the higher energy state the stimulated emission takes place with the emission of two photons of same energy that are highly directional and coherent. Thus stimulated emission could be used to generate a highly coherent directional beam of light.

1.4 Einstein's A and B co-efficients and expression for energy density

Consider a system containing N atoms and is under thermal equilibrium. Let E_1 and E_2 be the lower and higher energy levels that contain N_1 and N_2 number of atoms respectively. Let the incident energy density of the radiation be E_ν . Hence the system absorbs and emits the energy through the following processes. The energy of the photons absorbed and emitted by the atoms is $E = h\nu = (E_2 - E_1)$

Rate of induced absorption

The rate of induced absorption is defined as the number of induced absorption per second per unit volume in unit time. Rate of absorption depends on

1. Number of atoms in the lower energy state N_1 .
2. The incident energy density E_ν .

Hence

1. Rate of Induced absorption $\propto N_1 E_\nu$

2. Rate of Induced absorption $= B_{12} N_1 E_\nu$

Here B_{12} is proportionality constant called Einsteins coefficient of Induced absorption.

Rate of spontaneous emission:

The number of spontaneous emission per unit volume in unit time is called rate of spontaneous emission. Rate of spontaneous emission depends on

Since spontaneous emission is a voluntary process it is independent of energy density E_ν . The rate of spontaneous emission depends only on the number of atoms in the higher energy state N_2 . Thus

1. Rate of spontaneous emission $\propto N_2$
2. Rate of Spontaneous emission $= A_{21} N_2$

Here A_{21} is the proportionality constant called Einstein's co-efficient of spontaneous emission.

Rate of stimulated emission

The number of stimulated emission per unit volume in unit time is called rate of stimulated emission. Rate of stimulated emission depends upon,

1. Number of atoms in the higher energy state (N_2)
2. The energy density (E_ν).

Hence

1. The Rate of stimulated emission $\propto N_2 E_\nu$
2. Rate of stimulated emission $= B_{21} N_2 E_\nu$

Here the proportionality constant called B_{21} is Einstein's coefficient of stimulated emission.

Under Thermal Equilibrium the total Energy of the System remains unchanged. Hence Rate of Absorption is equal to rate of emission.

\therefore Rate of Induced Absorption = [Rate of Spontaneous emission + Rate of Stimulated Emission]

\therefore

$$B_{12} N_1 E_\nu = A_{21} N_2 + B_{21} N_2 E_\nu \quad (1.1)$$

$$(B_{12} N_1 - B_{21} N_2) E_\nu = A_{21} N_2$$

$$E_\nu = \frac{A_{21} N_2}{B_{12} N_1 - B_{21} N_2} \quad (1.2)$$

$$E_\nu = \frac{A_{21}}{B_{12} \frac{N_1}{N_2} - B_{21}} \quad (1.3)$$

$$E_\nu = \frac{A_{21}}{B_{21}} \left[\frac{1}{\frac{B_{12}}{B_{21}} \frac{N_1}{N_2} - 1} \right] \quad (1.4)$$

According to Boltzmann relation the we have

$$\frac{N_2}{N_1} = e^{-\frac{h\nu}{kT}} \quad (1.5)$$

or we can re-write as,

$$\frac{N_1}{N_2} = e^{\frac{h\nu}{kT}} \quad (1.6)$$

Here h is the Planck's constant, c is the speed of light in vacuum, λ is the wavelength of the photon, k is the Boltzmann constant and T is the absolute temperature. Substituting for $\frac{N_1}{N_2}$ in equation 1.4

$$E_\nu = \frac{A_{21}}{B_{21}} \left[\frac{1}{\frac{B_{12}}{B_{21}} \left(e^{\frac{h\nu}{kT}} \right) - 1} \right] \quad (1.7)$$

According to Planck's radiation law, the equation for energy density in the frequency domain is given by

$$E_\nu = \frac{8\pi h\nu^3}{c^3} \left[\frac{1}{e^{\frac{h\nu}{kT}} - 1} \right] \quad (1.8)$$

on comparing equations 1.7 and 1.8 we can get

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3}{c^3} \quad (1.9)$$

and

$$\frac{B_{12}}{B_{21}} = 1 \quad (1.10)$$

or $B_{12} = B_{21}$

This means that Probability of Induced absorption is equal to Probability of Stimulated emission. Hence A_{21} & B_{21} can be replaced by A & B . Thus equation 1.7 could be written as

$$E_\nu = \frac{A}{B} \left[\frac{1}{e^{\frac{h\nu}{kT}} - 1} \right] \quad (1.11)$$

Hence the expression for energy density in terms of Einstein's co-efficient A and B .

1.5 LASER Action and the Conditions for LASER action

Consider a LASER system. Let an atom in the excited state is stimulated by a photon of right energy so that atom makes stimulated emission. Two coherent photons are obtained. These two coherent photons if stimulate two atoms in the excited state to make emission then four coherent photons are emitted. These four coherent photons stimulate 4 more atoms in the excited state resulting in 8 coherent photons and so on. As the process continues number of coherent photons increases. These coherent photons constitute an intense beam of LASER. This phenomenon of building up of number of coherent photons so as to get an intense LASER beam is called lasing action.

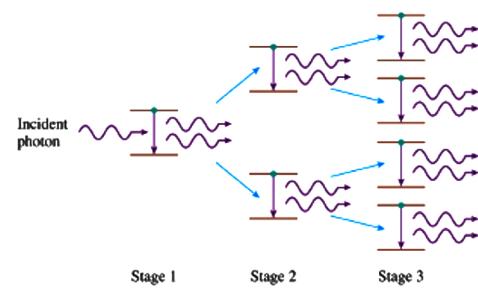


Figure 1.4: LASER action

LASER action could be achieved through the conditions population inversion and meta-stable state.

1.5.1 Population Inversion and Pumping

If a system is under thermal equilibrium the number of atoms in excited state is less than the number of atoms in the lower energy state. For the production of LASER number of stimulated emission must be more when compared to induced absorption and spontaneous emission. This is possible only if the number of atoms in the higher energy state is more than the number of atoms in the lower energy state and is called population inversion. The means of achieving population inversion by supplying energy from a suitable source is called Pumping. In addition,to have more stimulated emissions, the life time of atoms in the excited state must be longer. Thus the essential conditions for population inversion are

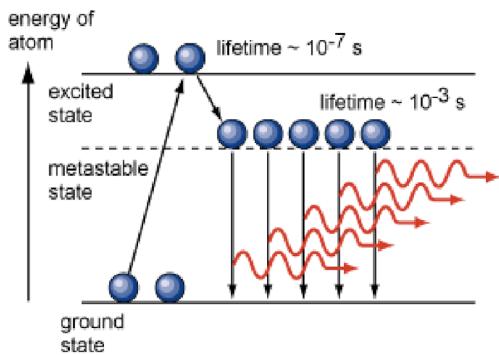
1. Higher energy state should posses a longer life time.
2. The number of atoms in the higher energy state must be greater than the number of atoms in the lower energy state.

1.5.2 meta-stable state

The life time of an energy level is of the order of 10^{-8} second. If an atom posses unusual longer life time in an energy state such a state is referred to as a meta-stable state. Usually the life time of meta-stable state varies from 10^{-2} s to 10^{-3} s. Population inversion could be achieved with the help of three energy state with one of them a meta-stable state and is as shown in the figure 1.5. The population inversion is achieved between the state E_2 and E_1 as state E_2 is a meta-stable state.

Note : The principles of Laser are

1. Stimulated Emission
2. Population Inversion
3. meta-stable State

Figure 1.5: Population inversion, E_2 is meta-stable state

1.6 Requisites of a LASER system

The three requisites of a LASER system are,

1. Excitation source for pumping action
2. Active medium that supports meta-stable states
3. LASER cavity

1.6.1 Energy Source or Pumping Mechanism

In order to achieve population inversion more and more atoms are to be moved to higher energy state and is called pumping. This is achieved by supplying suitable energy using an energy source. If optical energy is used then the pumping is called optical pumping and if electrical energy is used then the pumping is called electrical pumping.

1.6.2 Active medium

Population inversion occurs at certain stage in the active medium due to the absorption of energy. The active medium supports meta-stable states. After this stage the active medium is capable of emitting LASER light.

1.6.3 Resonant cavity (or) LASER cavity

The LASER Cavity consists of an active medium bound between two highly parallel mirrors. The reflection of photons from the mirrors results in multiple traverse of photons through the active medium inducing more and more stimulated emissions. Thus amplification of light is achieved. This also helps to tap certain permissible part of LASER energy from the active medium. The cavity resonates and the output will be maximum when the distance L between the mirrors is equal to an integral multiple of $\frac{\lambda}{2}$. Here λ is the wavelength of incident suitable radiation. The length of the LASER cavity is expressed as

$$L = \frac{n\lambda}{2} \quad (1.12)$$

1.7 Semiconductor LASER or Diode LASER

Introduction

Semiconductor diode LASER is an LED with heavily doped P and N sections. First semiconductor LASER was fabricated in 1962 using *Ga – As* by *Hall* with his co-workers. It is a low cost and high efficiency LASER.

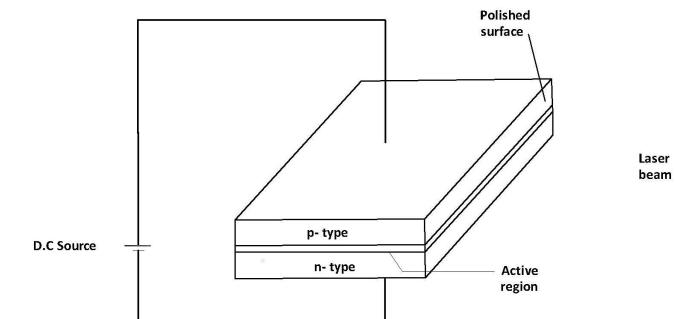
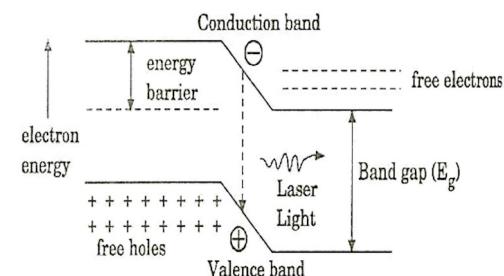


Figure 1.6: Semiconductor Diode LASER

Construction

Construction

The *Ga – As* LASER diode belongs to direct band gap semiconductors. The *n*-section is derived by doping the substrate with *Tellurium* and *p*-section is derived by doping the substrate with *Zinc*. The diode used is in the form of a cube with dimension 0.4 mm. The depletion region is of thickness 0.1 micrometer and lies horizontal as shown in the figure 1.6. The current is passed through the ohmic contacts provided to the top and bottom faces. The front and back faces are polished and made highly parallel to each other to have a LASER cavity. The other two faces are roughened.



Working

The Diode is forward biased using an external source. Therefore electrons and holes flow across junction. Hence

the current flows through the diode. When a hole meets an electron it recombines with electron emitting a photon. This could be considered as the transition of electron from conduction band to valence band. When the current is low spontaneous emission is predominant. If the current is sufficiently high population inversion is achieved. The photons liberated initially due to spontaneous emissions induce further stimulated emissions. The LASER cavity helps in the amplification of light. Finally this results in an avalanche of photons and hence the LASER action is achieved. If the GaAs semiconductor is used then the wavelength of the LASER emitted is 840nm.

Advantages

1. It has excellent efficiency
2. The output can be modulated
3. It produces both continuous wave output or pulsed output.
4. It is highly economical

Applications

1. It is used in optical fiber communication.
2. It is used in commercial CD recording and reading.
3. It is used in Barcode Reader, Laser printing and Laser Cooling.

1.8 Applications of LASER

LASER has wide range of applications pertaining all disciplines of engineering. Here in the syllabus only two applications are discussed relevant to computing.

1.8.1 LASER Barcode Reader

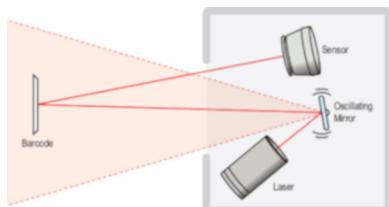


Figure 1.7: Barcode Reader



Figure 1.8: barcode

A barcode is a printed series of parallel bars or lines of varying width that is used for entering data into a computer system.

A barcode scanner/reader is a device with lights, lenses, and a sensor that decodes and captures the information contained in barcodes. Laser scanners use a laser beam as a light source and typically employ oscillating mirrors or rotating prisms to scan the laser beam back and forth across the barcode. A photodiode then measures the reflected light from the barcode. An analog signal is created from the photodiode, and is then converted into a digital signal.

1.8.2 LASER Printer

Laser printers were invented at XEROX in 1969 by researcher Gary Starkweather. Laser Printers are digital printing devices that are used to create high quality text and graphics on plain paper. A Diode Laser is used in the process of printing in LASER Printer.

Construction

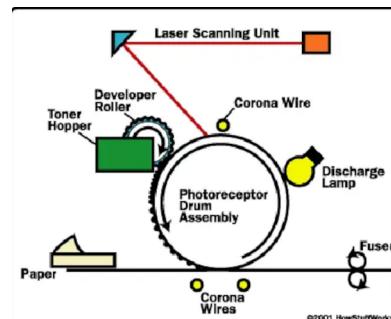


Figure 1.9: Laser Printer Schematic

Working Principle

1. A laser beam projects an image of the page to be printed onto an electrically charged rotating Photo sensitive drum coated with selenium.
2. Photo conductivity allows charge to leak away from the areas which are exposed to light and the area gets positively charged.
3. Toner particles are then electrostatically picked up by the drum's charged areas, which have been exposed to light.
4. The drum then prints the image onto paper by direct contact and heat, which fuses the ink to the paper.

Advantages

1. Laser printers are generally quiet and fast.
2. Laser printers can produce high quality output on ordinary papers.
3. The cost per page of toner cartridges is lower than other printers.

Disadvantages

1. The initial cost of laser printers can be high.
2. Laser printers are more expensive than dot-matrix printers and ink-jet printers

1.8.3 LASER Cooling

Principle of LASER Cooling Laser cooling is the use of dissipative light forces for reducing the random motion and thus the temperature of small particles, typically atoms or ions. Depending on the mechanism used, the temperature achieved can be in the millikelvin, microkelvin, or even nanokelvin regime.

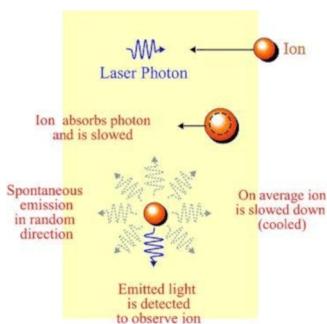


Figure 1.10: Laser Cooling

If an atom is traveling toward a laser beam and absorbs a photon from the laser, it will be slowed by the fact that the photon has momentum $p = \frac{E}{c} = \frac{\hbar}{\lambda}$. It would take a large number of such absorptions to cool the atoms to near 0K. The following are the types of laser cooling

- Doppler Cooling.
- Sisyphous Cooling.

1.9 Model Questions

1. What is LASER? Enumerate the Characteristics of a LASER Beam.
2. Discuss the three possible ways through which radiation and matter interaction can take place.

3. Explain the terms, (i) Induced absorption, (ii) Spontaneous emission, (iii) Stimulated emission, (iv) Population inversion, (v) Meta-stable state & (vi) Resonant cavity.
4. Explain the rates of absorption and emission and hence derive an expression for energy density using Einstein's A and B coefficients.
5. Explain requisites of LASER system.
6. What is Semiconductor LASER? Describe with energy band diagram the construction & working of Semiconductor diode LASER along with applications.
7. Discuss the working of LASER barcode reader.
8. With the help of a sketch describe the principle, construction and working of the LASER Printer.
9. Explain LASER Cooling and its application.

1.10 Numerical Problems

1. Find the ratio of population of two energy levels in a LASER if the transition between them produces light of wavelength 6493 Å, assuming the ambient temperature at 27°C.
2. Find the ratio of population of two energy levels in a medium at thermal equilibrium, if the wavelength of light emitted at 291 K is 6928 Å.
3. The ratio of population of two energy levels out of which one corresponds to metastable state is 1.059×10^{-30} . Find the wavelength of light emitted at 330 K.
4. Find the ratio of population of two energy levels in a medium at thermal equilibrium, if the wavelength of light emitted at 300 K is $10\mu m$. Also find the effective temperature when energy levels are equally populated.
5. The average power output of a LASER beam of wavelength 6500 Å is 10 mW. Find the number of photons emitted per second by the LASER source.
6. The average power of a LASER beam of wavelength 6328 Å is 5 mW. Find the number of photons emitted per second by the LASER source.
7. A pulsed LASER has an average power output 1.5 mW per pulse and pulse duration is 20 ns. The number of photons emitted per pulse is estimated to be 1.047×10^8 . Find the wavelength of the emitted LASER.
8. A pulsed LASER with power 1 mW lasts for 10 ns. If the number of photons emitted per pulse is 5×10^7 . Calculate the wavelength of LASER.

9. A Ruby LASER emits a pulse of 20 ns duration with average power per pulse being 100 kW. If the number of photons in each pulse is 6.981×10^{15} , calculate the wavelength of photons.
10. In a LASER system when the energy difference between two energy levels is 2×10^{-19} J, the average power output of LASER beam is found to be 4 mW. Calculate number of photons emitted per second.

Chapter 2

Optical Fibers

2.1 Introduction

Optical fibers are the wires and strands made of transparent dielectrics which guide light over longer distances using the phenomenon of **Total Internal Reflection**. Many optical fibers are bundled together and are given a protective layer of covering using an insulating material. This bundle is called Optical Fiber Cable or Fiber Bundle (Bundle Fiber).

Construction: The sectional view of a typical optical fiber is as shown in the figure. It has three regions named Core, Cladding and Sheath.

1. The innermost light guiding region is called Core.
2. The layer covering core and helps in total internal reflection of light is called Cladding or Clad.
3. The outermost protective layer is called Sheath (Coating). The sheath protects the fiber from mechanical stress and chemical reactions.

The optical fiber is designed to support total internal reflection and hence the RI of core n_1 is made greater than the RI of cladding n_2 . A typical fiber will be of the order of few microns.

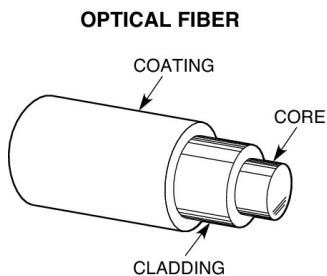


Figure 2.1: Optical fiber construction

2.2 Total Internal Reflection

Consider a ray of light moving from a denser medium to rarer medium. As a result the incident ray of light bends away from the normal. Hence the angle of refraction is greater than the angle of incidence. As the angle of incidence increases the angle of refraction also increases. For a particular angle of incidence θ_c the refracted ray grazes the interface separating the two media. The corresponding angle of incidence θ_c is called Critical Angle. If the angle of incidence is greater than the critical angle then all the light is turned back into the same medium and is called Total Internal Reflection.

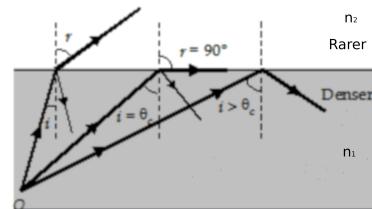


Figure 2.2: Total Internal Reflection

According to Snell's law

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

when $\theta_1 = \theta_c$ then, $\theta_2 = 90^\circ$

$$n_1 \sin\theta_c = n_2 \sin 90^\circ$$

$$\sin\theta_c = \frac{n_2}{n_1}$$

$$\theta_c = \sin^{-1} \left(\frac{n_2}{n_1} \right) \quad (2.1)$$

2.3 Angle of acceptance and Numerical aperture

Acceptance angle (θ_0) is the maximum angle of incidence with which the ray is sent into the fiber core which allows

the incident light to be guided by the core. It is also called as waveguide acceptance angle or acceptance cone half angle.

In optics, the numerical aperture (NA) of an optical fiber is a dimensionless number that characterizes the range of angles over which the fiber can accept light. Numerical aperture represents the light gathering capability of optical fiber and it is given by $NA = \sin\theta_0$.

2.3.1 Condition for propagation

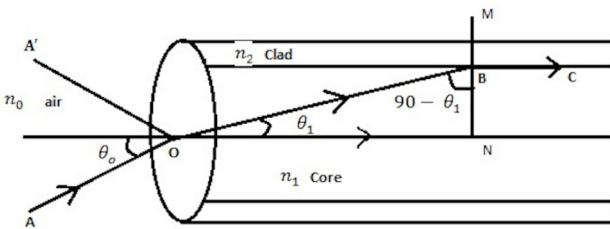


Figure 2.3: Ray propagation in the fiber

Consider an optical fiber with core made of refractive index n_1 & cladding made of material refractive index n_2 . Let n_0 be the refractive index of the surrounding medium. Let a ray of light AO entering into core at an angle of incidence θ_0 w.r.t fiber axis. Then it is refracted along OB at an angle θ_1 & meet core-cladding interface at critical angle of incidence ($\theta_c = 90 - \theta_1$). Then the refracted ray grazes along BC . On applying Snell's law at O, we get

$$\begin{aligned} n_0 \sin\theta_0 &= n_1 \sin\theta_1 \\ \therefore \sin\theta_0 &= \frac{n_1}{n_0} \sin\theta_1 \end{aligned} \quad (2.2)$$

On applying Snell's law at point B, we get

$$\begin{aligned} n_1 \sin(90^\circ - \theta_1) &= n_2 \sin 90^\circ \\ n_1 \cos\theta_1 &= n_2 \\ \therefore \cos\theta_1 &= \frac{n_2}{n_1} \end{aligned} \quad (2.3)$$

From trigonometric identity

$$\begin{aligned} \sin^2\theta_1 + \cos^2\theta_1 &= 1 \\ \sin\theta_1 &= \sqrt{1 - \cos^2\theta_1} \end{aligned}$$

using equation 1.25

$$\begin{aligned} \sin\theta_1 &= \sqrt{1 - \left(\frac{n_2}{n_1}\right)^2} \\ \sin\theta_1 &= \sqrt{\frac{n_1^2 - n_2^2}{n_1^2}} \end{aligned}$$

$$\sin\theta_1 = \frac{1}{n_1} \sqrt{n_1^2 - n_2^2} \quad (2.4)$$

use equation (1.26) in equation (1.24) we have,

$$\begin{aligned} \sin\theta_0 &= \frac{n_1}{n_0} \frac{1}{n_1} \sqrt{n_1^2 - n_2^2} \\ \sin\theta_0 &= \frac{1}{n_0} \sqrt{n_1^2 - n_2^2} \end{aligned} \quad (2.5)$$

Numerical aperture $N.A = \sin\theta_0$

$$N.A = \frac{1}{n_0} \sqrt{n_1^2 - n_2^2} \quad (2.6)$$

If the fiber is in air $n_0 = 1$ then,

$$N.A = \sin\theta_0 = \sqrt{n_1^2 - n_2^2} \quad (2.7)$$

Light is transmitted through the fiber only when

$$\theta_i \leq \theta_0 \quad (2.8)$$

$$\sin\theta_i \leq \sin\theta_0 \quad (2.9)$$

$$\sin\theta_i \leq \sqrt{n_1^2 - n_2^2} \quad (2.10)$$

$$\sin\theta_i \leq N.A \quad (2.11)$$

This is the condition for propagation. Light will be transmitted through the optical fiber with multiple total internal reflections when the above condition is satisfied.

2.4 Modes of propagation

Though optical fiber should support any numbers of rays for propagation practically. But it is found that the optical fiber allows only a certain restricted number of rays for propagation. The maximum number of rays or paths supported by the fiber for the propagation of light is called *Modes of propagation*. Based on the modes of propagation fibers are classified into Single mode and Multi-mode fibers.

2.5 RI Profile

The RI profile is a plot of variation of RI of the fiber with respect to radial distance from the axis of an optical fiber. Based on the RI profile fibers are classified into Step index and Graded index fibers. In case of Step index fibers RI of the core is constant. In case of Graded index fibers the RI decreases radially outwards.

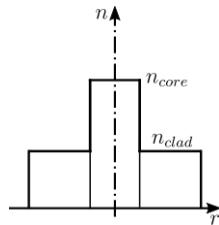


Figure 2.4: RI profile of step index fiber

2.5.1 Types of optical fibers

In any optical fiber, the whole material of the cladding has a uniform refractive index value. But the refractive index of the core material may either remain constant or subjected to variation in a particular pattern. The curve which represents the variation of refractive index with respect the radial distance from the axis of the fiber is called the *refractive index profile*. The optical fibers are classified under 3 categories,

1. Step index single mode fiber
2. Step index multi-mode fiber
3. Graded index multi-mode fiber

This classification is done depending on the refractive index profile, and the number of modes that the fiber can guide.

Step index single mode fiber

A single mode step index fiber consists of a very fine thin core of uniform RI surrounded by Cladding of RI lower than that of Core. Since there is abrupt change in the RI of Core and Cladding at the interface it is called step index fiber. Since the Core size is small the Numerical aperture is also small and hence support single mode. They accept light from LASER source. Splicing is difficult. They are used in submarine cables.

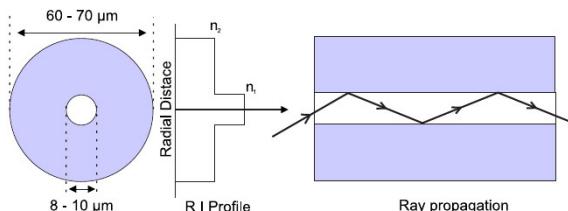


Figure 2.5: Step index single mode fiber

Step index multi-mode fiber

This is similar to single mode step index fiber with the exception that it has a larger core diameter. The core diameter

is very large as compared to single mode optical fiber. A typical multi-mode step index fiber is as shown in figure. The numerical aperture is large because of large core size and thus support multi-modes. They accept light from both LASER as well as from LED. They are used in data links.

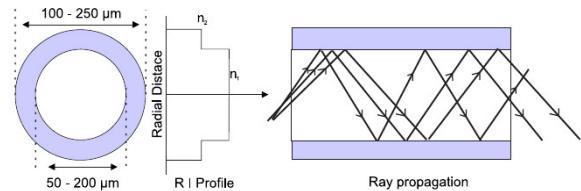


Figure 2.6: Step index multi-mode fiber

Graded index multi-mode fiber

A multi-mode fiber has concentric layers of RI is called GRIN fiber. It means the R I of the Core varies with distance from the fiber axis. The RI is maximum at the center and decreases with radial distance towards to core-cladding interface. The R I profile is as shown in fig. In GRIN fibers the acceptance angle and numerical aperture diminish with radial distance. The light transmission is as shown above. They accept light from both LASER as well as from LED. They are used for medium distance communication for example telephone link between central offices.

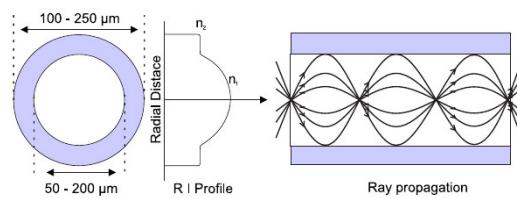


Figure 2.7: Graded index multimode fiber

2.6 Attenuation

The optical energy (signal) passing through the optical fiber gets reduced progressively. This is due to attenuation. It is also called the fiber loss or significant loss. The attenuation is measured in terms of attenuation co-efficient. The attenuation co-efficient α is defined as the ratio of optical power output to the optical power input for a fiber of length L and for a given wavelength of propagating light. It is expressed in dB/km . Attenuation co-efficient is given by

$$\alpha = \frac{-10}{L} \log_{10} \left(\frac{P_{out}}{P_{in}} \right) \quad dB/km \quad (2.12)$$

Here L is the length of the cable in km , P_{in} is Power of optical signal at launching end (input power) & P_{out} is Power of optical signal at receiving end (output power)

The attenuation in fibers gives is due to the following three losses

1. Absorption losses
2. Scattering loss (due to Rayleigh Scattering)
3. Geometric Effects (Radiation losses)

2.6.1 Absorption loss

In this type of loss, the loss of signal power occurs due to absorption of photons associated with the signal. Photons are absorbed either by impurities in the glass fiber or by pure glass material itself. Absorption loss is wavelength dependent. Thus absorption loss is classified in to two types.

Extrinsic absorption : Extrinsic loss in an optical fiber is due to the absorption of light by the impurities such as hydroxide ions and transition metal ions such as iron, chromium, cobalt and copper.

Intrinsic absorption Intrinsic loss in fiber is due to the absorption of light by the material of the fiber glass itself. The intrinsic losses are insignificant.

2.6.2 Scattering loss

Light traveling through the core can get scattered by impurities or small regions with sudden change in refractive index. Rayleigh scattering varies as $\alpha = \frac{1}{\lambda^4}$ and leads to significant power loss at smaller wavelengths. The scattering results in loss of photons. Rayleigh scattering is responsible for maximum losses in optical fibers.

2.6.3 Geometric effects

These may occur due to manufacturing defects like irregularities in fiber dimensions during drawing process or during coating, cabling or insulation processes. The microscopic bends are the bends with radii greater than fiber diameter. The microscopic bends couple light between the various guided modes of the fiber and some of them then leak through the fiber.

2.7 Applications of Optical Fibers

2.7.1 Fiber Optic Networking

Local Area Network

A Local Area Network (LAN) is a type of computer network that interconnects multiple computers and computer-

driven devices in a particular physical location. Traditionally copper coaxial cables are used for LAN.

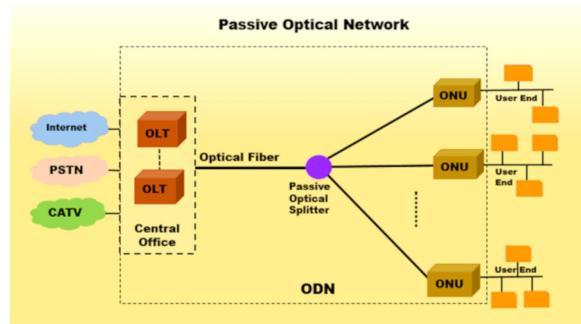


Figure 2.8: Fiber Optic LAN

Abbreviations

1. PON - Passive Optical Network
2. ONT - Optical Network Terminal
3. ODN - Optical Distribution Network
4. OLT - Optical Line Terminal
5. ONU - Optical Network Unit

Passive Optical LAN

A passive optical network refers to a fiber-optic network utilizing a point-to-multipoint topology and optical splitters to deliver data from a single transmission point to multiple user endpoints. Passive here refers to the unpowered condition of the fiber and splitting/combing components. Passive optical LANs are built entirely using Optical fiber cables. The passive optical LAN works on the concept of optical network terminals (ONT) and passive optical splitters. Network switches act as passive splitters and the commercial media converters act as optical network terminals in a real-time application of passive optical LAN.

Advantages

1. High speeds and bandwidth
2. Longer distances are possible
3. Less chance of errors

2.7.2 Point to point communication using Optical Fibers

In an optical fiber communication system, the input signals (audio, video or other digital data) are used to modulate light from a source like a LED or a semiconductor LASER and is transmitted through optical fiber. At the

receiving end the signal is demodulated to reproduce the input signal. If data transfer takes place between only two devices then, it is called point to point communication.

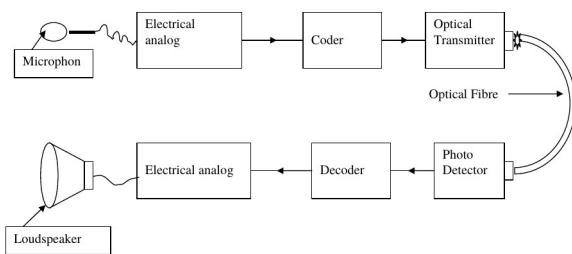


Figure 2.9: Point to point fiber optic communication system

Optical fiber communication process : The communication using Optical fiber is as follows. First voice is converted into electrical signal using a transducer. It is digitized using a Coder. The digitized signal, which carries the voice information, is fed to an optical transmitter. The light source in optical transmitter (LED or LASER Diode) emits modulated light, which is transmitted through the optical fiber. At the other end the modulated light signal is detected by a photo detector and is decoded using a decoder. Finally the information is converted into analog electrical signal and is fed to a loud speaker, which converts the signal to voice (sound).

Advantages

1. Optical fibers can carry very large amounts of information in either digital or analog form.
2. The raw material for optical fiber is of low cost and abundant.
3. It has low cost /meter/ channel
4. Cables are very compact
5. Signals are protected from radiation from lightning or sparking
6. There is no energy radiation from fiber
7. No sparks are generated

Disadvantages

1. The optical connectors are very costly
2. Maintenance cost is high
3. They cannot be bent too sharply
4. They undergo structural changes with temperature

2.8 Model Questions

1. Define the terms: (i) angle of acceptance, (ii) numerical aperture, (iii) modes of propagation & (iv) refractive index profile.
2. Obtain an expression for numerical aperture and arrive at the condition for propagation.
3. Explain modes of propagation and RI profile.
4. What is attenuation? Explain the factors contributing to the fiber loss.
5. Discuss the types of optical fibers based on modes of propagation and RI profile.
6. Explain attenuation along with the expression for attenuation coefficient and also discuss the types of fiber losses.
7. Explain the Fiber Optic Networking and mention its advantages.
8. Discuss point to point optical fiber communication system and mention its advantages over the conventional communication system.
9. Discuss the advantages and disadvantages of an optical communication.

2.9 Numerical Problems

1. Calculate the numerical aperture and angle of acceptance for an optical fiber having refractive indices 1.563 and 1.498 for core and cladding respectively.
2. The refractive indices of the core and cladding of a step index optical fiber are 1.45 and 1.4 respectively and its core diameter is $45\mu m$. Calculate its fractional refractive index change and numerical aperture.
3. Calculate numerical aperture, acceptance angle and critical angle of a fiber having a core RI 1.50 and cladding RI 1.45.
4. An optical fiber has a numerical aperture of 0.32. The refractive index of cladding is 1.48. Calculate the refractive index of the core, the acceptance angle of the fiber and the fractional index change.
5. An optical signal propagating in a fiber retains 85% of input power after traveling a distance of 500 m in the fiber. Calculate the attenuation coefficient.
6. An optical fiber has core RI 1.5 and RI of cladding is 3% less than the core index. Calculate the numerical aperture, angle of acceptance critical angle.

7. The numerical aperture of an optical fiber is 0.2 when surround by air. Determine the RI of its core, given the RI of the cladding is 1.59. Also find the acceptance angle when the fiber is in water of RI 1.33.
8. The angle of acceptance of an optical fiber is 30° when kept in air. Find the angle of acceptance when it is in medium of refractive index 1.33.
9. An optical fiber of 600 m long has input power of 120 mW which emerges out with power of 90 mW. Find attenuation in fiber.
10. The attenuation of light in an optical fiber is 3.6 dB/km. What fraction of its initial intensity is remains after i) 1 km and ii) 3 km ?
11. The attenuation of light in an optical fiber is 2.2 dB/km. What fraction of its initial intensity is remains after i) 2 km and ii) 6 km ?

Part II

MODULE 2 : Quantum Mechanics

Chapter 3

Quantum Mechanics

3.1 Wave-Particle dualism

The phenomena like Interference, Diffraction and Polarization are attributed to the wave properties of radiation. The Quantum theory of radiation and experiments like Photoelectric effect and Compton Effect describe the particle nature of radiation. Thus radiation behaves like waves and like particles under different suitable circumstances. Hence radiation exhibits dual nature.

3.2 de Broglie hypothesis

In the year 1924 French physicist Louis de Broglie extended wave-particle dualism through a hypothesis stating *If radiant energy could behave like waves in some experiments and particles or photons in others and since nature loves symmetry, then one can expect the particles like protons and electrons to exhibit wave nature under suitable circumstances.* This is well known as de Broglie's hypothesis.

Therefore some sort of waves can be even associated with moving material particles called *Matter waves* or *de-Broglie waves* and the wavelength associated with matter waves is called *de Broglie wavelength*. The wavelength of a photon in-terms of its momentum is given by $\lambda = \frac{h}{p}$. Hence by analogy the de Broglie wavelength of matter waves is given by $\lambda = \frac{h}{p} = \frac{h}{mv}$. Here m is the mass of the moving particle and v is its velocity.

Note

- For a particle, charged or uncharged, moving with kinetic energy E the de Broglie wavelength is given by $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$.
- For a charged particle accelerated with a potential V volt, the de Broglie wavelength is given by $\lambda = \frac{h}{\sqrt{2mqV}}$.
- For an electron accelerated through a potential difference of V volt, the de Broglie wavelength is given by $\lambda = \frac{h}{\sqrt{2meV}}$. Further substituting the values of h, m

and e , the de Broglie wavelength is given by the expression $\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$.

3.3 Matter waves and its properties

3.3.1 Phase velocity

The velocity with which a wave travels is called phase velocity (v_p) and is also called wave velocity. If a point is marked on the wave representing the phase of the particle then the velocity with which the phase propagates from one point to another is called phase velocity.

$$v_p = \frac{\omega}{k} = \frac{E}{P} = \frac{c^2}{v} \quad (3.1)$$

Here c is the velocity of light in vacuum and v is the velocity of the matter wave. It is also evident, from the above equation 3.1, that the phase velocity is not only greater than the particle velocity it is also greater than the velocity of light. Hence there is no physical meaning for phase velocity of matter waves.

3.3.2 Wave packet and Group velocity

Since the velocity of matter waves must be equal to that of the particle velocity and since no physical meaning can be associated with phase velocity, the concept of group velocity is introduced.

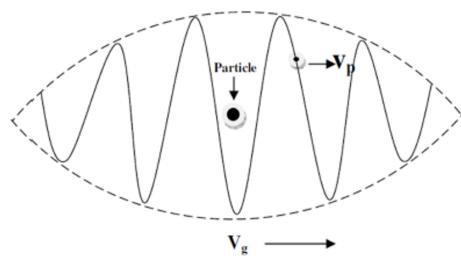


Figure 3.1: Wave group or wave packet

Matter wave can be considered as a resultant wave due to the superposition of many component waves whose velocities differ slightly. Thus a wave group or wave packet is formed. The velocity with which the wave group travels is called group velocity which is same as particle velocity. It is denoted by v_g and is as given in the equation 3.2.

$$v_g = \frac{d\omega}{dk} \quad (3.2)$$

3.3.3 Properties of matter waves

The following are the properties associated with the matter waves

1. Matter waves are associated only with particles in motion
2. They are not electromagnetic in nature
3. Group velocity is associated with matter waves
4. As a result of superposition of large number of component waves which slightly differ in frequency, matter waves are localized.
5. The phase velocity has no physical meaning for matter waves
6. The amplitude of the matter wave at a given point is associated with the probability density of finding the particle at that point.
7. The wave length of matter waves is given by $\lambda = \frac{h}{mv}$

3.4 Heisenberg's Uncertainty Principle

Statement: The simultaneous determination of the exact position and momentum of a moving particle is impossible.

Explanation : According to this principle if Δx is the error involved in the measurement of position and Δp_x is the error involved in the measurement of momentum during their simultaneous measurement, then the product of the corresponding uncertainties is given by

$$\Delta x \Delta p_x \geq \frac{h}{4\pi} \quad (3.3)$$

$$\Delta E \Delta t \geq \frac{h}{4\pi} \quad (3.4)$$

$$\Delta \theta \Delta L \geq \frac{h}{4\pi} \quad (3.5)$$

The product of the errors is of the order of Planck's constant. If one quantity is measured with high accuracy then the simultaneous measurement of the other quantity becomes less accurate.

Physical significance : According to Newtonian physics the simultaneous measurement of position and momentum are *exact*. But the existence of matter waves induces serious problems due to the limit to accuracy associated with the simultaneous measurement. Hence the *exactness* in Newtonian physics is replaced by *probability* in quantum mechanics.

3.4.1 Application of uncertainty principle

Non-existence electrons inside the nucleus : Beta rays are emitted by the nucleus. When it was first observed it was believed that electrons exist inside the nucleus and are emitted at certain instant. If the electron can exist inside the atomic nucleus then uncertainty in its position must not exceed the diameter of the nucleus. The diameter of the nucleus is of the order of Δx_{max} is $10^{-14}m$. Applying Heisenberg's uncertainty principle for an electron expected to be inside the nucleus we get

$$\Delta x_{max} \Delta p_{min} \geq \frac{h}{4\pi} \quad (3.6)$$

$$\Delta p_{min} \geq \frac{h}{4\pi \Delta x_{max}} \quad (3.7)$$

$$\Delta p_{min} \geq \frac{6.625 \times 10^{-34}}{4 \times 3.142 \times 10^{-14}} = 5.276 \times 10^{-21} kgms^{-1} \quad (3.8)$$

Therefore, the electron should possess momentum

$$p_{min} \approx \Delta p_{min} = 5.276 \times 10^{-21} kgms^{-1} \quad (3.9)$$

Non-relativistic equation of energy of the electron is given by

$$E = \frac{(p_{min})^2}{2m_e} = 1.53 \times 10^{-11} J \quad (3.10)$$

here m_e is the rest mass of the electron

$$E_{min} = \frac{1.53 \times 10^{-11}}{1.6 \times 10^{-19}} = 95 \text{ MeV} \quad (3.11)$$

Conclusion : According to experiments, the energy associated with the beta ray (electron) emission is around 3 MeV which is much lesser than the energy of the electron expected to be inside the nucleus 95 MeV. Hence electrons do not exist inside the nucleus.

Note : Equations 3.4 and 3.5 represent the uncertainty relationship between the conjugate physical quantities (Energy, time) and (Angular displacement, Angular momentum).

3.5 Principle of Complementarity

Statement Bohr stated as “*In a situation where the wave aspect of a system is revealed, its particle aspect is concealed; and, in a situation where the particle aspect is revealed, its wave aspect is concealed. Revealing both simultaneously is impossible; the wave and particle aspects are complementary.*”

Explanation We know that the consequence of the uncertainty principle is both the Wave and particle nature of the matter can not be measured simultaneously. In other words, we can not precisely describe the dual nature of Light.

- If an experiment is designed to measure the particle nature of the matter, during this experiment, errors of measurement of both position and the time coordinates must be zero and hence the momentum, energy and the wave nature of the matter are completely unknown.
- Similarly, if an experiment is designed for measuring the wave nature of the particle, then the errors in the measurement of the energy and the momentum will be zero, whereas the position and the time coordinates of the matter will be completely unknown. unknown.

From the above explanation, we can conclude that, when the particle nature of the matter is measured or displayed, the wave nature of the matter is necessarily suppressed and vice versa.

3.6 Wave Function

According to the de Broglie's hypothesis the relation between momentum and wavelength is found to be experimentally valid for both photons and particles. The quanta of matter or radiation can be represented in agreement with uncertainty principle by wave packets. Thus it suggests that concentrated bunches of waves might be used to describe localized particles and quanta of radiation. **The variations of which make up the matter wave is called wave function.** Hence we shall consider a wave function that depends on space (x, y and z) and time(t) and is denoted by $\psi(r, t)$. The wave function for a wave packet moving along +ve x axis is given by

$$\psi = \psi_0 e^{i(kx - \omega t)} \quad (3.12)$$

The quantity ψ is assumed to have the following three basic properties

1. It can interfere with itself so that it can account for diffraction experiments.

2. It is large in magnitude where is particle or photon is likely to be found and small else where.
3. It will be regarded as describing the behavior of single particle or photon and not statistical distribution of number of quanta.

3.7 Time Independent Schrödinger Wave Equation

The wave equation which has variations only with respect to position and describes the steady state is called Time Independent Schrodinger wave equation. Consider a particle of mass m moving with velocity v along +ve x-axis. The de Broglie wave length λ is given by

$$\lambda = \frac{h}{mv} \quad (3.13)$$

The wave equation for one dimensional propagation of waves is given by

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \quad (3.14)$$

The wave function is given by

$$\psi = \psi_0 e^{i(kx - \omega t)} \quad (3.15)$$

here ψ_0 is the amplitude at the point of consideration, ω is angular frequency and k is the wave number. Differentiating ψ twice with respect to t , we get

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi_0 e^{i(kx - \omega t)} \quad (3.16)$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi \quad (3.17)$$

substituting equation 3.17 in equation 3.14

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} (-\omega^2 \psi) \quad (3.18)$$

substituting for ω and v we get

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{(f\lambda)^2} (-(2\pi f)^2 \psi) \quad (3.19)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \psi \quad (3.20)$$

substituting for λ from equation 3.13

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{(\frac{h}{mv})^2} \psi \quad (3.21)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2 (mv)^2}{h^2} \psi \quad (3.22)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{8\pi^2 m (\frac{1}{2} mv^2)}{h^2} \psi \quad (3.23)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{8\pi^2 m(E-U)}{h^2} \psi \quad (3.24)$$

here

$$\frac{1}{2}mv^2 = E - U \quad (3.25)$$

here E is the total and U is potential energy of the particle.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m(E-U)}{h^2} \psi = 0 \quad (3.26)$$

This can be extended to three dimension

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m(E-U)}{h^2} \psi = 0 \quad (3.27)$$

$$\nabla^2 \psi + \frac{8\pi^2 m(E-U)}{h^2} \psi = 0 \quad (3.28)$$

here the operator ∇^2 is given by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3.29)$$

Hence the Time Independent Schrodinger equation.

3.8 Physical significance of Wave Function : Physical Interpretation

The wave function ψ just as itself has no direct physical meaning. It is more difficult to give a physical interpretation to the amplitude of the wave. The amplitude of the wave function ψ is certainly not like displacement in water wave or the pressure wave nor the waves in stretched string. It is a very different kind of wave. The quantity squared absolute value of the amplitude gives the probability of finding the particle per unit volume at the given location in space and is referred to as probability density. This is also referred to as *Born interpretation*. It is given by

$$P(x) = |\psi|^2 \quad (3.30)$$

Thus, in one dimension the probability of finding a particle in the width dx of length x

$$P(x)dx = |\psi|^2 dx \quad (3.31)$$

Similarly, in three dimension, the probability of finding a particle in a given small volume dV of volume V is given by

$$P dV = |\psi|^2 dV \quad (3.32)$$

here $dv = dx dy dz$ and P is the probability of finding the particle at given location per unit volume and is called *Probability Density*. Since ψ is a complex quantity $|\psi|^2 = \psi\psi^*$ and the product is a real number. ψ^* is the complex conjugate of ψ .

3.9 Expectation Value

In quantum mechanics ***The expectation value is the probabilistic expected value of the result (measurement) of an experiment. It can be thought of as an average of all the possible outcomes of a measurement as weighted by their likelihood.*** Expectation value as such it is not the most probable value of a measurement. In the real sense the expectation value may have zero probability of occurring. Let us consider a particle moving along the x axis.

The result of a measurement of the position x is a continuous random variable. Consider a wave function $\psi(x, t)$. The $|\psi(x, t)|^2$ value is a probability density for the position observable and $|\psi(x, t)|^2 dx$ is the probability of finding the particle between x and $x + dx$ at time t . Thus, if a measurement of position is repeated many times in an identical way on an identical particle in identical circumstances, many possible outcomes are possible and the expectation value of these outcomes is, according to the following equation

$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\psi(x, t)|^2 dx \quad (3.33)$$

3.10 Eigen values and eigen functions

The Schrodinger wave equation is a second order differential equation. Thus solving the Schrodinger wave equation to a particular system we get many expressions for wave function (ψ). However, all wave functions are not acceptable. Only those wave functions which satisfy certain conditions are acceptable. Such wave functions are called ***Eigen functions*** for the system. The energy values corresponding to the Eigen functions are called ***Eigen values***. The wave functions are acceptable if they satisfy the following conditions.

1. ψ must be finite everywhere (Cannot be infinite)
2. ψ must be single valued which implies that solution is unique for a given position in space.
3. ψ and its first derivatives with respect to its variables must be continuous everywhere.

3.11 Applications of schrödinger wave equation

3.11.1 Particle in one-dimensional potential well of infinite height

Consider a particle of mass m bouncing back and forth between the walls of one dimensional potential well as shown in figure 3.2. The particle is said to be under bound state. Let the motion of the particle be confined along the x -axis

in between two infinitely hard walls at $x = 0$ and $x = a$. Since the walls are infinitely hard, no energy is lost by the particle during the collision with walls and the total energy remains constant.

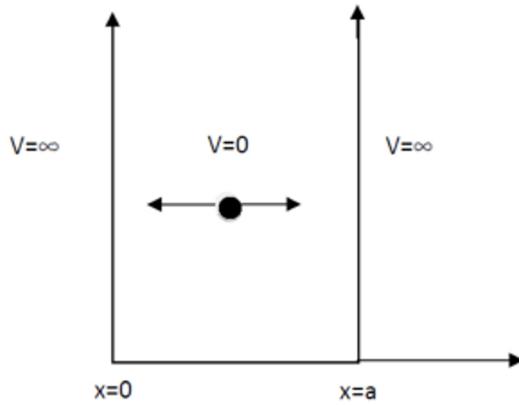


Figure 3.2: One dimensional potential well of infinite height

The description of the potential well is as follows. In between walls i.e. $0 < x < a$, the potential $V = 0$. Beyond the walls i.e. $x \leq 0$ and $x \geq a$, the potential $V = \infty$.

Beyond the walls or outside the potential well

Since the particle is unable to penetrate the hard walls it exists only inside the potential well. Hence $\psi = 0$ and the probability of finding the particle outside the potential well is also zero.

In between the walls or inside the potential well

The Schrodinger wave equation is given by

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2m(E - U)}{\hbar^2}\psi = 0 \quad (3.34)$$

Since the potential inside the well $V = 0$, hence potential energy $U = 0$, the Schrodinger wave equation becomes

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2m(E - 0)}{\hbar^2}\psi = 0 \quad (3.35)$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2mE}{\hbar^2}\psi = 0 \quad (3.36)$$

$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0 \quad (3.37)$$

$$k^2 = \frac{8\pi^2mE}{\hbar^2} \quad (3.38)$$

here k is a constant for a given value of energy E . The general solution for equation 3.37 is given by

$$\psi(x) = A \sin kx + B \cos kx \quad (3.39)$$

Here in the above equation A and B are arbitrary constants which can be evaluated by applying boundary conditions.

Applying Boundary Conditions

1. The first boundary condition is, at $x = 0$, $\psi(x) = 0$.

Applying this to equation 3.39, we get $0 = A \sin 0 + B \cos 0 \implies B = 0$ hence equation 3.39 reduces to

$$\psi(x) = A \sin kx \quad (3.40)$$

2. The second boundary condition is, at $x = a$, $\psi(x) = 0$.

Applying this to equation 3.40, we get $0 = A \sin ka$. Since $A \neq 0$ then $\sin ka = 0$. This results in $ka = n\pi$ which further could be written as $k = \frac{n\pi}{a}$. n can take integer values. Hence equation 3.40 could be written as

$$\psi(x) = A \sin \left(\frac{n\pi x}{a} \right). \quad (3.41)$$

also from equation 3.38

$$k^2 = \frac{n^2\pi^2}{a^2} = \frac{8\pi^2mE_n}{\hbar^2} \quad (3.42)$$

$$E_n = \frac{n^2\hbar^2}{8ma^2} \quad (3.43)$$

Quantization of Energy States

Substituting for $n = 1, 2, 3, 4, \dots$ in the above equation **Energy Eigen Values** are obtained. The lowest energy state corresponds to lowest integral value of $n = 1$ which is also called as **Zero Point Energy** is given by $E_1 = \frac{\hbar^2}{8ma^2}$. The energy values of a bound particle in one dimensional potential well are quantized (discrete) and are represented by the equation $E_n = n^2 E_1$.

Normalization of wave function

The wave function for a particle in one dimensional potential well of infinite height is given by the equation 3.41 $\psi(x) = A \sin \left(\frac{n\pi x}{a} \right)$. In this equation A is an arbitrary constant and it can take any value. The process of determination of value of the arbitrary constant is called *Normalization of wave function*. The particle has to exist somewhere inside the potential the probability of the finding the particle inside the potential well is given by

$$\int_0^a |\psi(x)|^2 dx = \int_0^a P dx = 1 \quad (3.44)$$

Substituting for the wave function in the integral

$$\int_0^a A^2 \sin^2 \left(\frac{n\pi x}{a} \right) dx = 1 \quad (3.45)$$

from trigonometry $\sin^2 \theta = \frac{1}{2}(1 - \cos 2\theta)$. Therefore the above equation could be written as

$$\int_0^a \frac{A^2}{2} \left[1 - \cos \left(\frac{2n\pi x}{a} \right) \right] dx = 1 \quad (3.46)$$

integrating the above equation we get

$$\frac{A^2}{2} \left[x - \frac{a}{2n\pi} \sin \left(\frac{2n\pi x}{a} \right) \right]_0^a = 1 \quad (3.47)$$

$$\implies A = \sqrt{\frac{2}{a}} \quad (3.48)$$

Substituting this in equation 3.41 the normalized wave function or eigen function for a particle in one dimensional potential well of infinite height is given by

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \left(\frac{n\pi x}{a} \right). \quad (3.49)$$

The wave functions and the probability densities for the first three values of n are as shown in fig 3.3

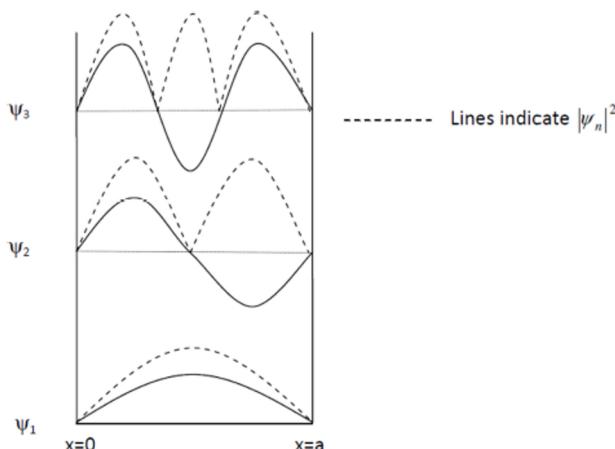


Figure 3.3: Wave function and Probability density for $n = 1, 2, 3$

Thus for ground state ($n = 1$). The probability of finding the particle at the walls is zero and at the center $\frac{a}{2}$ is maximum. The first excited state has three nodes and the second excited state has four nodes.

Summary

Black Body radiation spectrum posed challenges during the early 19th century. Many experiments were conducted and theories were put forward to understand the

phenomenon. Wein and Rayleigh-Jeans were able to explain the black-body radiation spectrum in the lower and higher wavelength region respectively. Planck's radiation law, based on discrete energy packet 'Quanta' or 'Photon', is able to explain the energy distribution in the black body radiation spectrum completely. Several experiments and theories were put forward to understand the particle and wave nature of radiations. This proved dual nature of radiation. Further, based on analogy, Louis de Broglie extended the same concept to moving particles and proposed a hypothesis which indicates the wave nature of moving particles. Diffraction experiments prove the wave nature of moving particles. Attempts were successful in knowing the different quantities related to the wave associated with particles called matter waves. Irwin Schrodinger set up a differential equation for the moving particle implementing de Broglie hypothesis. The Schrodinger wave equation is set up for a bound particle and free particles. Subsequent solutions prove that the energies of bound particles are quantized and that of free particles is continuous.

3.12 Model Questions

1. State and Explain de Broglie hypothesis.
2. What are matter waves and mention the properties.
3. Derive the relation between Phase velocity and Group velocity.
4. Derive the relation between Group velocity and Particle velocity.
5. State and Explain Heisenberg's uncertainty principle. Mention its physical significance.
6. Explain why electron cannot exist inside the nucleus?
7. State and Explain the Principle of Complementarity.
8. Define wave function? Mention its basic properties.
9. Derive Time independent Schrodinger wave equation for a particle moving in three dimension.
10. Discuss the physical interpretation of wave function?
11. Elucidate expectation value.
12. Describe Eigen functions and Eigen values.
13. Discuss the motion of a particle in one dimensional potential well of infinite height.
14. Discuss the energies of a free particle using time independent schrodinger equation.

3.13 Numerical Problems

1. Calculate the momentum of the particle and the de Broglie wavelength associated with an electron with a kinetic energy of 1.5keV .
2. Calculate the wavelength associated with an electron having kinetic energy 100eV .
3. Calculate de Broglie wavelength associated with electron carrying energy 2000eV .
4. Find the energy of the neutron in eV whose de Broglie wavelength is 1\AA .
5. Calculate de Broglie wavelength associated with neutron of mass $1.674 \times 10^{-27}\text{kg}$ with $\frac{1}{10}^{\text{th}}$ part of speed of light.
6. Calculate de Broglie wavelength associated with electrons whose speed is 0.01 part of the speed of light.
7. What is the de Broglie wavelength of a proton whose energy is 3eV given mass of proton is $1.67 \times 10^{-27}\text{kg}$.
8. Find the kinetic energy and group velocity of an electron with de Broglie wavelength of 0.2nm .
9. Calculate the de Broglie wavelength of particle of mass $0.65 \frac{\text{MeV}}{c^2}$ has a kinetic energy 80eV .
10. Find de Broglie wavelength of a particle of mass $0.58 \frac{\text{MeV}}{c^2}$ has a kinetic energy 90eV , Where c is speed of light.
11. A particle of mass $940 \frac{\text{MeV}}{c^2}$ has kinetic energy 0.5keV . Find its de Broglie wavelength, where c is speed of light.
12. Find the de Broglie wavelength of an electron accelerated through a potential difference of 182V and object of mass 1kg moving with a speed of 1ms^{-1} . Compare the results and comment.
13. The position and momentum of an electron with energy 0.5keV are determined. What is the minimum percentage uncertainty in its momentum if the uncertainty in the measurement of position is 0.5\AA .
14. The speed of electron is measured to be with an uncertainty of $2.2 \times 10^4\text{ms}^{-1}$ in one dimension. What is the minimum width required by the electron to be confined in an atom?
15. Estimate the time spent by an atom in the excited state during the excitation and de-excitation processes, when a spectral line of wavelength 546nm and width 10^{-14}m is emitted.
16. An electron is confined to a box of length 10^{-9}m , calculate the minimum uncertainty in its velocity.
17. The position and momentum of 1 keV electron are simultaneously determined. If its position is located within 1\AA , find the uncertainty in the determination of its momentum.
18. A spectral line of wavelength 4000\AA has a width of $8 \times 10^{-5} \text{\AA}$. Evaluate the minimum time spent by the electrons in the upper energy state between the excitation and de-excitation processes.
19. The inherent uncertainty in the measurement of time spent by Iridium 191 nuclei in the excited state is found to be $1.4 \times 10^{-10}\text{s}$. Estimate the uncertainty that results in its energy in eV in the excited state.
20. An electron is bound in one dimensional potential well of width 0.18nm . Find the energy value in eV of the second excited state.
21. The first excited state energy of an electron in an infinite well is 240eV . What will be its ground state energy when the width of the potential well is doubled?
22. A quantum particle confined to one-dimensional box of width a is in its first excited state. What is the probability of finding the particle over an interval of $\frac{a}{2}$ marked symmetrically at the center of the box.

Part III

MODULE 3 : Quantum Computing & Quantum Gates

Chapter 4

Principles of Quantum Information & Quantum Computing

4.1 Introduction to Quantum Computing

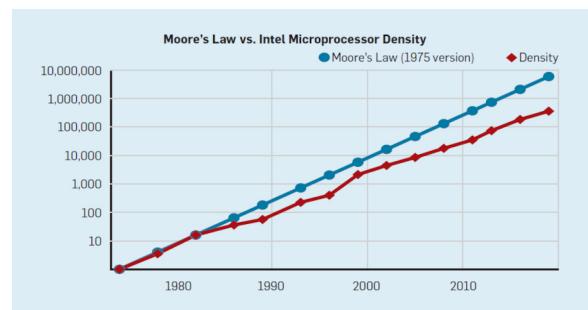
Quantum Computing is the area of study focused on developing computing methods based on the principle of quantum theory. Quantum computing is based on the principle of quantum superposition. In Quantum computing, the information is encoded in quantum system such as atoms, ions or quantum dots. One quantum rule in particular creates an enormous incentives to apply quantum mechanics to computing.

The algorithms are also written based on quantum principles in which, Shor's algorithm for factorization and Grover's search algorithm are basic. (Grover is an Indian born Physicist working in Bell Labs). The process of computation is incredibly fast but it has to be done by the help of quantum computers which are yet to be realized in practice. It is expected that 140 digit log number could be factored a billion (10^9) times faster than is possible with classical computation. It is so powerful that a search engine can search every part of internet in half an hour.

4.2 Moore's law & its end

In the year 1965, Gordon Moore observed increasing performance in the first few generations of the integrated-circuit (IC) technology. Moore's Law is not a law of nature, but an observation of a long-term trend in how technology is changing. Moore's Law is an observation that predicted that the number of transistors in an IC doubles about every two years. The following plot shows the number of transistors on a logarithmic scale over 50 years of Moore's law.

The question that arises is how long can Moore's law continues to hold and what are the ultimate limitations?. According to the semiconductor size data the size has reached 5 nanometer in 2021. The Demise of the Transistor in the quantum scale could be expected as the dimensions decrease further. Quantum effects can cascade into



the micro scale realm causing problems for current microelectronics. The most typical effects are electron tunneling among the circuit lines. Thus Quantum Computation is the option for the further generation.

Table 2-3. Semiconductor Size Data for Figure 2-2

Year	Size in nanometers
1995	600
2001	130
2010	32
2014	14
2019	7
2021	5

4.3 Differences Between Classical and Quantum Computing

4.3.1 Classical Computing

1. Used by large scale,multipurpose and devices.
2. Information is stored in bits.
3. There is a discrete number of possible states. Either 0 or 1.

4. Calculations are deterministic. This means repeating the same inputs results in the same output.
5. Data processing is carried out by logic and in sequential order.
6. Operations are governed by Boolean Algebra.
7. Circuit behavior is defined by Classical Physics.

4.3.2 Quantum Computing

1. Used by high speed, quantum mechanics-based computers.
2. Information is based on Quantum Bits.
3. There is an infinite, continuous number of possible states. They are the result of quantum superposition.
4. The calculations are probabilistic, meaning there are multiple possible outputs to the same inputs.
5. Data processing is carried out (by) quantum logic at parallel instances.
6. Operations are defined by linear algebra by Hilbert Space.
7. Circuit behavior is defined by Quantum Mechanics.

4.4 Concept of Qubit and its properties

4.4.1 Concept of Qubit

The counterpart of a classical binary bit in quantum computing is Qubit. A qubit (quantum bit) is a basic unit of information in quantum computing. Superposition, Entanglement, and Tunneling are all special properties that define a qubit.

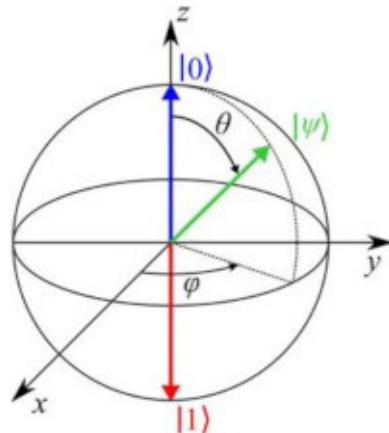
4.4.2 Properties of Qubits

1. A qubit can be in a superposed state of the two states 0 and 1.
2. If measurements are carried out with a qubit in superposed state then the results that we get will be probabilistic unlike how it's deterministic in a classical computer.
3. Owing to the quantum nature, the qubit changes its state at once when subjected to measurement. This means, one cannot copy information from qubits the way we do in the present computers and is known as "*no cloning principle*".

A Qubit can be physically implemented by the two states of an electron or horizontal and vertical polarizations of photons as $| \downarrow \rangle$ and $| \uparrow \rangle$

4.5 Representation of Qubits by Bloch Sphere

The **pure state space qubits** (Two Level Quantum Mechanical Systems) can be visualized using an imaginary sphere called **Bloch Sphere**. It has a unit radius.



The Arrow on the sphere represents the state of the Qubit. The north and south poles are used to represent the basis states $|0\rangle$ and $|1\rangle$ respectively. The other locations are the superpositions of $|0\rangle$ and $|1\rangle$ states and represented by $\alpha|0\rangle + \beta|1\rangle$ with $\alpha^2 + \beta^2 = 1$. Thus a Qubit can be any point on the Bloch Sphere.

The Bloch sphere allows the state of the qubit to be represented using spherical coordinates. They are the polar angle θ and the azimuthal angle ϕ . The Bloch sphere is represented by the equation

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle \quad (4.1)$$

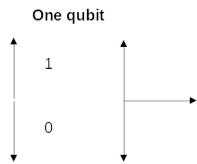
here $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. The normalization constraint is given by

$$\left|\cos\frac{\theta}{2}\right|^2 + \left|\sin\frac{\theta}{2}\right|^2 = 1 \quad (4.2)$$

4.6 Single and Two qubits and Extension to N qubits

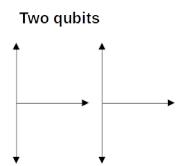
4.6.1 Single qubit

A Single Qubit has two computational basis states $|0\rangle$ and $|1\rangle$. The pictorial representation of the single qubit is as follows. $\alpha|0\rangle + \beta|1\rangle$



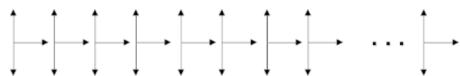
4.6.2 Two qubit

A two-qubit system has 4 computational basis states denoted as $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. The pictorial representation of two qubit is as follows. $\alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$



4.6.3 Extension to N qubits

A multi-qubit system of N qubits has 2^N computational basis states. For example a state with 3 qubits has 2^3 computational basis states. Thus for N qubits the computational basis states are denoted as $|00\cdots 00\rangle$, $|00\cdots 01\rangle$, $|00\cdots 10\rangle$, $|00\cdots 11\rangle \cdots |11\cdots 11\rangle$. The block diagram of representation of N qubits is as follows.



Chapter 5

Dirac Representation and Matrix Operations

5.1 Linear Algebra

Linear Algebra is the study of vector spaces and operations on vector spaces. The Standard quantum mechanical notation for a quantum state ψ in a vector space is $|\psi\rangle$. The notation $| \rangle$ indicates that the object is a vector and is called a *ket vector*. The examples of ket vectors are $|\psi\rangle$, $|\phi\rangle$ and $|u\rangle$ etc.

5.2 Matrix Representation of 0 and 1 States

The wave function could be expressed in ket notation as $|\psi\rangle$ (ket Vector), ψ is the wave function. The $|\psi\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$

The matrix for of the states $|0\rangle$ and $|1\rangle$. $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

5.2.1 Identity Operator

The operator of type $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is called *identity operator*. When an identity operator acts on a state vector its keeps the state intact. By analogy we study identity operator as an identity matrix.

Let us consider the operation of Identity operator on $|0\rangle$ and $|1\rangle$ states. As per the principle of identity operation $I|0\rangle = |0\rangle$ and $I|1\rangle = |1\rangle$

$$I|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (5.1)$$

$$I|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.2)$$

Thus the operation of identity matrix(operator) on $|0\rangle$ and $|1\rangle$ leaves the states unchanged.

5.2.2 Pauli Matrices

Pauli Matrices and Their operation on $|0\rangle$ and $|1\rangle$ States

There are four extremely useful matrices called Pauli Matrices. The Pauli matrices of the following form

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.3)$$

This is an identity matrix.

$$\sigma_1 = \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (5.4)$$

$$\sigma_2 = \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (5.5)$$

$$\sigma_3 = \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (5.6)$$

Pauli Matrices operating on $|0\rangle$ and $|1\rangle$ States

$$1. \sigma_0 |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle.$$

$$\sigma_0 |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle.$$

$$2. \sigma_x |0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

$$\sigma_x |1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle.$$

$$3. \sigma_y |0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i |1\rangle$$

$$\sigma_y |1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i |0\rangle.$$

$$4. \sigma_z |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

$$\sigma_z |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = - |1\rangle.$$

5.3 Conjugate of a Matrix

It is possible to find the conjugate for a given matrix by replacing each element of the matrix with its complex conjugate. For example consider a matrix A as given below.

$$A = \begin{pmatrix} i & 1 \\ 0 & 2 - 3i \end{pmatrix} \quad (5.7)$$

The conjugate of the matrix A is given by

$$A^* = \begin{pmatrix} -i & 1 \\ 0 & 2 + 3i \end{pmatrix} \quad (5.8)$$

Thus A^* is the conjugate of A

5.4 Transpose of a Matrix

The transpose of a matrix is found by interchanging its rows into columns or columns into rows. The Transpose of a matrix A is denoted by using the superscript as A^T . Consider a matrix A as given below.

$$A = \begin{pmatrix} i & 1 \\ 0 & 2 - 3i \end{pmatrix} \quad (5.9)$$

The Transpose of the matrix A is given by

$$A^T = \begin{pmatrix} i & 0 \\ 1 & 2 - 3i \end{pmatrix} \quad (5.10)$$

Thus A^T is the Transpose of A

5.5 The Conjugate Transpose of a Matrix

The complex conjugate transpose of a matrix interchanges the row and column index for each element, reflecting the elements across the main diagonal. The operation also negates the imaginary part of any complex numbers. It is denoted by a \dagger symbol as a super script.

$$A = \begin{pmatrix} i & 1 \\ 0 & 2 - 3i \end{pmatrix} \quad (5.11)$$

The Transpose of the matrix A is given by

$$A^\dagger = (A^*)^T = \begin{pmatrix} -i & 0 \\ 1 & 2 + 3i \end{pmatrix} \quad (5.12)$$

Thus A^\dagger is the Conjugate-Transpose of A .

5.6 Hermitian

The matrix that is equal to its conjugate-transpose is called Hermitian. Thus If $A^\dagger = A$ then it is called **Hermitian** or **Self-Adjoint** matrix.

$$A = \begin{pmatrix} 3 & 3+i \\ 3-i & 2 \end{pmatrix} \quad (5.13)$$

The conjugate of A is given by

$$A^* = \begin{pmatrix} 3 & 3-i \\ 3+i & 2 \end{pmatrix} \quad (5.14)$$

The transpose of A^* is given by

$$A^\dagger = \begin{pmatrix} 3 & 3+i \\ 3-i & 2 \end{pmatrix} \quad (5.15)$$

Hence $A^\dagger = A$

5.7 Unitary Matrix

A matrix is said to be Unitary if the condition $U^\dagger U = I$ is satisfied. Thus an operator is said to be Unitary if each of its matrix representations are unitary. Consider an operator in matrix form U .

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{bmatrix} \quad (5.16)$$

Then

$$U^\dagger = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{bmatrix} \quad (5.17)$$

$$U^\dagger U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (5.18)$$

Thus

$$U^\dagger U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I \quad (5.19)$$

Hence U is unitary.

5.8 Column and Row Matrices

The **Column Vectors** are called **ket Vectors** denoted by $|\psi\rangle$ and are represented by **Column Matrices**. The **Row Vectors** are called **Bra Vectors** denoted by $\langle\phi|$ and are represented by **Row Matrices**. Let us consider a ket vector represented in the form of a column matrix.

$$|\psi\rangle = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} \quad (5.20)$$

The Row Matrix is represented as

$$\langle\psi| = [\alpha_1^* \quad \beta_1^*] \quad (5.21)$$

Here

$$\begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix}^\dagger = [\alpha_1^* \quad \beta_1^*] \quad (5.22)$$

Thus the Bra is the complex conjugate of ket and vice-versa. For example

$$\begin{bmatrix} 1 \\ i \end{bmatrix}^\dagger = [1 \quad -i] \quad (5.23)$$

Flipping between **kets** and **bras** is called "**Taking the Dual**".

Thus for $|0\rangle$ state the corresponding $\langle 0|$ is given by

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (5.24)$$

$$\langle 0| = [1 \quad 0] \quad (5.25)$$

and similarly for and $|1\rangle$ states we have $\langle 1|$ as follows.

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (5.26)$$

$$\langle 1| = [0 \quad 1] \quad (5.27)$$

5.9 Inner Product - Multiplication of Row and Column Matrices

Let us consider two states $|\psi\rangle$ and $|\phi\rangle$ as follows

$$|\psi\rangle = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} \quad (5.28)$$

$$|\phi\rangle = \begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix} \quad (5.29)$$

here

$$\langle \psi | = [\alpha_1^* \quad \beta_1^*] \quad (5.30)$$

The multiplication of the $|\psi\rangle$ and $|\phi\rangle$ is possible only by taking the inner product and is given by $\langle \psi | \phi \rangle$

$$\langle \psi | \phi \rangle = [\alpha_1^* \quad \beta_1^*] \begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix} \quad (5.31)$$

$$\langle \psi | \phi \rangle = \alpha_1^* \alpha_2 + \beta_1^* \beta_2 \quad (5.32)$$

The inner product always results in a **scalar product**.

5.10 Probability

Let us consider a Quantum State

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad (5.33)$$

The above equation represents the Quantum Superposition of states $|0\rangle$ and $|1\rangle$.

$$|\psi\rangle = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad (5.34)$$

Using equation 5.31 the inner product $\langle \psi | \psi \rangle$ is given by,

$$\langle \psi | \psi \rangle = [\alpha^* \quad \beta^*] \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha \alpha^* + \beta \beta^* \quad (5.35)$$

Thus

$$\alpha \alpha^* + \beta \beta^* = |\alpha|^2 + |\beta|^2 \quad (5.36)$$

This could also be written as

$$|\psi|^2 = \psi \psi^* \quad (5.37)$$

Thus the above equation represents **Probability Density**. As per the principle of Normalization

$$|\psi|^2 = \psi \psi^* = \langle \psi | \psi \rangle = 1 = |\alpha|^2 + |\beta|^2 \quad (5.38)$$

Thus it implies $|\psi\rangle$ is normalized.

5.11 Orthogonality

Two states $|\psi\rangle$ and $|\phi\rangle$ are said to be **orthogonal** if their inner product is Zero. Mathematically

$$\langle \phi | \psi \rangle = 0 \quad (5.39)$$

The two states are orthogonal means they are mutually exclusive. Like Spin Up and Spin Down of an electron.

Consider $\langle 0 | 1 \rangle$

$$\langle 0 | 1 \rangle = [1 \quad 0] \begin{bmatrix} 0 \\ 1 \end{bmatrix} = (0 + 0) = (0) \quad (5.40)$$

5.12 Orthonormality

The states $|\psi\rangle$ and $|\phi\rangle$ are said to be **orthonormal** if

1. $|\psi\rangle$ and $|\phi\rangle$ are *normalized*.
2. $|\psi\rangle$ and $|\phi\rangle$ are *orthogonal* to each other.

Chapter 6

Quantum Gates

6.1 Introduction to Quantum Gates

In quantum computing a quantum logic gate is a basic quantum circuit operating on a small number of qubits. A qubit is useless unless it is used to carry out a quantum calculation. The quantum calculations are achieved by performing a series of fundamental operations, known as quantum logic gates. They are the building blocks of quantum circuits similar to the classical logic gates in conventional digital circuits.

6.2 Single Qubit Gates

6.2.1 Quantum Not Gate

In Quantum Computing the quantum NOT gate for qubits takes the state $|0\rangle$ to $|1\rangle$ and vice versa. It is analogous to the classical not gate.

The Matrix representation of Quantum Not Gate is given by

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6.1)$$

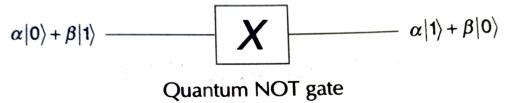
$$X |0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle \quad (6.2)$$

$$X |1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \quad (6.3)$$

A Quantum State is given by $\alpha|0\rangle + \beta|1\rangle$ and its matrix representation is given by $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$. Hence the operation of Quantum Not Gate on quantum state is given by

$$X \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix} \quad (6.4)$$

Thus the quantum state becomes $\alpha|1\rangle + \beta|0\rangle$. Similarly, The input $\alpha|1\rangle + \beta|0\rangle$ to the quantum not gates changes the state to $\alpha|0\rangle + \beta|1\rangle$. The quantum not gate circuit and the truth table are as shown below.



Truth table of NOT gate	
Input	Output
$ 0\rangle$	$ 1\rangle$
$ 1\rangle$	$ 0\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$\alpha 1\rangle + \beta 0\rangle$

6.2.2 Pauli-X,Y and Z Gates

X Gate

The **Pauli-X Gate** is nothing but **Quantum Not Gate**.

6.2.3 Y Gate

Y Gate is represented by Pauli matrix σ_y or Y . This gate Maps $|0\rangle$ state to $i|1\rangle$ state and $|1\rangle$ state to $-i|0\rangle$ state. The Y Gate and its operation is as given below

$$Y |0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = 0|0\rangle + i|1\rangle = i|1\rangle \quad (6.5)$$

$$Y |1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i|0\rangle + 0|1\rangle = -i|0\rangle \quad (6.6)$$

Thus the Y-Gate defines the transformation

$$Y(\alpha|0\rangle + \beta|1\rangle) = \alpha Y|0\rangle + \beta Y|1\rangle = -i\beta|0\rangle + i\alpha|1\rangle \quad (6.7)$$

Quantum Y-Gate is represented by



Truth Table of Y-Gate	
Input	Output
$ 0\rangle$	$i 1\rangle$
$ 1\rangle$	$-i 0\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$-i\beta 0\rangle + i\alpha 1\rangle$

6.2.4 Z-Gate

The Z-gate is represented by Pauli Matrix σ_z or Z. Z-Gate maps input state $|k\rangle$ to $(-1)^k |k\rangle$.

- For input $|0\rangle$ the output remains unchanged.
- For input $|1\rangle$ the output is $-|1\rangle$.

The Matrix representation and the operation of Z-Gate on $|0\rangle$ and $|1\rangle$ are as follows

$$Z|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \quad (6.8)$$

$$Z|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|1\rangle \quad (6.9)$$

$$Z(\alpha|0\rangle + \beta|1\rangle) = \alpha Z|0\rangle + \beta Z|1\rangle = \alpha|0\rangle - \beta|1\rangle \quad (6.10)$$

The circuit symbol and the truth table of Z-Gate are as follows.



Truth table of Z gate	
Input	Output
$ 0\rangle$	$ 0\rangle$
$ 1\rangle$	$- 1\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$\alpha 0\rangle - \beta 1\rangle$

6.2.5 Hadamard Gate

The Hadamard Gate is a truly quantum gate and is one of the most important in Quantum Computing. It has similar characteristics of \sqrt{NOT} Gate. It is a **self inverse gate**. It is used to create the superpositions of $|0\rangle$ and $|1\rangle$ states. The Matrix representation of Hadamard Gate is as follows

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (6.11)$$

The Hadamard Gate and the output states for the $|0\rangle$ and $|1\rangle$ input states are represented as follows. The Hadamard Gate satisfies Unitary Condition.

$$H^\dagger H = I \quad (6.12)$$

The truth-table for the Hadamard Gate is as follows.

$$\begin{aligned} |0\rangle &\xrightarrow{H} \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \\ |1\rangle &\xrightarrow{H} \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle \end{aligned}$$

Input	Action of Hadamard gate	Output
$ 0\rangle$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\frac{ 0\rangle + 1\rangle}{\sqrt{2}}$
$ 1\rangle$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$	$\frac{ 0\rangle - 1\rangle}{\sqrt{2}}$
$\alpha 0\rangle + \beta 1\rangle$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} \alpha + \beta \\ \alpha - \beta \end{bmatrix}$	$\frac{\alpha 0\rangle + \beta 1\rangle}{\sqrt{2}} + \frac{\alpha 0\rangle - \beta 1\rangle}{\sqrt{2}}$ or $\alpha \frac{ 0\rangle + 1\rangle}{\sqrt{2}} + \beta \frac{ 0\rangle - 1\rangle}{\sqrt{2}}$

6.2.6 Phase Gate or S Gate

The phase gate turns a $|0\rangle$ into $|0\rangle$ and a $|1\rangle$ into $i|1\rangle$. The Matrix representation of the S gate is given by

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \quad (6.13)$$

The effect of S gate on input $|0\rangle$ is given by

$$S|0\rangle = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \quad (6.14)$$

Similarly the effect of S gate on input $|1\rangle$ is given by The effect of S gate on input $|0\rangle$ is given by

$$S|1\rangle = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix} = i|1\rangle \quad (6.15)$$

The transformation of state $|\psi\rangle$ is given by

$$S|\psi\rangle = S(\alpha|0\rangle + \beta|1\rangle) = \alpha S|0\rangle + \beta S|1\rangle = \alpha|0\rangle + i\beta|1\rangle \quad (6.16)$$

The S Gate and the Truth table are given by For S gate

Input	Output
$ 0\rangle$	$ 0\rangle$
$ 1\rangle$	$ 1\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$\alpha 0\rangle + i\beta 1\rangle$



$S^\dagger S = I$ and hence it is Unitary.

6.2.7 T Gate or $\frac{\pi}{8}$ Gate

The T Gate is represented by the matrix as follows

$$T = \begin{bmatrix} 1 & 0 \\ 0 & \exp \frac{i\pi}{4} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \left(\frac{1+i}{\sqrt{2}} \right) \end{bmatrix} \quad (6.17)$$

It is also called $\frac{\pi}{8}$ gate as it could be represented in the following form

$$T = \exp \frac{i\pi}{8} \begin{bmatrix} \exp \frac{-i\pi}{8} & 0 \\ 0 & \exp \frac{i\pi}{8} \end{bmatrix} \quad (6.18)$$

Another Important Feature of T gate is it could be related to S gate as

$$T^2 = S \quad (6.19)$$

The Operation of T gate on $|0\rangle$ and $|1\rangle$ are given by

$$T|0\rangle = \begin{bmatrix} 1 & 0 \\ 0 & \left(\frac{1+i}{\sqrt{2}}\right) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \quad (6.20)$$

$$T|1\rangle = \begin{bmatrix} 1 & 0 \\ 0 & \left(\frac{1+i}{\sqrt{2}}\right) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ \left(\frac{1+i}{\sqrt{2}}\right) \end{bmatrix} = \left(\frac{1+i}{\sqrt{2}}\right)|1\rangle \quad (6.21)$$

The T Gate and the Truth Table are as follows.

Input	Output
$ 0\rangle$	$ 0\rangle$
$ 1\rangle$	$\exp(i\pi/4) 1\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$\alpha 0\rangle + \beta \exp(i\pi/4) 1\rangle$

$\alpha|0\rangle + \beta|1\rangle$ —————  ————— $\alpha|0\rangle + \beta \exp(i\pi/4)|1\rangle$

6.3 Multiple Qubit Gates

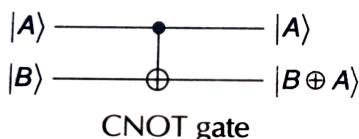
Multiple Qubit Gates operate on Two or More input Qubits. Usually one of them is a control qubit.

6.3.1 Controlled Gates

A Gate with operation of kind "If 'A' is True then do 'B'" is called Controlled Gate. The ' $|A\rangle$ ' Qubit is called **Control qubit** and ' $|B\rangle$ ' is the **Target qubit**. The target qubit is altered only when the control qubit is $|1\rangle$. The control qubit remains unaltered during the transformations.

6.3.2 Controlled Not Gate or CNOT Gate

The CNOT gate is a typical multi-qubit logic gate and the circuit is as follows. The Matrix representation of CNOT



Gate is given by

$$U_{CN} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad (6.22)$$

The Transformation could be expressed as

$$|A, B\rangle \rightarrow |A, B \oplus A\rangle \quad (6.23)$$

Consider the operations of CNOT gate on the four inputs $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$.

Operation of CNOT Gate for input $|00\rangle$

Here in the inputs to the CNOT Gate the control qubit is $|0\rangle$. Hence no change in the state of Target qubit $|0\rangle$

$$|00\rangle \rightarrow |00\rangle \quad (6.24)$$

Operation of CNOT Gate for input $|01\rangle$

Here in the inputs to the CNOT Gate the control qubit is $|0\rangle$. Hence no change in the state of Target qubit $|1\rangle$

$$|01\rangle \rightarrow |01\rangle \quad (6.25)$$

Operation of CNOT Gate for input $|10\rangle$

Here in the inputs to the CNOT Gate the control qubit is $|1\rangle$. Hence the state of Target qubit flips from $|0\rangle$ to $|1\rangle$.

$$|10\rangle \rightarrow |11\rangle \quad (6.26)$$

Operation of CNOT Gate for input $|11\rangle$

Here in the inputs to the CNOT Gate the control qubit is $|1\rangle$. Hence the state of Target qubit flips from $|1\rangle$ to $|0\rangle$.

$$|11\rangle \rightarrow |10\rangle \quad (6.27)$$

The Truth Table of operation of CNOT gate is as follows.

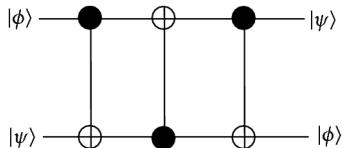
Input	Output
$ 00\rangle$	$ 00\rangle$
$ 01\rangle$	$ 01\rangle$
$ 10\rangle$	$ 11\rangle$
$ 11\rangle$	$ 10\rangle$

6.3.3 Swap Gate

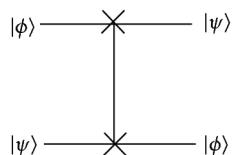
The SWAP gate is two-qubit operation. Expressed in basis states, the SWAP gate swaps the state of the two qubits involved in the operation. The Matrix representation of the Swap Gate is as follows

$$U_{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (6.28)$$

The schematic symbol of swap gate circuit is as follows



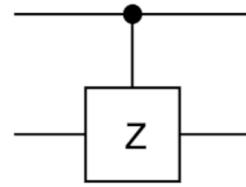
which is equivalent to The swap gate is a combined cir-



cuit of 3 CNOT gates and the over all effect is that two input qubits are swapped at the output. The Action and truth table of the swap gate is as follows.

Gate	Input to gate	Output of gate
1	$ a, b\rangle$	$ a, a \oplus b\rangle$
2	$ a, a \oplus b\rangle$	$ b, a \oplus b\rangle$
3	$ b, a \oplus b\rangle$	$ b, a\rangle$

Truth table of SWAP gate	
Input	Output
$ 00\rangle$	$ 00\rangle$
$ 01\rangle$	$ 10\rangle$
$ 10\rangle$	$ 01\rangle$
$ 11\rangle$	$ 11\rangle$



Input	Output
$ 00\rangle$	$ 00\rangle$
$ 01\rangle$	$ 01\rangle$
$ 10\rangle$	$ 10\rangle$
$ 11\rangle$	$- 11\rangle$

6.3.5 Toffoli Gate

The Toffoli Gate is also known as CCNOT Gate (Controlled-Controlled-Not). It has three inputs out of which **two are Control Qubits** and one is the Target Qubit. **The Target Qubit flips** only when both the Control Qubits are $|1\rangle$. The two Control Qubits are not altered during the operation.

The matrix representation, Gate Circuit and the Truth Table of Toffoli Gate are as follows.

$$U_T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

6.3.4 Controlled Z Gate

In Controlled Z Gate, The operation of Z Gate is controlled by a **Control Qubit**. If the control Qubit is $|A\rangle = |1\rangle$ then only the Z gate transforms the **Target Qubit** $|B\rangle$ as per the Pauli-Z operation. The action of Controlled Z-Gate could be specified by a matrix as follows.

$$U_Z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \quad (6.29)$$

The controlled Z gate and the truth table are as follows.

Inputs					
a	a'	b	b'	c	c'
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	1
1	1	1	1	1	0



The Toffoli matrix is unitary. The Toffoli Gate is its own inverse. It could be used for NAND Gate Simulation.

6.4 Question Bank and Numerical Problems

6.4.1 Principles of Quantum Information and Quantum Computing

1. Describe briefly the Quantum Computing and its importance.
2. Elucidate the differences between classical and quantum computing.
3. Define a bit and qubit and explain the differences between them. Mention the properties of Qubit.
4. Discuss the representation of qubit by Bloch Sphere.
5. Explain single, two qubits and extension to N qubits.

6.4.2 Dirac Representation and Matrix Operations

1. Mention the matrix representation of $|0\rangle$ and $|1\rangle$ states and apply the Identity operator to show there is no change in states.
2. State the Pauli matrices and apply Pauli matrices on the states $|0\rangle$ and $|1\rangle$.
3. Explain conjugate and Transpose of a matrix.
4. Describe unitary matrix and along with an example.
5. Describe row and column matrices and the inner product.
6. Discuss probability and quantum superposition.
7. Explain the conditions for orthogonality and orthonormality.

6.4.3 Quantum Gates

1. Illustrate the principle and working of Quantum Not Gate.
2. Discuss the Pauli X,Y and Z gates and their operations on quantum states.
3. Describe the Phase gate along with matrix representation and truth table.
4. Discuss the CNOT gate and its operation on four different input states.
5. Explain the matrix form and operation of Toffoli gate.
6. Describe the Swap gate with the matrix and truth table.
7. Elucidate the working of controlled-Z gate mentioning its matrix representation and truth table.

8. Distinguish between single qubit and multiple qubit gates.
9. Describe Quantum Gates with three examples.
10. Discuss the functioning of Hadamard gate with matrix representation and truth table.
11. Explain the working of T gate with its matrix and truth table.

6.5 Numerical Problems

6.5.1 Dirac Representation and Matrix Operations

1. A Linear Operator ' X ' operates such that $X|0\rangle = |1\rangle$ and $X|1\rangle = |0\rangle$. Find the matrix representation of ' X '.
2. Given $A = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, Prove that $A^\dagger = A$.
3. Show that the Matrix $U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{bmatrix}$ is Unitary.
4. Find the inner product of states $|1\rangle$ and $|0\rangle$ and draw conclusions on the result.
5. Given $|\psi\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$ Prove that $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$

6.5.2 Quantum Gates

1. Using Matrix multiplication show that on applying Hadamard gate twice to a $|0\rangle$ results in its original state.
2. Using two X-gates in series show that two not gates in series are equivalent to a quantum wire.
3. Show the Hadamard Gate is Unitary.
4. Two Qubits are passed through CNOT gate. If the first qubit is the control qubit then what is the output for the following initial states 1. $|00\rangle$, 2. $|01\rangle$, and 3. $|11\rangle$.
5. Show that S gate can be formed by connecting two T gates in Series.

Part IV

MODULE 4 : Electrical Properties of Materials

Chapter 7

Classical and Quantum Free Electron Theory of Metals

7.1 Electrical Conductivity and Resistivity

Consider a conductor carrying electric current I with area of cross section A perpendicular to the current. The current density J is defined as the ration of current I to the area of cross section A . Hence

$$J = \frac{I}{A} \quad (7.1)$$

It is observed that the current density is proportional to the applied electric field in a conductor. And hence

$$J \propto E \quad (7.2)$$

$$J = \sigma E \quad (7.3)$$

The constant of proportionality σ is called **Electrical Conductivity** of the conductor. The Electrical Resistivity $\rho = \frac{1}{\sigma}$ of the material is the reciprocal of the Electrical Conductivity of the material and is the property of the material by the virtue of which it opposes the flow of current through it.

7.2 Mobility of conduction electrons

It is found that the drift velocity depends on the applied field strength and is mathematically given by $v_d = \mu E$. Here μ is called the mobility of the free electrons. It is defined as the drift velocity acquired by the conduction electrons per unit field strength.

$$\mu = \frac{v_d}{E} = \frac{e\tau}{m} = \frac{\sigma}{ne} = \frac{1}{\rho ne} m^2 V^{-1} s^{-1} \quad (7.4)$$

7.3 Concept of Phonon

A Phonon is a quantum of lattice vibration, the collective motion of atoms constituting a crystal. The Energies and Momenta of Phonons are quantized. It is often characterized as Heat Energy. The study of phonon is an important

part of solid state physics. The phonon plays an important role in many of the physical properties of solids such as the thermal conductivity and the electrical conductivity. The conduction electrons in a metal collide against lattice ions during the motion. The interaction is considered to be of type phonon exchange. This results in non-radioactive transitions.

7.4 Mathiesen's Rule

A Metal consists of lattice ions and impurity atoms that are held together by free electrons. Free electrons wander inside the crystal. During the motion electrons undergo scattering by lattice ions and impurity atoms. The resistivity ρ of a conductor is mainly attributed to two reasons

1. Scattering of electrons with the vibrating lattice ions. The resistivity of the metal due to electron lattice ion scattering is given by

$$\rho_{ph} = \frac{m}{ne^2 \tau_{ph}} \quad (7.5)$$

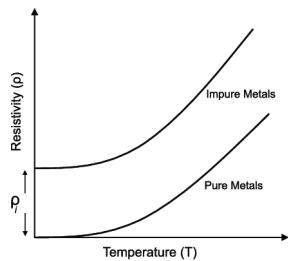
2. Scattering of electrons by the presence of impurities present in the metal. The scattering also occurs from the lattice dislocations and grain boundaries. The resistivity of the metal due to such scattering is given by

$$\rho_i = \frac{m}{ne^2 \tau_i} \quad (7.6)$$

Thus net resistivity of the conductor is given by

$$\rho = \rho_{ph} + \rho_i = \frac{m}{ne^2 \tau_{ph}} + \frac{m}{ne^2 \tau_i} \quad (7.7)$$

The above equation is called Matthiessen's Rule, Which states that the net resistivity of conductor is equal to the sum of the resistivity due to the phonon scattering which is temperature dependent and resistivity due to the presence of impurity which is temperature independent. Graphically the variation of resistance with temperature and impurity is as follows.



7.5 Failures of classical free electron theory of metals

Classical free electron theory of metal is successful in explaining the certain experimentally observed facts of electronic conduction in solids and thermal conductivity. This theory fails to explain certain other experimental observations. The following are the failures of classical free electron theory of metals.

7.5.1 Electronic specific heat of solids

According to the Classical Free Electron Theory Metals the electronic specific heat is given by

$$C_v = \frac{3}{2}R = 12.5 \text{ J mole}^{-1} \text{ K}^{-1} \quad (7.8)$$

The experimental value of electronic specific heat is $C_v = 10^{-4}RT$. It is very small and also temperature dependent. Hence Classical theory fails to explain the electronic specific heat of solids.

7.5.2 Dependence of σ on temperature

According to classical free electron theory of metals the electrical conductivity σ is inversely proportional to square root of temperature (\sqrt{T}). But experiments reveal that electrical conductivity (σ) is inversely proportional to temperature (T). Hence classical free electron theory fails to explain dependence of electrical conductivity (σ) on the temperature (T).

7.5.3 Dependence of σ on n , the number density

The theory predicts the direct dependence of electrical conductivity (σ) on number of free electrons per unit volume (n) called number density. But experiments have revealed different with $\sigma_{Cu} > \sigma_{Al}$ even though the the number densities $n_{Cu} < n_{Al}$. Hence it fails to explain the dependence of electrical conductivity σ on the number free electrons per unit volume n . The experimental observations are as in the table below.

Metal	$\sigma(\Omega^{-1} m^{-1})$	$n(m^{-3})$
Copper	5.88×10^7	8.45×10^{28}
Aluminium	3.65×10^7	18.06×10^{28}

7.6 Quantum free electron theory of metals

The failures of classical free electron theory led to the rise of Quantum Free electron theory and was proposed by Sommerfeld in the year 1928. The quantum free electron theory is based on the following assumptions.

7.6.1 Assumptions

1. Unlike classical free electron theory, in quantum free electron theory, energy values of free electrons are quantized. The energy values of free electrons are discrete since their motion is confined within the boundaries of the metal.
2. Thus in a metal there exists large number of closely spaced energy levels for free electrons which form a band.
3. The distribution of free electrons in the energy levels is as per the Pauli's exclusion principle. Only a maximum of two electrons can occupy a given an energy level. This also suggests the availability of two energy states for free electrons in an energy level corresponding to spin up and spin down states.
4. The potential setup by the lattice ions is assumed to be constant throughout the metal.
5. The mutual repulsion between electrons and the attraction between electrons and lattice ions are neglected.

7.6.2 Fermi energy

For a metal consisting of N atom there exists N number of energy levels in each band. These energy levels are very closely spaced. The energy levels in bands fillup as per Pauli's exclusion principle. Thus free electrons in a metal start filling up the available energy levels from the lower most level of the valence band. **The highest filled energy level in a metal at absolute zero by free electrons is called Fermi Level and the corresponding energy is called Fermi Energy (E_F)**. Thus, at absolute zero and with no electric field applied, all levels below Fermi level are completely filled and above Fermi level are empty.

7.6.3 Density of States (DoS)

According to band theory Energy bands are formed in solids and in a band the spacing between two successive energy levels decreases with increase in energy.

The Density of States is defined as the number of energy states available per unit volume of the material in the unit energy range in the valence band of the material. It is mathematically a continuous function denoted

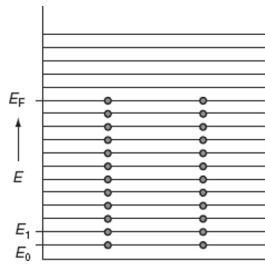


Figure 7.1: Energy Band diagram and Fermi Energy

by $g(E)$. The number of energy levels in the energy range E and $E + dE$ per unit volume of the material is given by $g(E)dE$.

$$g(E)dE = \left(\frac{8\sqrt{2}\pi m^{3/2}}{h^3} \right) E^{-\frac{1}{2}} dE \quad (7.9)$$

The variation of $g(E)dE$ as a function of E is given by

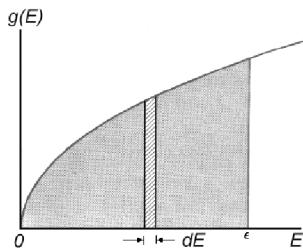


Figure 7.2: Density of states function vs Energy

7.6.4 Fermi-Dirac distribution and Fermi factor

The occupation of energy levels by free electrons in the valence band of a metal is according to Pauli's exclusion principle. This distribution of electrons is not random. It follows a certain universal rule of distribution called Fermi-Dirac Statistics. ***The probability of occupation of an energy level of energy (E) at temperature (T) under thermal equilibrium is evaluated using an expression called Fermi Factor.***

$$f(E) = \frac{1}{e^{\left(\frac{E-E_f}{kT}\right)} + 1} \quad (7.10)$$

7.6.5 Dependence of Fermi factor on energy and temperature

As described, the Fermi factor is a function of energy and temperature. This dependence could be explained for energy levels below and above Fermi level at absolute zero and higher temperatures.

Probability of occupation of levels with energy $E < E_F$ and at $T = 0K$

The Fermi factor or Fermi function is given by

$$f(E) = \frac{1}{e^{\left(\frac{E-E_f}{kT}\right)} + 1} \quad (7.11)$$

Here $E - E_f$ is negative. Substituting the value for $T = 0$

$$f(E) = \frac{1}{e^{\left(\frac{E-E_f}{k*0}\right)} + 1} = \frac{1}{e^{-\infty} + 1} = \frac{1}{0 + 1} = 1$$

Therefore $f(E) = 1$. Hence, at $T = 0K$, all energy levels below the Fermi level are completely filled.

Probability of occupation of levels with energy $E > E_F$ and at $T = 0K$

The Fermi factor or fermi function is given by Here $E - E_f$ is positive. Substituting the value for $T = 0$

$$f(E) = \frac{1}{e^{\left(\frac{E-E_f}{k*0}\right)} + 1} = \frac{1}{e^{\infty} + 1} = \frac{1}{\infty + 1} = 0$$

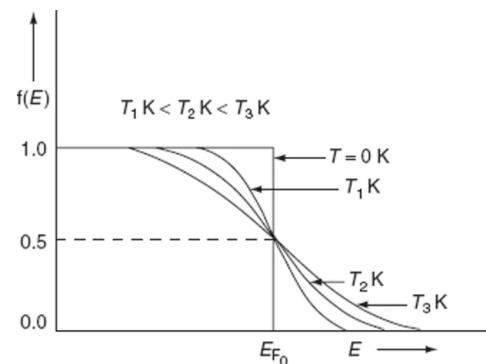
Therefore $f(E) = 0$. Hence, at $T = 0K$, all energy levels above the Fermi level are empty.

Probability of occupation of levels with energy $E = E_F$ and at $T > 0K$

Here $E - E_f = 0$. Substituting the values

$$f(E) = \frac{1}{e^{\left(\frac{0}{kT}\right)} + 1} = \frac{1}{1 + 1} = \frac{1}{2} = 0.5 \quad (7.12)$$

Thus for all temperatures above 0 K the probability of occupation of Fermi level is $\frac{1}{2}$. Thus the variation of Fermi factor with temperature is as shown in the graph 7.3

Figure 7.3: Variation of $f(E)$ as a function of Temperature and Energy

Numerical Problems

1. Calculate the probability of an electron occupying an energy level $0.02eV$ above the Fermi level at $200K$ and $400K$.
2. Calculate the probability of an electron occupying an energy level $0.02eV$ below the Fermi level at $400K$.
3. The Fermi level for silver is $5.5eV$. What is the energy for which probability of occupancy at $300K$ is 0.01
4. Find the temperature at which there is 1% probability that a state with an energy $0.5eV$ above Fermi energy is occupied.
5. Find the probability that an energy level at $0.2eV$ below Fermi level being occupied at temperature $300K$ and $1000K$
6. Calculate the probability that an electron occupies an energy level $0.02 eV$ above Fermi level at $300 K$.

Chapter 8

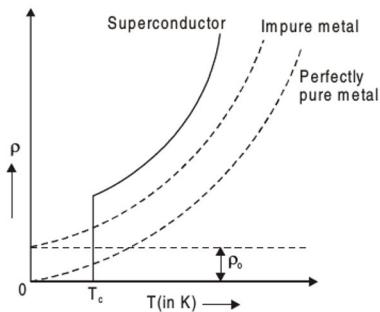
Superconductivity

8.1 Introduction to Superconductivity

Discovery : Lord Kamerlingh Onnes discovered the phenomenon of superconductivity in the year 1911. When he was studying the temperature dependence of resistance of Mercury at very low temperature he found that resistance of Mercury decreases with temperature with the decrease in temperature up to a particular temperature $T_c = 4.15\text{K}$. Below this temperature the resistance of mercury abruptly drops to zero. Between 4.15K and 0K Mercury offered no resistance for the flow of electric current. This phenomenon is reversible and material becomes normal once again when temperature was increased above 4.15K . This phenomenon is called superconductivity and material which exhibits the property is named superconductor.

Definition : Thus the Superconductivity is defined as “*The phenomenon in which resistance of certain metals, alloys and compounds drops to zero abruptly, below certain temperature is called superconductivity*

Variation of Resistivity with Temperature The variation of the resistivity of a superconductor, pure and impure metals with temperature is as shown below.



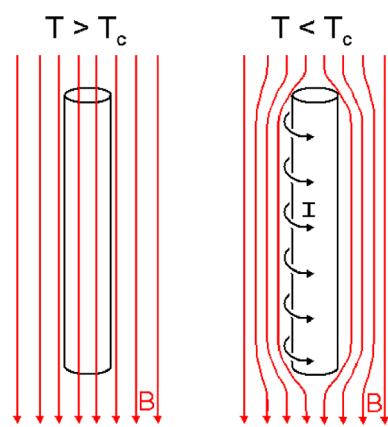
Critical Temperature : The temperature, below which materials exhibit superconducting property is called critical temperature, denoted by T_c . Critical temperature T_c is different for different substances. The materials, which

exhibit superconducting property, are called superconductors.

Above critical temperature material is said to be in normal state and offers resistance for the flow of electric current. Below critical temperature material is said to be in superconducting state. Thus T_c is also called as transition temperature.

8.2 Meissner's Effect

In 1933, Meissner and Ochsenfeld showed that when a superconducting material is placed in a magnetic field it allows magnetic lines of force to pass through, if its temperature is above T_c . If the temperature is reduced below the critical temperature T_c then it expels all the flux lines completely out of the specimen and exhibits perfect diamagnetism. This is known as Meissner's effect. Since superconductor exhibits perfect diamagnetism below the critical temperature T_c , magnetic flux density inside the material is zero.



The expression for magnetic flux density is given by

$$B = \mu_0(M + H) \quad (8.1)$$

Here B is Magnetic Flux Density, M is Magnetization and H is the applied magnetic field strength. For a supercon-

ductor, $B = 0$ at $T < T_c$. Thus we get

$$M = -H \quad (8.2)$$

Thus Meissner's Effect signifies the negative magnetic moment associated with superconductors.

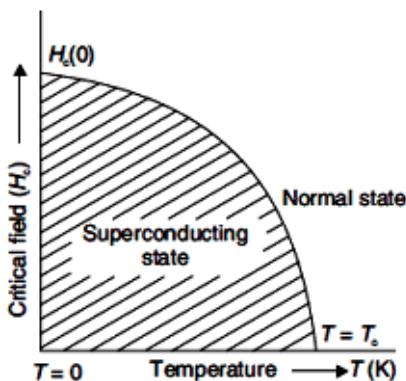
8.3 Critical Field and its Temperature Dependence

Critical field We know that when superconductor is placed in a magnetic field it expels magnetic flux lines completely out of the body and exhibits a perfect diamagnetism. But if the strength of the magnetic field is further increased, it is found that for a particular value of the magnetic field, material loses its superconducting property and becomes a normal conductor. The value of the magnetic field at which the transition occurs from the Superconducting state to Normal Conducting state is called **Critical Field or Critical Magnetic Field** and is denoted by H_c . It is found that by reducing the temperature of the material further superconducting property of the material could be restored. Thus, critical field does not destroy the superconducting property of the material completely but only reduces the critical temperature of the material.

The variation of Critical field with temperature below the critical temperature is given by

$$H_c = H_0 \left[1 - \frac{T^2}{T_c^2} \right] \quad (8.3)$$

Here H_c is the Critical field at any temperature T less than T_c , H_0 is the Critical field at $T = 0K$.



8.4 Types of Superconductors

Superconductors are classified into two types

1. Type I Superconductor or Soft Superconductor
2. Type II Superconductor or Hard Superconductor

Type I Superconductors

paragraph Type I superconductors exhibit complete Meissner's Effect and posses a single value of critical field . The graph of magnetic moment Vs magnetic field is as shown in the Fig.8.1. As the field strength increases the material becomes more and more diamagnetic until H becomes equal to H_c . Above H_c the material allows the flux lines to pass through and exhibits normal conductivity. The value of H_c is very small for soft superconductors. Therefore soft superconductors cannot withstand high magnetic fields. Therefore they cannot be used for making superconducting magnets. Ex. Hg, Pb and Zn.

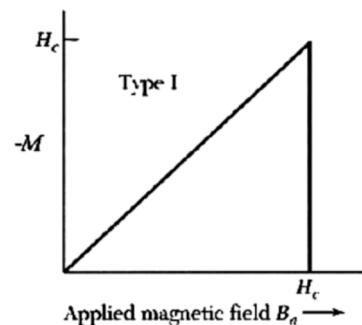


Figure 8.1: Type1 Superconductor

Type II Superconductors

paragraph Superconducting materials, which can withstand high value of critical magnetic fields, are called Hard Superconductors.

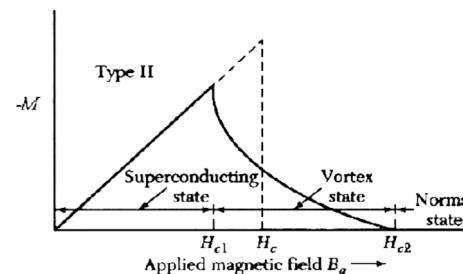
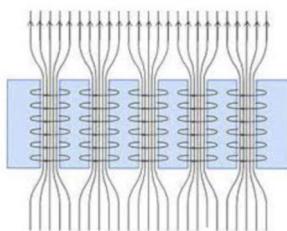


Figure 8.2: Type2 Superconductor

The graph of magnetic moment Vs magnetic field is as shown in the Fig.8.2. Hard superconductors are characterized by two critical fields H_{c1} and H_{c2} . When applied magnetic field is less than H_{c1} material exhibits perfect diamagnetism. Beyond H_{c1} partial flux penetrates and the material is said to be **Vortex State**. Thus flux penetration occurs through small-channelized regions called filia-

ments. As the strength of the field increases further, more and more flux fills the body and thereby decreasing the diamagnetic property of the material. At H_{c2} flux fills the body completely and material loses its diamagnetic property as well as superconducting property completely.



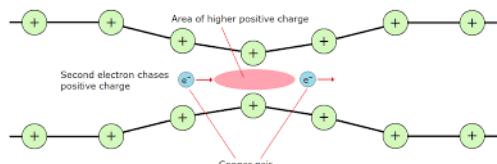
The value of H_{c2} is hundreds of times greater than H_c of soft superconductors. Therefore they are used for making powerful superconducting magnets. Examples: $NbTi$, Nb_3Sn

8.5 BCS Theory of Superconductivity

Bardeen, Cooper and Schrieffer explained the phenomenon of superconductivity in the year 1957. The essence of the BCS theory is as follows.

Consider an electron approaching a positive ion core and suffers attractive coulomb interaction. Due to this attraction ion core is set in motion and thus distorts that lattice. Let a second electron come in the way of distorted lattice and interaction between the two occurs which lowers the energy of the second electron. The two electrons therefore interact indirectly through the lattice distortion or the phonon field which lowers the energy of the electrons. The above interaction is interpreted as electron - Lattice - electron interaction through phonon field.

It was shown by Cooper that, this attractive force becomes maximum if two electrons have opposite spins and momentum. The attractive force may exceed coulombs repulsive force between the two electrons below the critical temperature, which results in the formation of bound pair of electrons called cooper pairs.



Below the critical temperature the dense cloud of Cooper pairs form a collective state and the motion all Cooper pairs is correlated resulting in zero resistance of the material.

8.6 High Temperature Superconductivity

Superconducting materials which exhibit superconductivity at relatively higher temperatures are called high temperature superconductors. Thus high temperature superconductors posses higher value of critical temperature compared to conventional superconductors. Most of the high temperature superconductors are found to fall into the category of ceramics. In 1986 George Bednorz and Alex Muller discovered a compound containing Lanthanum, Barium, Copper and Oxygen having $T_c = 30K$ was developed. In 1987 scientists developed a compound which is an oxide of the form $YBa_2Cu_3O_7$ which is referred to as 1-2-3 compound with $T_c > 90K$ was discovered.

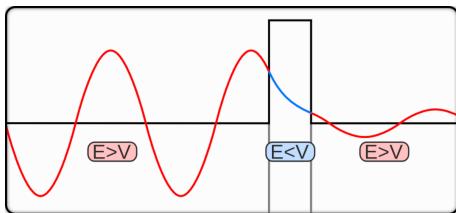
All high temperature superconductors are oxides of copper and bear Perovskite crystal structure characterized by large number of copper-oxygen layers. It was found that addition of extra copper-oxygen layer pushes the critical temperature T_c to higher values. The super currents are strong in the copper-oxygen layer and weak in the direction perpendicular to the planes. Following is the list of High Temperature Superconductors.

Superconductor	Year	T_c (K)
K_3WO_6	1967	6.0
$LiTi_{2+y}O_4$	1973	1.2
$BaPb_{1-y}Bi_yO_3$	1975	13
$La_{2-y}Ba_yCuO_4$	1986	30
$YBa_2Cu_3O_{7-y}$	1987	90
$Ba_{1-y}K_yBiO_3$	1988	20
$BiSrCaCu_2O_{6+y}$	1988	105
$TlBa_2Ca_2Cu_3O_{9+y}$	1989	110
$HgBa_2CaCu_2O_{6+y}$	1993	120
$GdFeAsO_{1-y}$	2008	53.5

8.7 Quantum Tunneling

In classical mechanics, when a particle has insufficient energy, it would not be able to overcome a potential barrier. In the quantum world the particles can often behave

like waves. On encountering a barrier, a quantum wave will not end abruptly. Rather its amplitude decrease exponentially. This drop in amplitude corresponds to a drop in the probability of finding a particle further into the barrier. If the barrier is thin enough, then the amplitude may be non-zero on the other side. This would imply that there is a finite probability that some of the particles will tunnel through the barrier.



In regions where the potential energy is higher than the wave's energy, the amplitude of the wave decays exponentially. If the region is narrow enough, the wave can have a non-zero amplitude on the other side.

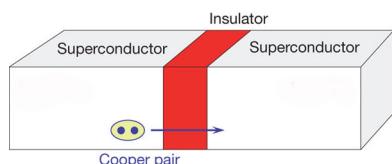
8.8 AC and DC Josephson Junctions

8.8.1 Josephson Junction

In 1962, Brian Josephson predicted that Cooper pairs could tunnel through a very thin insulating layer separating two superconductors. The superconductor-insulator-superconductor layer constitutes the Josephson junction.

8.8.2 DC Josephson Effects

Consider a Josephson junction consisting of two superconducting metal films separated by a thin oxide barrier of 10 to 20 Å thick. The Cooper pairs tunnel from one side of the junction to the other side easily. This due to the phase difference introduced by the insulator between the wave function of Cooper pairs on both sides the junction. Due to the phase difference a super current flows through the junction even if the applied voltage is zero. This is known as the **DC Josephson effect**. Josephson showed that the super current through the junction is given by



$$I_S = I_C \sin \phi_0 \quad (8.4)$$

Here ϕ_0 is the phase difference between the wave functions describing Cooper pairs on both sides of the barrier, and I_C is the critical current at zero voltage condition. I_C

depends on the thickness and width of the insulating layer and the temperature.

8.8.3 AC Josephson Effect

If we apply a dc voltage across the Josephson junction, it introduces an additional phase on Cooper pairs during tunneling. As a result a strikingly new phenomenon will be observed. The dc voltage generates an alternating current I given by

$$I_S = I_C \sin(\phi_0 + \Delta\phi) \quad (8.5)$$

Because of the dc voltage V applied across the barrier, the energies of Cooper pairs on both sides of the barrier differ in energy by $2eV$.

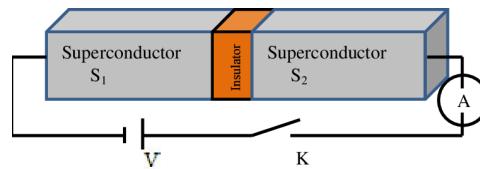


Figure 8.3: DC and AC Josephson Effects

8.9 DC and RF Squids

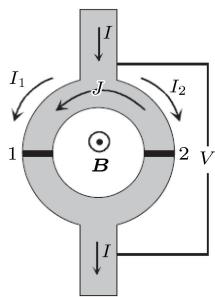
8.9.1 SQUID

A superconducting quantum interference device (SQUID) is a device used to measure extremely weak magnetic flux. Thus, it is basically a sensitive magnetometer made of a superconducting ring. The flux penetrating a superconducting loop is quantized in steps of $\phi_0 = \frac{h}{2e}$. The heart of a SQUID is a superconducting ring, which contains one or more Josephson junctions. There are two main types of SQUID: DC SQUID and RF (or AC) SQUID.

8.9.2 DC SQUID

The DC SQUID was invented in 1964 by Robert Jaklevic, John Lambe, Arnold Silver, and James Mercereau. It has two Josephson junctions in parallel in a superconducting loop. It is based on the DC Josephson effect. It relies on the interference of currents from each junction.

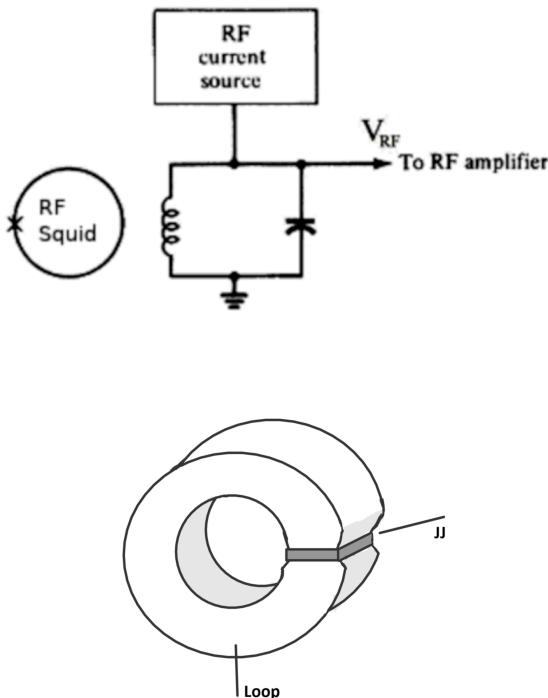
The dc SQUID is biased with a dc current equal to about twice the superconducting current I_c . Dc voltage across the junctions is created. Change in the flux penetrating the loop enhances the current through one JJ and reduces the current through the other. This leads to JJs working asymmetrically, one JJ is driven normally and one is superconducting. This asymmetry provides a feedback current that nulls the flux penetrating the SQUID loop. Total flux



within the loop is multiples of ϕ_0 . The feedback current is a direct measure of changes in flux applied to the SQUID.

8.9.3 RF (AC) Squid

The RF SQUID was invented in 1965 by Robert Jaklevic, John J. Lambe, Arnold Silver, and James Edward Zimmerman at Ford. It is based on the AC Josephson effect and uses only one Josephson junction. It is less sensitive compared to DC SQUID but is cheaper and easier to manufacture in smaller quantities.



In RF SQUID the flux is coupled into a loop containing a single JJ through an input coil and an RF coil. RF coil is part of a high-Q resonant circuit to read out current changes due to induced flux in the SQUID loop. The tuned circuit is driven by a constant RF oscillator which is weakly coupled to the loop. Measuring the change in the input coil current is done by counting the number of peri-

ods the coil produces in the detected RF output, because the detected RF output is a periodic function.

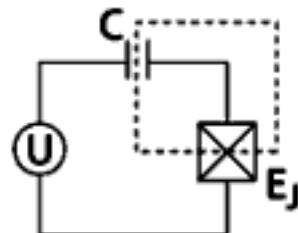
Note : The DC SQUIDs offer higher sensitivity, but RF SQUIDs have lower sensitivity. RF SQUIDs are commonly used form of the sensor, because of their ease and low price of manufacturing in small batches.

8.10 Applications of Superconductivity in Quantum Computing

Squids find application of magnetometers to measure very small fields like human brain magnetic fields. But the applications of SQUIDs in Quantum computing are as follows.

8.10.1 Charge Qubit

In quantum computing, a charge qubit is also known as Cooper-pair box. it is a qubit whose basis states are charge states. The states represent the presence or absence of excess Cooper pairs in the island (dotted region in the figure). In superconducting quantum computing, a charge qubit is formed by a tiny superconducting island coupled by Josephson Junction to a superconducting reservoir.

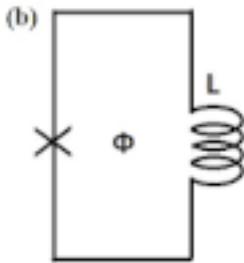


8.10.2 Flux Qubit

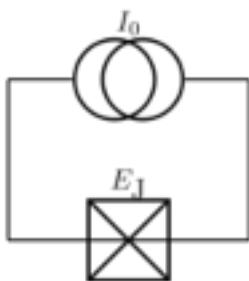
Flux qubits (also known as persistent current qubits) are micrometer sized loops of superconducting metal that is interrupted by a number of Josephson junctions. These devices function as quantum bits. The Josephson junctions are designed so that a persistent current will flow continuously when an external magnetic flux is applied. Only an integer number of flux quanta are allowed to penetrate the superconducting ring.

8.10.3 Phase Qubit

A phase qubit is a current-biased Josephson junction, operated in the zero voltage state with a non-zero current bias.



This employs a single Josephson junction and the two levels are defined by quantum oscillations of the phase difference between the electrodes of the junction. DC SQUID is a type of phase qubit.



8.11 Model Questions

1. Define Phonon. Describe Mathiessen's rule.
2. Explain the failures of Classical Free Electron Theory of Metals.
3. Mention the Assumptions of Classical Free electron theory of metals.
4. Explain the concept of Fermi Level, Fermi Energy, Density of States.
5. Define Fermi Factor. Discuss the variation of Fermi Factor with Energy and Temperature and represent graphically.
6. Discuss the discovery of Superconductivity and hence discuss the variation of resistivity with temperature in superconductor with critical temperature as reference.
7. State and explain Meissner's Effect.
8. Define Critical field and hence explain its variation with temperature below critical temperature.
9. Distinguish between/Explain Type-1 and Type-2 superconductors.
10. Describe the evolution of high temperature of superconductivity.

11. Elucidate the BCS Theory of Superconductivity.
12. Explain the phenomenon of quantum tunneling.
13. Define a Josephson Junction and hence explain the DC and AC Josephson effects.
14. Define Squid and describe DC and RF Squids.
15. Brief the applications of superconductivity in quantum computing.

8.12 Numerical Problems

1. Lead has superconducting transition temperature of $7.26K$. If the initial field at $0K$ is $50 \times 10^3 Am^{-1}$ Calculate the critical field at $6K$.
2. A superconducting tin has a critical temperature of $3.7K$ at zero magnetic field and a critical field of 0.0306 tesla at $0K$. Find the critical field at $2K$.
3. The superconducting transition temperature of Lead is $7.26K$. Calculate the initial field at $0K$ given the critical field at $5 K$ as $33.644 \times 10^3 Am^{-1}$
4. Calculate the ratio of critical fields for a superconductor at $7K$ and $5K$ give the critical temperature $8K$.
5. The critical field for niobium is $1 \times 10^5 Am^{-1}$ at $8K$ and $2 \times 10^5 Am^{-1}$ at $0K$. Calculate the transition temperature of the element.