UNIT 1 - QUANTUM MECHANICS

INTRODUCTION:

Quantum mechanics is a physical science dealing with the behaviour of matter and energy on the scale of atoms and subatomic particles or waves.

The term "quantum mechanics" was first coined by Max Born in 1924. The acceptance by the general physics community of quantum mechanics is due to its accurate prediction of the physical behaviour of systems, including systems where Newtonian mechanics fails.

DUAL NATURE OF LIGHT:

There are some phenomena such as interference, diffraction and polarization which can be explained by considering light as **wave** only.

On the other hand phenomenon such as photoelectric effect and Compton Effect can be explained by considering light as a **particle** only.

When we visualize light as a wave, we need to forget its particle aspect completely and vice versa. This type of behavior of light as a wave as well as particle is known as dual nature of light.

Einstein's theory of photoelectric effect: When a photon of energy $h\upsilon$ is incident on the surface of the metal, a part of energy Φ is used in liberating the electron from the metal. This energy is known as the work function of the metal. The rest of energy is given to the electron so that is acquires kinetic energy $\frac{1}{2} mv^2$. Thus a photon of energy $h\upsilon$ is completely absorbed by the emitter.
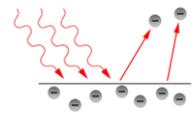
Energy of photon = Energy needed to liberate the electron + Maximum K.E of the liberated electron

$$h\upsilon = \Phi + KE_{max}$$
$$h\upsilon = \Phi + \tfrac{1}{2} mv^2_{max}$$

The above equation is called Einstein's photoelectric equation. This equation can explain all the features of the photoelectric effect.

Compton Effect

When a beam of high frequency radiation (x-ray or gamma-ray) is scattered by the loosely bound electrons present in the scatterer, there are also radiations of longer wavelength along with original wavelength in the scattered radiation. This phenomenon is known as Compton Effect.

When a photon of energy $h\nu$ collides with the electron, some of the energy is given to this electron. Due to this energy, the electron gains kinetic energy and photon loses energy. Hence scattered photon will have lower energy $h\nu'$ that is longer wavelength than the incident one.
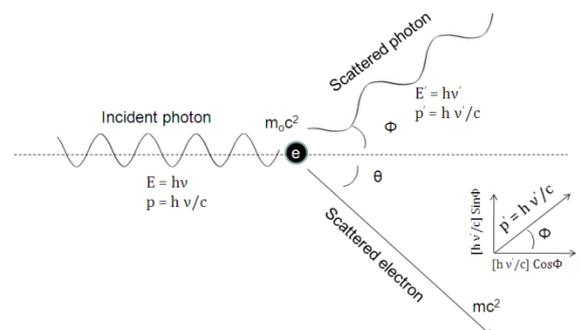
$$(\lambda' - \lambda) = h/mc \; [1-cos\Phi] \quad \text{where } h/mc = \lambda_C = \textbf{Compton wavelength} = 0.02424\text{Å}$$

De Broglie hypothesis:

Louis De Broglie a French Physicist put forward his bold ideas like this

   "Since nature loves symmetry, if the radiation behaves as a particle under certain circumstances and waves under other circumstances, then one can even expect that entities which ordinarily behave as particles also exhibit properties attributable to waves under appropriate circumstance and those types of waves are termed as matter waves.

All matter can exhibit wave-like behavior. For example, a beam of electrons can be diffracted just like a beam of light or a water wave. The concept that matter behaves like a wave was proposed by Louis de Broglie in 1924. It is also referred to as the de Broglie hypothesis of matter waves. On the other hand de Broglie hypothesis is the combination of wave nature and particle nature.

If ' E ' is the energy of a photon of radiation and the same energy can be written for a wave as follows

$E = mc^2$ ---(1) (particle nature)   and $E = h\nu = hc/\lambda$ ---(2) (wave nature)

Comparing eqns (1) & (2) we get

$mc^2 = hc/\lambda$ or $\lambda = h/mc = h/p$

$\lambda = h/p$; where λ = De Broglie wavelength

Particles of the matter also exhibit wavelike properties and those waves are known as matter waves.

Expression for de Broglie wavelength of an accelerated electron

De Broglie wavelength for a matter wave is given by

$\lambda = h/p$; where λ = De Broglie wavelength -------------(1)

From eqn. (1) we find that, if the particles like electrons are accelerated to various velocities, we can produce waves of various wavelengths. Thus higher the electron velocity, smaller will be the de-Broglie wavelength. If velocity v is given to an electron by accelerating it through a potential difference V, then the work done on the electron is eV. This work done is converted to kinetic energy of electron. Hence, we can write

$\frac{1}{2} mv^2 = eV$

$mv = (2meV)^{1/2}$ -------------(2)

But eqn.(1) can be written as

$\lambda = h/mv$ ------------------(3)

Substituting eqn.(2) in eqn.(3) we get

$$\boxed{\lambda = h/(2meV)^{1/2}}$$

PROPERTIES OF MATTER WAVES:

1. The wavelength of a matter wave is inversely related to its particles momentum
2. Matter wave can be reflected, refracted, diffracted and undergo interference
3. The position and momentum of the material particles cannot be determined accurately and simultaneously.
4. The amplitude of the matter waves at a particular region and time depends on the probability of finding the particle at the same region and time.

Wave packet:

Two or more waves of slightly different wavelengths alternately interfere and reinforce so that an infinite succession of groups of waves or wave packets are produced.

The velocity of the individual wave in a wave packet is called phase velocity of the wave and is represented by V_p.
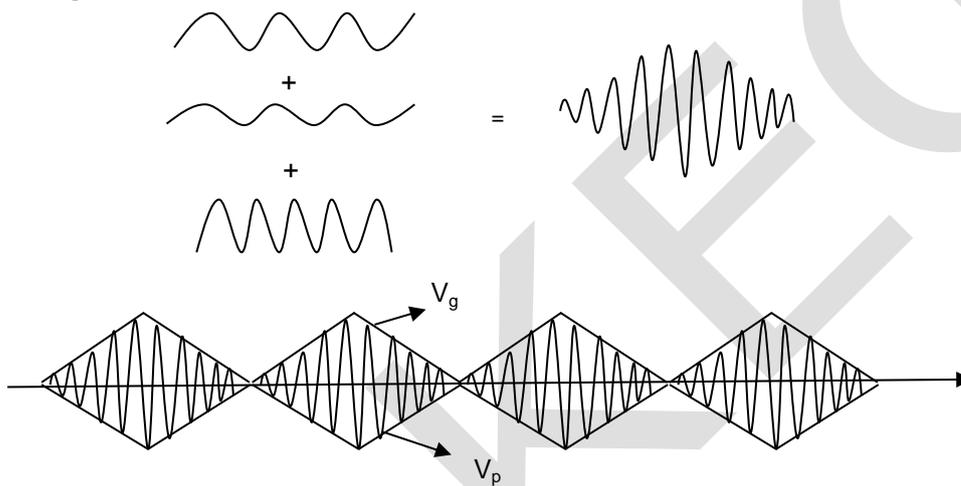
Phase, Group and particle velocities:

According to de Broglie each particle of matter (like electron, proton, neutron etc) is associated with a de Broglie wave; this de Broglie wave may be regarded as a wave packet, consisting of a group of waves. A number of frequencies mixed so that the resultant wave has a beginning and an end forms the group. Each of the component waves propagates with a definite velocity called wave velocity or **phase velocity**.

Expression for Phase velocity:

A wave can be represented by

Y= A sin ($\omega t – kx$) ---------- (1)

Where k = ω/v = wave number (rad/m) ; ω = Angular frequency (rad/s)

When a particle moves around a circle ν times/s, sweeps out $2\pi\nu$ rad/s

In eqn.(1) the term ($\omega t – kx$) gives the phase of the oscillating mass

($\omega t – kx$) = constant for a periodic wave

d ($\omega t – kx$) /dt = 0   or $\omega – k(dx/dt) = 0$ or   dx/dt =ω/k

$$\boxed{v_p = \omega/k}$$

When a wave packet or group consists of a number of component waves each traveling with slightly different velocity, the wave packet (group) travels with a velocity different from the velocities of component waves of the group; this velocity is called **Group velocity**.

Expression for Group velocity:

A wave group can be mathematically represented by the superposition of individual waves of different wavelengths. The interference between these individual waves results in the variation of amplitude that defines the shape of the group. If all the waves that constitute a group travel with the same velocity, the group will also travel with the same velocity.

If however the wave velocity is dependent on the wavelength the group, velocity will be different from the velocity of the individual waves.

The simplest wave group is one in which two continuous waves are superimposed. Let the two waves be represented by

$y_1 = a \cos(\omega_1 t - k_1 x)$ and $y_2 = a \cos(\omega_2 t - k_2 x)$

The resultant

$y = y_1 + y_2 = a \cos(\omega_1 t - k_1 x) + a \cos(\omega_2 t - k_2 x)$

$$y = 2a \cos\left[\left(\frac{\omega_1 - \omega_2}{2}\right)t - \left(\frac{k_1 - k_2}{2}\right)x\right] \cos\left[\left(\frac{\omega_1 + \omega_2}{2}\right)t - \left(\frac{k_1 + k_2}{2}\right)x\right]$$

$Let \quad \left(\frac{\omega_1 + \omega_2}{2}\right) = \omega$ and $\left(\frac{k_1 + k_2}{2}\right) = k$

$$y = 2a \cos\left[\left(\frac{\omega_1 - \omega_2}{2}\right)t - \left(\frac{k_1 - k_2}{2}\right)x\right] \cos(\omega t - kx)$$

This equation represents a wave of angular frequency ω and wave number k whose amplitude is modulated by a wave of angular frequency $(\omega_1 - \omega_2)/2$ and wave number $(k_1 - k_2)/2$ and has a maximum value of 2a. The effect of this modulation is to produce a succession of wave groups as shown below:

The velocity with which this envelope moves, i.e., the velocity of the maximum amplitude of the group is given by $\quad v_g = \dfrac{\omega_1 - \omega_2}{k_1 - k_2} = \dfrac{\Delta\omega}{\Delta k}$

If a group contains a number of frequency components in an infinitely small frequency interval (for $\Delta k \to 0$), then the above expression may be written as

$v_g = \dfrac{d\omega}{dk}$ This is the expression for group velocity

Two or more waves of slightly different wavelengths alternately interfere and reinforce so that an infinite succession of groups of waves or wave packets are produced. The de Broglie wave group associated with a particle travels with a velocity equal to the **particle velocity.**

Relation between group velocity (v_g) and phase velocity(v_p)

We know that

$$v_p = \frac{\omega}{k} \quad \text{------ (1)} \qquad \text{and} \qquad v_g = \frac{d\omega}{dk} \quad \text{------ (2)}$$

$$\therefore \quad \omega = k\, v_p$$

$$\therefore \quad v_g = \frac{d}{dk}(k\, v_p) = k\frac{dv_p}{dk} + v_p$$

$$\therefore \quad v_g = v_p + k\frac{dv_p}{dk} = v_p + k\left(\frac{dv_p}{d\lambda}\right)\left(\frac{d\lambda}{dk}\right)$$

$$= v_p + \left(\frac{2\pi}{\lambda}\right)\left(\frac{-\lambda^2}{2\pi}\right)\left(\frac{dv_p}{d\lambda}\right)$$

$$v_g = v_p - \lambda\left(\frac{dv_p}{d\lambda}\right)$$

Relation between the particle velocity of a matter wave and is its group velocity

$$v_g = \frac{d\omega}{dk} \text{ - - - - - - - (1)}$$

where $\omega = 2\pi v = 2\pi\left(\dfrac{E}{h}\right)$

$$d\omega = \left(\frac{2\pi}{h}\right)dE \text{ - - - - - - -(2)}$$

Also, we know that

$$k = \frac{2\pi}{\lambda} = 2\pi\left(\frac{p}{h}\right) = \left(\frac{2\pi}{h}\right)p$$

$$dk = \left(\frac{2\pi}{h}\right)dp \text{ - - - - - - - - (3)}$$

$$\therefore \frac{d\omega}{dk} = \frac{dE}{dp} \text{ - - - - - - - - - - - - - - -(4)}$$

From eqn.(1) and (4) one can write

$$v_g = \frac{dE}{dp}$$

Expression for kinetic energy can be written as

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

$$dE = \frac{p}{m}dp$$

$$\frac{dE}{dp} = \frac{p}{m} = v_{particle} - - - - - - - (5)$$

comparing eqns.(1),(4) & (5) we get

$$v_{group} = v_{particle}$$

Expression for de Broglie wavelength using group velocity

We know that the expression for group velocity is given by

$$v_g = \frac{d\omega}{dk} \quad \text{-------} (1)$$

where $\omega = 2\pi\nu \Rightarrow d\omega = 2\pi d\upsilon$

$$k = \frac{2\pi}{\lambda} \Rightarrow dk = 2\pi d\left(\frac{1}{\lambda}\right)$$

$$\therefore v_g = \frac{d\upsilon}{d\left(\frac{1}{\lambda}\right)}$$

Also, we know that $v_{group} = v_{particle}$

$$\therefore v_{particle} = \frac{d\upsilon}{d\left(\frac{1}{\lambda}\right)} \quad \text{-----} (2)$$

We can write

Total energy $=$ potential energy $+$ kinetic energy

i.e $E = \frac{1}{2}mv^2 + V$ ----(3)   also one can write $E = h\upsilon$ -----(4)

Equating eqn. (3) & (4)

$$h\upsilon = \frac{1}{2}mv^2 + V \text{--------}(5)$$

Taking derivative on both sides of eqn.(5) we get

$h\, d\upsilon = mv\, dv$ (If we treat $V = $ constant then $dV = 0$)

$$\therefore d\upsilon = \left(\frac{mv}{h}\right)dv \text{----------} (6)$$

Substituting eqn.(6) in eqn.(2) we get

$$d\left(\frac{1}{\lambda}\right) = \left(\frac{m}{h}\right)dv$$

Taking integration on both sides we get

$$\frac{1}{\lambda} = \frac{mv}{h} + \text{const.}$$

$$\therefore \lambda = \frac{h}{mv}$$

Relation between phase velocity, particle velocity and velocity of light

Since de Broglie wave is associated with a moving particle therefore, it is very much essential to know that if both the particle and wave associated with them travel with the same velocity or with different velocity.

$$v_p = \omega/k = 2\pi\upsilon/(2\pi/\lambda) = \lambda\nu = (h/mv)(mc^2/h)$$

$$\therefore \mathbf{v_p = c^2/v}$$

As the velocity of material particle is always less than the velocity of light c, it means that the propagation velocity of de Broglie wave is always greater than c. Thus it seems that both the particle & de Broglie wave associated with the particle do not travel together with the same velocity & the wave would leave the particle behind. However, these difficulties can be ruled by considering that a moving material particle is equivalent to a wave packet rather than a single wave.

Principle of complimentarity :

The experiment of Davisson & Germer demonstrated the diffraction of electron beams. The wave nature of electrons can also be demonstrated by interference with a double slit. But it is an extremely difficult task to prepare a suitable double slit that can transmit an electron beam.

But the experiment was done by Jönson in 1961. He passed a 50,000eV beam of electron through a double slit. The pattern obtained by him was very similar to the interference pattern obtained by Young with visible light.

In an experiment of the above type it is rather tempting to try to find out through which slit an electron has passed. If we design a suitable device for detecting the passage of an electron through one of the slits, the interference pattern is found to vanish.

If the electron is to behave like a classical particle, it has to pass through one of the two slits. On the other hand, if it is a wave, it can pass through both the slits!

When we try observing the passage of electron through one of the slits, we are examining its particle aspect. However, when we observe the interference pattern we are investigating the wave aspect of electron.

At a given moment and under given circumstances the electron will behave either as a particle or as a wave but not as both.

In other words, the particle and wave nature of a physical entity cannot be observed simultaneously.

Heisenberg's Uncertainty principle.

Physical quantities like position, momentum, time, energy etc. can be measured accurately in macroscopic systems (i.e. classical mechanics). However, in the case of microscopic systems, the measurement of physical quantities for particles like electrons, protons, neutrons, photons etc are not accurate. If the measurement of one is certain and that of other will be uncertain.

A wave packet that represents and symbolizes all about the particle and moves with a group velocity describes a de Broglie wave. According to Bohr's probability interpretation, the particle may be found anywhere within the wave-packet. This implies that the position of the particle is uncertain within the limits of the wave packet. As the wave packet has a velocity spread, there is an uncertainty about the momentum of the particle. Thus according to uncertainty principle states that *the position and the momentum of a particle in an atomic system cannot be determined simultaneously and accurately. If Δx is the uncertainty associated with the position of a particle and Δpₓ the uncertainty associated with its momentum, then the product of these uncertainties will always be equal or greater than h/4π. That is*

$$\Delta x \ \Delta p_x \geq h/4\pi$$

Different forms of uncertainty principle

$$\Delta E \ \Delta t \geq h/4\pi$$
$$\Delta \omega \ \Delta \theta \geq h/4\pi$$

Applications Heisenberg's Uncertainty principle (Nonexistence of electron in the nucleus)

The radius 'r' of the nucleus of any atom is of the order of 10^{-14}m so that if an electron is confined in the nucleus, the uncertainty in its position will be of the order of $2r = \Delta x$ (say) i.e diameter of the nucleus

But according to HUP

$\Delta x \ \Delta p \geq h/4\pi$ (Δp = uncertainty in momentum)

$\Delta x \sim 2\times10^{-14}$m

Therefore,

$\Delta p = h/(4\pi \ \Delta x) = 6.625\text{E-}34 / (4\pi \times 2\times10^{-14}) = $ **2.63 x 10⁻²¹ kg-m/s**

Taking $\Delta p \sim p$ we can calculate energy using the formula

$E^2 = c^2(p^2 + m_o^2c^2) = (3\times10^8)^2 \times [(2.63 \times 10^{-21})^2 + (9.1\times10^{-31})^2 \times (3\times10^8)^2]$
$\qquad = 7.932\times10^{-13}\text{J} = 4957745 \text{ eV} \sim \textit{5 MeV}$

However, the experimental investigations on beta decay reveal that the kinetic energies of electrons must be equal to 4MeV. Since there is a disagreement between theoretical and experimental energy values we can conclude that electrons cannot be found inside the nucleus.

a) Wave function (ψ)**:**

Water waves ------------ height of water surfaces varies

Light waves -------------- electric & magnetic fields vary

Matter waves -------------- wave function (ψ)

Ψ is related to the probability of finding the particle. Max Born put these ideas forward for the first time.

➢ The wave function ψ indicates the state of the particle. However it has no direct physical significance. There is a simple reason why ψ cannot be interpreted in terms of an experiment. The probability that something be in a certain place at a given time must lie between 0 & 1 i.e. the object is definitely not there and the object is definitely there respectively.

➢ An intermediate probability, say 0.2, means that there is a 20% chance of finding the object. However, the amplitude of a wave can be negative as well as positive and a negative probability -0.2 is meaningless. Hence ψ by itself cannot be an observable quantity.

➢ Because of this the square of the absolute value of the wave function ψ is considered and is known as probability density denoted by $|\psi|^2$

➢ The probability of experimentally finding the body described by the wave function ψ at the point x, y, z at the time t is proportional to the value of $|\psi|^2$.

• Small value of $|\psi|^2$ ----- Less possibility of presence
• As long as $|\psi|^2$ is not actually zero somewhere however, there is a definite chance, however small, of detecting it there. Max Born first made this interpretation in 1926.
• If we know the momentum of a particle, we can find the wavelength of the associated matter wave by using the equation $\lambda = h/mv$. We have now to realize how we can describe the amplitude of a matter wave. That is we have to find out just what is waving.

A particle of mass 'm' traveling in the increasing x- direction with no force acting on it is called a free particle.

According to Schrodinger the wave function ψ(x,t) for a free particle moving in the positive x direction is given by

$\psi(x,t) = \psi_o\, e^{i(kx - \omega t)}$, here ψ_o = amplitude and ψ(x,t) = complex

b) Probability density :

If ψ is a complex no. then its complex conjugate is obtained by replacing i by –i, ψ alone don't have any meaning but only ψψ* gives the probability of finding the particle. In quantum mechanics we cannot assert where exactly a particle is. We cannot say where it is likely to be

$P(x) = \psi\psi^* = [\psi_o\, e^{i(kx - \omega t)}]\,[\psi_o\, e^{-i(kx - \omega t)}] = |\psi_o|^2$

➢ Large value of $|\psi|^2$ ----- Strong possibility of presence of particle
➢ Small value of $|\psi|^2$ ----- Less possibility of presence of particle

c) Normalization of wave function:

The probability of finding the particle between any two coordinates x_1 & x_2 is determined by

summing the probabilities in each interval dx. Therefore there exists a particle between x_1 & x_2 in any interval dx. This situation can be mathematically represented by

$$\int_{x_1}^{x_2} |\psi(x)|^2 dx = 1$$
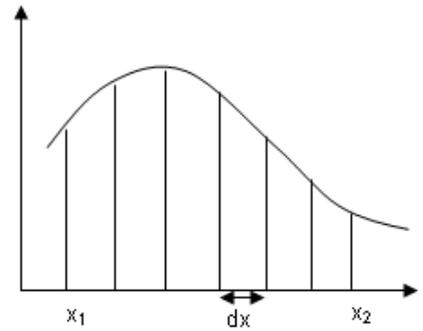
If a particle exists anywhere in a region of space within a small volume element dv, then the normalized condition can be represented as

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$$

Time independent one dimensional Schrodinger wave equation :

A wave eqn. for a debroglie wave is given by

$\psi = A\, e^{i(kx-\omega t)}$ ------------- (1)

Differentiating twice eqn.(1) with respect to t we get

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \left[A\, e^{i(kx-\omega t)} \right]$$

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

Displacement 'y' of a wave is given by $\quad y = A\sin[\omega t - kx]$ -------(A)

Differentiating twice w.r.t 't' we get $\quad \dfrac{\partial^2 y}{\partial t^2} = -\omega^2 y$ ----------(B)

Similarly differentiating twice w.r.t 'x' we get $\quad \dfrac{\partial^2 y}{\partial x^2} = -k^2 y = -\left(\dfrac{\omega}{v}\right)^2 y = -\left(\dfrac{1}{v}\right)^2 \omega^2 y$ ----(C)

Comparing eqns (B) & (C) we get $\quad \dfrac{\partial^2 y}{\partial x^2} = \left(\dfrac{1}{v^2}\right)\dfrac{\partial^2 y}{\partial t^2}$ ------ (3)

By analogy eqn. for a traveling de Broglie wave is given by

$$\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{1}{v^2}\right)\frac{\partial^2 \psi}{\partial t^2}$$ ------ (4)

Comparing eqns. (2) & (4) $\dfrac{\partial^2 \psi}{\partial x^2} = -\left(\dfrac{\omega}{v}\right)^2 \psi$; where $\omega = 2\pi v$ and $v = \nu\lambda$

$$\frac{\partial^2 \psi}{\partial x^2} = -\left[\frac{4\pi^2}{\lambda^2}\right]\psi \quad \text{or} \quad \frac{1}{\lambda^2} = -\left[\frac{1}{4\pi^2 \psi}\right]\frac{\partial^2 \psi}{\partial x^2}$$ --------(5)

For a particle of mas 'm' moving with a velocity 'v'

Kinetic energy = ½ mv² = m²v²/2m = p²/2m

But p = h/λ

Therefore, $KE = [1/\lambda^2][h^2/2m]$

Substituting for $1/\lambda^2$ from eqn (5) we get

$$KE = -\left[\frac{1}{4\pi^2\psi}\right]\left[\frac{h^2}{2m}\right]\frac{\partial^2\psi}{\partial x^2} = -\left[\frac{h^2}{8\pi^2m}\right]\left[\frac{1}{\psi}\right]\frac{\partial^2\psi}{\partial x^2}$$

Total energy is given by

$$E = PE + KE = V - \left[\frac{h^2}{8\pi^2m}\right]\left[\frac{1}{\psi}\right]\frac{\partial^2\psi}{\partial x^2}$$

$$\frac{\partial^2\psi}{\partial x^2} = (E - V)\left[\frac{-8\pi^2m}{h^2}\right]\psi$$

$$\mathbf{\frac{\partial^2\psi}{\partial x^2} + \left[\frac{8\pi^2m}{h^2}\right](E - V)\psi = 0}$$

Properties of wave function.

Ψ should

• satisfy the law of conservation of energy i.e Total energy = PE + KE
• be consistent with de Broglie hypothesis i.e $\lambda = h/p$
• be single valued (because probability is unique)
• be continuous
• be finite
• be linear so that de Broglie waves have the important superposition property

Eigen value & Eigen function:

A wave function Ψ, which satisfies all the properties is said to be *Eigen function* (Eigen = proper)

An operator $\hat{O}$ is a mathematical operator (differentiation, integration, addition, multiplication, division etc.) which may be applied on a function $\Psi(x)$, which changes the function to another function $\Phi(x)$. This can be represented as

$$\hat{O}\,\psi(x) = \phi(x)$$

If a function is Eigen function, then by result of operation with an operator $\hat{O}$, we get the same function as

$$\hat{O}\,\psi(x) = \lambda\psi(x)$$

$\Psi(x)$ = eigen function, λ = eigen value, $\hat{O}$ = operator and $\Psi(x)$ = operand

Eg. $-\dfrac{d^2}{dx^2}(\sin 2x) = 4(\sin 2x)$, Here $\hat{O} = -\dfrac{d^2}{dx^2}$; $\lambda = 4$; $\psi(x) = \sin 2x$
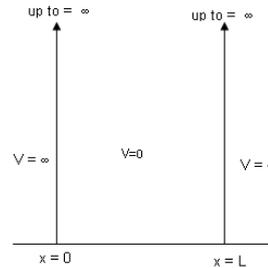
Energy Eigen values and Eigen function for a particle trapped in a potential well of infinite height

A particle moving freely in one-dimensional "box" of length 'L' trapped completely within the box is imagined to be as a particle in a potential well of infinite depth.

Initial conditions

$V(x) = 0 \; ; \; 0 < x < L$

$V(x) = \infty \; ; \; x < 0, \; x > L$

If the walls of the box are perfectly rigid, the particle must always be in the box and the probability for finding it elsewhere must be zero. Thus outside the box we have

$\Psi(x) = 0 \; ; \; x < 0, \; x > L$

Schrodinger wave equation is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \text{--------------- (1)}$$

Inside the well V = 0, thus equation (1) becomes

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

Let $\quad \dfrac{8\pi^2 m}{h^2} E = k^2 \quad \text{---------------- (3)}$

Substituting eqn.(3) in eqn.(2) we get

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{----------------- (4)}$$

The solution for above differential eqn. can be written as

$\Psi(x) = A \sin kx + B \cos kx \quad \text{---------------- (5)}$

Let us solve equation (5) outside the boundaries

Case I : For $x \leq 0, \; \Psi = 0$

Therefore, $\quad \Psi(0) = A \sin 0 + B \cos 0$

$\Rightarrow \quad \textbf{B = 0} \quad \text{------------------- (6)}$

Case II : For x ≥ L, Ψ = 0

Therefore, $\Psi(L) = A \sin kL$

$\Rightarrow$ $A \sin kL = 0$

$\Rightarrow$ Either $A = 0$ or $\sin kL = 0$

 $A \neq 0$ because Ψ is finite inside the box

Therefore, $\sin kL = 0$

$\Rightarrow k L = n \pi$

$\Rightarrow$ **k = n π / L** ----------------- (7)

Where   n = 1,2,3…………

Thus the solution to the Schrodinger equation for a particle trapped in a linear region of length 'L' is a series of standing de Broglie waves.

Only certain values of k are permitted and thus only certain values of E may occur. Thus the energy is quantized.

Substituting eqn.(6) in eqn.(3) we get

$$\frac{8\pi^2 m}{h^2} E = \left(\frac{n\pi}{L}\right)^2 \qquad \text{or}$$

$$\boxed{E_n = \frac{n^2 h^2}{8mL^2}}$$ ------------------- (8)   where   n = 1,2,3……….

Equation (8) is the expression for energy Eigen values for a particle trapped in a potential well of infinite depth.

However, the particle must be present somewhere inside the well, thus

$$\int_0^L |\psi|^2 \, dx = 1$$

Substituting eqn.(6) & eqn.(7) in eqn.(5) we get

$\Psi(x) = A \sin[n\pi / L]x$

$$\int_0^L A^2 \sin^2\left(\frac{n\pi}{L}\right)x \; dx = 1 \qquad \text{However, we know that } \sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$$

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

$$\frac{A^2}{2}\left[x\big]_0^L - \left\{ \left(\frac{L}{2n\pi}\right)\sin\left(\frac{2n\pi}{L}\right)x \right\}\Big]_0^L \right] = 1$$
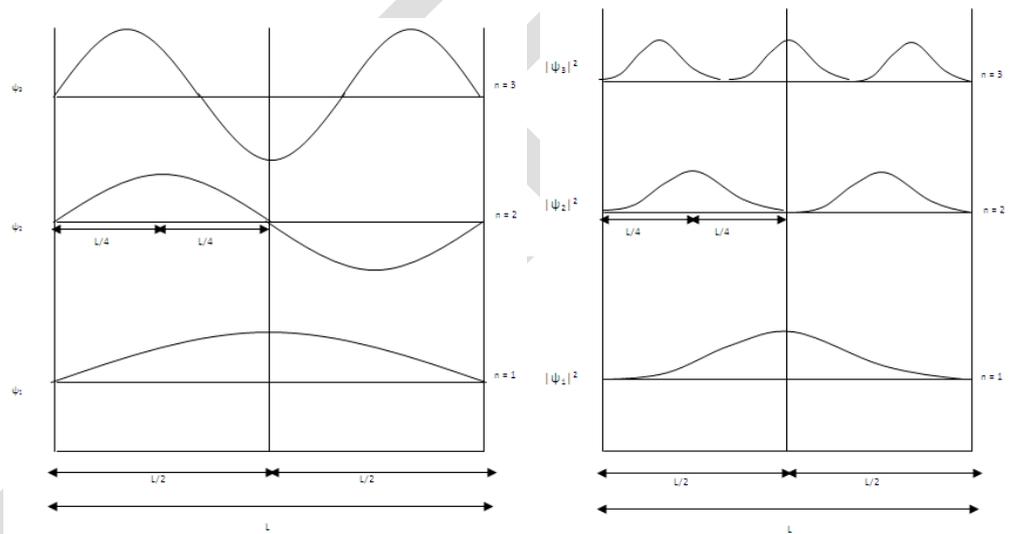
$$\frac{A^2}{2}\left[L - \left(\frac{L}{2n\pi}\right)\sin(2n\pi)L \right] = 1 \qquad \text{But} \quad \sin 2n\pi = 0$$

Therefore,

$$\frac{A^2 L}{2} = 1 \qquad \text{or} \qquad \boxed{A = \sqrt{\frac{2}{L}}}$$

Hence, we can write the wave function as

$$\boxed{\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x}$$

Energy Eigen values for a free particle

A particle moving in any region of space without the influence of force is called as a free particle.

We know that Schrodinger wave equation can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \text{--------------- (1)}$$

Let us treat $V = 0$, thus equation (1) becomes

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

Let $\quad \dfrac{8\pi^2 m}{h^2}E = k^2 \quad$ ---------------- (3)

Substituting eqn.(3) in eqn.(2) we get

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{---------------- (4)}$$

The solution for above differential eqn. can be written as

$$\Psi(x) = A \sin kx + B \cos kx \quad \text{---------------- (5)}$$

It is not possible to apply the boundary condition and solve the eqn. (5). Because Ψ is finite everywhere in the space. Hence energy eigen value for a free particle can be written as

$$E = \frac{h^2 k^2}{8\pi^2 m} = \frac{h^2}{8\pi^2 m}\left(\frac{2\pi}{\lambda}\right)^2 = \frac{h^2}{2m\lambda^2} = \frac{\mathbf{p}^2}{\mathbf{2m}}$$

Therefore for a free particle, the energy Eigen values are not quantized and is equal to the kinetic energy of the particle itself.
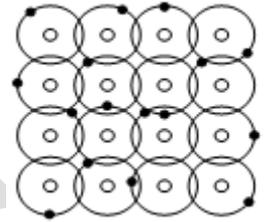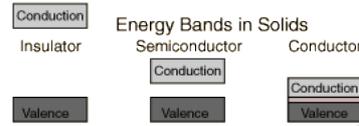
Postulates of Classical Free Electron Theory (CFET) or Drude-Lorentz theory

Electrical conductivity in Metals:

Drude-Lorentz theory

- Large number of atoms combines to form a metal; the boundaries of the neighbouring atoms slightly overlap on each other. Due to such an overlapping, though the core electron remain unaffected, the valence electron find continuity from atom to atom and thus can move easily throughout the body of the metal.
- The free movement of electrons means that none of them belongs to any atom in particular, but each of them belongs to the metal to which they are confined to. Thus, each such electron is named a free electron.
- The electrons in the closed shells are called core electrons and those in the outer incomplete shell are called valence electrons.
- The core electrons are strongly attracted by comparatively immobile nucleus (+vely charged metallic ions). The valence electrons in the constituent atoms are free electrons.
- In 1900, Drude assumed that the electrons in a metal are free to move and form 'electron gas'.Lorentz predicted that the kinetic theory of gases could be applied to the free electron gas. When the atoms are brought closer to form metal, the valence electrons get detached and move freely through the metal. Hence, they are called free or conduction electrons. The concentration of the free electrons is ~ $10^{28}/m^3$.

Assumptions of classical free electron theory:

1. A metal is imagined as a structure of 3-dimensional array of ions in between which, there are freely moving valence electrons confined to the body of the material. Such freely moving electrons cause electrical conduction under an applied field and hence referred to as conduction electrons.
2. The free electrons are treated as equivalent to gas molecules and thus they are assumed to obey the laws of kinetic theory of gases. In the absence of the field, the energy associated with each electron at a temp.T is given by $(3/2) kT$, where k is Boltzmann constant. It is related to the KE through the relation $(3/2)kT = (1/2)m(v_{th})^2$, where v_{th} = thermal velocity.
3. The electric potential due to the ionic cores is taken to be essentially constant throughout the body of the metal and the effect of repulsion between the electrons is considered insignificant.
4. The electric current in a metal due to an applied field is a consequence of the drift velocity in a direction opposite to the direction of the field.

What do you understand by Drift velocity?

Drift velocity:
The disconnection of a valence electron from the parent atom results in a virtual loss of one negative charge for that atom. Consequently, the electrical neutrality of the atom is lost and it becomes an ion. The structure formulation due to the array of such fixed ions in 3-dimensions is called lattice.

"The nucleus of an atom together with the electrons in the inner shells is called the ionic core"

A free e⁻ while moving across the metal, knocks against the lattice corners. Its direction of motion will be continuously changing.

The random motion of the free e⁻ will be retained in the metal even after the application of an electric field. As the e⁻s have –ve charge, the net motion or drift of the e⁻s will be in a direction opposite to that of the applied electric field. The velocity of this overall motion of the e⁻s is called drift velocity. In the absence of an electric field, the free electrons in a metal will be moving at random in all directions and will be at thermal equilibrium. Then by the kinetic theory of gases

$$\frac{1}{2}mv^2 = 3/2kT$$

The force acting on an electron under the application of field E will Ee. The resulting acceleration will be Ee/m. The drift velocity is small compared to the random velocity v. Further, the drift velocity is not retained after a collision with an atom because of the relatively large mass of the atom. Hence, just after a collision, the drift velocity is zero. If the mean free path is λ then the time that elapses before the next collision takes place is λ/v. Hence the drift velocity acquired just before the next collision takes place is

Drift velocity = (acceleration)x(time constant) = (Ee/m)x(λ/v)

Define the term and Mean free path, Mean collision time and Relaxation time.

The average distance traversed by the free electron between two successive collisions with the lattice corners is called *Mean free path (λ)*.

The average time interval between two successive collisions of an electron with the lattice corners is called *Mean collision time (τ)*.
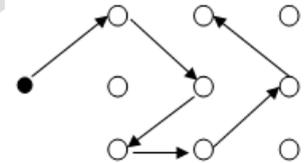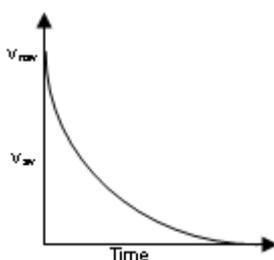
Relaxation time:
In the absence of an external electric field, the free electrons in a metal will be moving at random in all directions. Hence, the average velocity v_{av} in any particular direction will be zero. When an external electric field is applied, the electrons will have a net average velocity v_{nav} in a direction opposite to the direction of the applied field. If the external field is turned off, the average velocity reduces exponentially from the value v_{nav} to zero.

$V_{av} = 0$ (in the absence of the field)

$V_{av} = V_{nav}$ (in the presence of the field due to drift velocity)

If the field is turned off suddenly, the average velocity V_{av} reduces exponentially to zero from V_{nav}

$$v_{av} = v_{nav}\, e^{-(t/\tau_r)} \quad ; where\ \tau_r = \text{Re}\ laxation\ time,\ t = time\ counted\ when\ the\ field\ is\ turned\ off$$

at $t = \tau_r$

$$v_{av} = \frac{1}{e}(v_{nav})$$

When the external electric field is removed then the time required for the average velocity of the conduction electrons in a metal to be reduced to (1/e) times its initial value at the time of removal of the field is called Relaxation time.

Expression for electrical conductivity in metals:

Under the influence of electric field E on a conductor, the electrons having charge e will get a force

F = eE ----------- (1)

If m is the mass of the electron, then from Newton's II law of motion

F = ma = m(dv/dt) ------------ (2)

Comparing eqns. (1) & (2)

eE = m(dv/dt)   →   dv = (Ee/m)dt

By taking integration on both sides we get

v = (Ee/m)t ------------ (3)

Let t = τ = collision time (average)

Since by definition, the collision time applies to an average value, the corresponding velocity in eqn.(3) also becomes the average velocity v_{av}.

Therefore, v_{av} = (Ee/m) τ --------------(4)

We know that

Current density (J) α Applied field (E)

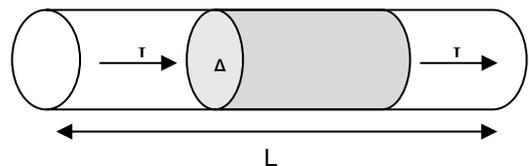J = σ E   ; where σ = electrical conductivity

Therefore, σ = J/E -----------(5)

But J = I/A   current per unit cross sectional area

σ AE = I ------------- (6)

Conductor cross section

Let a current carrying conductor of length L

& area of cross section A is having 'n' number of e^{-s} .

Then we can write total charge

$q = (nAL) e$; $t = L/v_{av}$; $I = q/t$

Now the average velocity of electrons is given by

v_{av} = distance/time

v_{av} = distance for a unit time

Therefore,   volume = v_{av} x area

&   current $(I) = [(nAL)e]/[L/v_{av}] = nA\, v_{av}\, e$ ------------(7)

Substituting the values of 'I' and 'v_{av}' from eqns. (4) & (6) we get

$\sigma\, AE = nA[(Ee/m)\, \tau]e$

$\boldsymbol{\sigma = [ne^2/m]\, \tau}$ ------------- **(8)**

Explain the failures of classical free electron theory

Molar specific heat at constant volume (C_V)

Specific heat capacity is the measure of heat energy required to increase the temperature of a substance by one degree Kelvin (when the unit quantity is mole then the term molar specific heat capacity is used).

Molar specific heat of a gas is $C_V = (3/2)R$ but

Specific heat of a metal by its conduction e^- is

$C_V = 10^{-4}\, RT$

This deviation in the results of C_v is not explained by the classical theory.

Temperature dependence of σ

We know that

$$\frac{1}{2}mv_{th}^2 = \frac{3}{2}kT$$

$$v_{th} = \sqrt{\frac{3kT}{m}}$$

$$v_{th} \alpha \sqrt{T}$$

However, mean collision time τ is inversely proportional to $v_{th.}$ Therefore,

$$\tau \alpha \frac{1}{v_{th}} \quad \Rightarrow \quad \tau \alpha \frac{1}{\sqrt{T}}$$

$$But \quad \sigma = \frac{ne^2\tau}{m}$$

$$\Rightarrow \quad \sigma \alpha \tau$$

$$\Rightarrow \quad \sigma \alpha \frac{1}{\sqrt{T}}$$

But experiment ally it is observed that $\sigma \alpha \dfrac{1}{T}$

Dependence of electrical conductivity on concentration of electrons

We have $\sigma = [ne^2/m]\ \tau \implies \sigma\ \alpha\ n$

According to this dependence σ will be high for the metals having large electron concentration. But some of the metals having less electron concentration is found to have higher σ and vice versa. These experimental observations were not explained by classical free electron theory.

Write a short note on Fermi-Dirac statistics

Fermi-Dirac statistics:

Particles of half integral spin (1/2, 3/2……..) which obey Pauli's exclusion principle such as electrons or nucleons are known as fermions and their distribution function is the Fermi-Dirac distribution. Fermi-Dirac distribution function is given by

$$f_{FD}(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$$
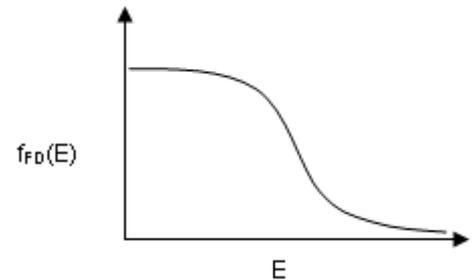
- General observation is that all of the distribution functions fall to zero at large values of E
- When $E \gg kT$, the occupation probability is very small
- f_{FD} never becomes larger than one just as we expect for particles that obey the Pauli's exclusion principle.
- At T = 0, all energy levels up to E_F are occupied (f_{FD} = 1.0) and all energy levels above E_F are empty (f_{FD} = 0).
- As T increases, some levels above E_F are partially occupied ($f_{FD} > 0$), while some levels below E_F are partially empty ($f_{FD} < 1$). At higher temperature, the "Spread out" of f_{FD} becomes more.
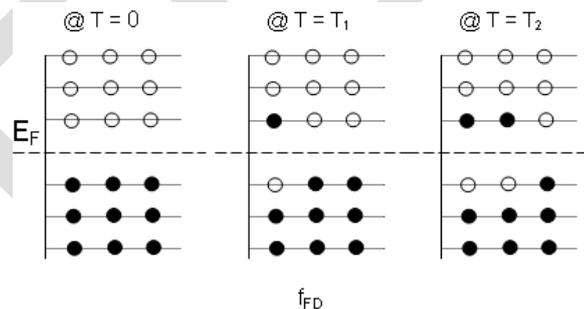
- When $E = E_F$ and $T \sim 0K$ f_{FD} = 0.5. Thus an alternative definition of E_F is " the point at which the occupation probability is exactly 0.5 or 50%.
- E_F is almost constant for most materials. For semi-conductors, the density of conduction electrons can change significantly with temperature and thus E_F in these materials is temperature dependent.
- f(E) is the Fermi factor which gives the probability of occupation of a given energy state for a material in thermal equilibrium.
- Probability of occupation for $E < E_F$ at T = 0

$$f_{FD}(E) = \frac{1}{e^{-\infty} + 1} = \frac{1}{\left(\frac{1}{e^{\infty}}\right) + 1} = \frac{1}{0 + 1} = 1$$

$f_{FD}(E) = 1$ for $E < E_F$

Energy levels are certainly occupied and $E < E_F$ applies to all the energy levels below E_F

- Probability of occupation for $E > E_F$ at T = 0

$$f_{FD}(E) = \frac{1}{e^{\infty} + 1} = \frac{1}{\infty + 1} = \frac{1}{\infty} = 0$$

$f_{FD}(E) = 0$ for $E > E_F$

Energy levels are not occupied at $E > E_F$

- When $E = E_F$ and $T \sim 0K$ f_{FD} = 0.5. Thus an alternative definition of E_F is " the point at which the occupation probability is exactly 0.5 or 50%.

Define Fermi energy (E_F) and Fermi velocity (V_F)

Fermi Energy (E_F): The energy of the electron in the highest occupied state is known as Fermi energy of the metal.

Fermi velocity (V_F):

The energy of the electrons which are at the Fermi level is E_F. The velocity of the electrons which occupy Fermi level is known as Fermi velocity

$$E_F = \tfrac{1}{2} mv_F^2 \qquad \text{or} \qquad v_F = (2E_F/m)^{1/2}$$

Failures of classical free electron theory

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According to this dependence σ will be high for the metals having large electron concentration. But some of the metals having less electron concentration is found to have higher σ and vice versa. These experimental observations were not explained by classical free electron theory.

Assumptions of quantum free electron theory (QFET):

Concept of free electron:

The total energy of the electron is contributed by

1. Potential energy of the electron which depends on its distance from the proton and

2. Kinetic energy due to its motion round the proton.

When an electron absorbs some energy given o it, it moves to a larger distance from proton and finds itself in a larger orbit, due to which there will be an increase in the total energy.

All the energy levels except the ground level are known as excited energy levels or excited states. For instance, the electron can never be found in an orbit in which its energy is of any value between -1.51eV & -3.40eV. This kind of restriction on energy values is called the **quantization of energy.** However, it must be noted that the quantization of energy occurs because of the reason that the electron is under the influence of field due to proton. A free electron can of course, have continuous energy values.

Assumptions of Quantum theory of free electron:

Two assumptions of the classical free electron theory are retained in the quantum theory. They are

1. The electrons travel under a constant potential. However, their movement is confined to the boundaries of the metal.

2. The attraction between the e^{-s} and the ions at the lattice corners as well as the repulsion between e^{-s} are ignored.

There are two more assumptions which are peculiar to the quantum theory. They are

3. The energy levels of the conduction electrons are quantized

4. The distribution of electrons among the various permitted energy levels is subject to Pauli's exclusion principle

Merits of QFET

- Only the electrons whose energies differ from E_F by kT can absorb heat and that there are $2kT/E_F$ such electrons. These electrons are the one which are very close to the Fermi level. But free electron theory assumes that all the valence electrons in a metal can absorb thermal energy. For one kmol of a metal, there will be N_A free electrons. The total energy of the electron is given by

$$U = 3/2\ N_A kT$$

When heat is supplied to the material, the free electrons also absorb part of that heat

$$\therefore C_V = dU/dT = 3/2\ N_A k = 3/2\ R = 3/2 \times 6.023 \times 10^{26} \times 1.38 \times 10^{-23} = \textbf{12.5 kJ/mol/K}$$

This calculated value of molar specific heat at constant volume is found to be hundred times greater than experimentally predicted value.

- In a high quality metal, when the atoms vibrate, the lattice is no longer ideal and presents an effective cross sectional area of πr^2 for scattering, where r is the amplitude of vibration. The electron mean free path λ is inversely proportional to the scattering cross section

$$\lambda = 1/\ \pi r^2$$

But the energy of the vibrating atom $E \sim r^2 \sim kT$

$\therefore\ \lambda \sim 1/T\ $ but $\sigma\ \alpha\ \lambda$

$\Rightarrow \lambda\ \alpha\ 1/T\ $ or $\quad \boldsymbol{\sigma\ \alpha\ 1/T}$

- If we compare the cases of Cu & Al, the value of 'n' for Al is 2.13 times higher than that of Cu. But the value of the ratio (λ/v_F) for Cu is 3.73 times higher than that of Al. Hence not only $\sigma\ \alpha\ \lambda$ but also $\sigma\ \alpha\ (\lambda/v_F)$.

Density of States

- The Fermi function does not by itself gives us the number of electrons, which have certain energy. It gives us only the probability of occupation of an energy state by a single electron.
- Since even at the highest energy the difference between neighboring energy levels is as small as 10^{-6} eV, we can say that in a macroscopically small energy interval dE, there are still many discrete energy levels.
- To know the actual number of electrons with a given energy, one must know the number of states in the system, which has the energy under consideration.
- Then by multiplying the number of states by the probability of occupation, we get the actual number of electrons.

Evaluation of density of states for the electrons in a 3-dimensional solid of unit volume
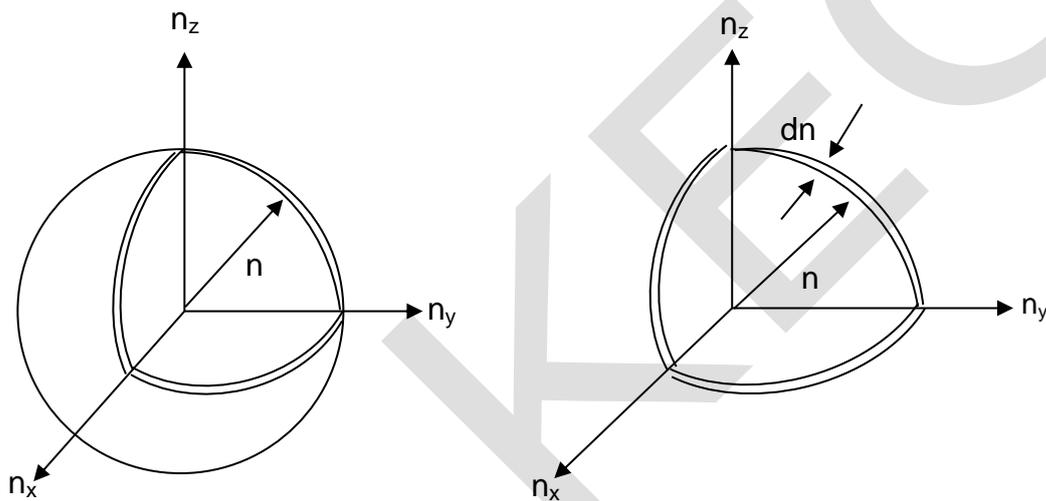
We have the equation for the allowed energy for a particle in one-dimensional potential well is

$$E = \frac{n^2 h^2}{8mL^2} \text{ ------- (1)}$$

For 3-dimensional well

$$E = \frac{(n_x^2 + n_y^2 + n_z^2)h^2}{8mL^2} \text{ ----------- (2)}$$ where $n^2 = n_x^2 + n_y^2 + n_z^2$

The number of available states within a sphere of radius 'n' is given by 1/8[4/3πn³]. The factor 1/8 accounts for the fact that only +ve integers are allowable & thus only one octant of the sphere is available. Again the no. of states within a sphere of radius (n+dn) is therefore 1/8[4/3π(n+dn)³]. Thus the no. of energy states having energy values between E & E+dE is

Z(E)dE = 1/8[4/3π(n+dn)³] - 1/8[4/3πn³] = π/6 (3n²dn) = π/2 (n²dn) ------------ (3)

From eqn.(1) we can write

$$n^2 = \frac{8mL^2 E}{h^2} \qquad \Rightarrow \qquad n = \left(\frac{8mL^2}{h^2}\right)^{1/2} E^{1/2}$$

Differentiating w.r.t E we get

$$2n\, dn = \left(\frac{8mL^2}{h^2}\right) dE \qquad \Rightarrow \qquad dn = \frac{1}{2n}\left(\frac{8mL^2}{h^2}\right) dE$$

Eqn.(4) in eqn.(3) leads to

$$Z(E)\, dE = \frac{\pi}{2} n^2 \left(\frac{1}{2n}\right) \left(\frac{8mL^2}{h^2}\right) dE = \left(\frac{\pi}{4}\right) n \left(\frac{8mL^2}{h^2}\right) dE$$

$$Z(E)\, dE = \left(\frac{\pi}{4}\right) \left(\frac{8mL^2}{h^2}\right)^{1/2} \left(\frac{8mL^2}{h^2}\right) E^{1/2} dE$$

$$Z(E)\, dE = \left(\frac{\pi}{4}\right) \left(\frac{8mL^2}{h^2}\right)^{3/2} E^{1/2} dE$$

If should be now remembered that the Pauli's exclusion principle permits two electrons in each state, so that the no. of energy levels actually available are

$$Z(E)\, dE = \left(\frac{2\pi}{4}\right) \left(\frac{8mL^2}{h^2}\right)^{3/2} E^{1/2} dE$$

The actual no. of electrons N(E) dE in a given energy interval dE will now be obtained by multiplying the no. of energy states in the interval by Fermi distribution function
N(E) dE = Z(E) F(E) dE

$$N(E)\, dE = \left(\frac{\pi}{2}\right) \left(\frac{8m}{h^2}\right)^{3/2} E^{1/2} \frac{dE}{1 + \exp[(E - E_F)/kT]}$$

At T=0K when E<E_F, F(E) =1
$\therefore$ N(E)dE = Z(E) dE

$$= \left(\frac{\pi}{2}\right) \left(\frac{8mL^2}{h^2}\right)^{3/2} E^{1/2} dE$$

$$\int N(E)dE = \left(\frac{\pi}{2}\right) \left(\frac{8mL^2}{h^2}\right)^{3/2} \int_0^{E_F} E^{1/2} dE = \left(\frac{\pi}{2}\right) \left(\frac{8mL^2}{h^2}\right)^{3/2} \left(E_F^{3/2}\right)_0^{E_F} \left(\frac{2}{3}\right)$$

$$n = \left(\frac{\pi}{3}\right) \left(\frac{8m}{h^2}\right)^{3/2} E_F^{3/2} \qquad\qquad\qquad\qquad a^3 = 1(\text{unit volume})$$

$$E_F^{3/2} = \left(\frac{3n}{\pi}\right) \left(\frac{h^2}{8m}\right)^{3/2}$$

$$\therefore E_F = \left[\left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right)\right] n^{2/3}$$

Thermal Properties

Thermal conductivity (K) of a material is equal to the amount of heat energy (Q) conducted per unit area of cross section to the temperature gradient (dT/dx).

i.e., $Q \, \alpha \, \dfrac{dT}{dx}$ Or $Q = K \, \dfrac{dT}{dx}$

So, Thermal conductivity, $K = \dfrac{Q}{(dT/dx)}$ ------ (1)

The unit of 'K' is W/m/K. In solids, the conductivity takes place by both free electrons and thermally excited lattice vibrations known as phonons.

$$K_{total} = K_{electrons} + K_{phonons}$$

Expression for Thermal conductivity

Consider a uniform rod HC with temperature of the hot end H as T_1 and the temperature of the cold end C as T_2 as shown in figure. Heat is flowing from H to C. Lat A be the area of cross section, which is at a distance equal to the mean free path λ; of the electrons between the two ends H and C. The kinetic energy of the electrons at the hot end H is greater than that of the electrons at the cold end C.
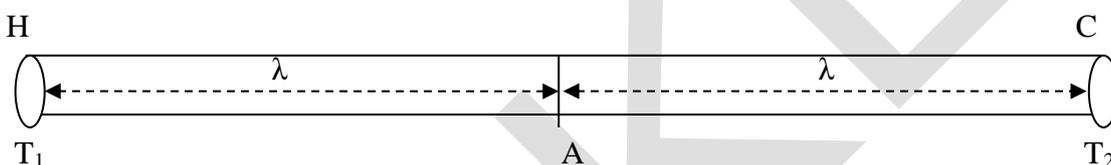
Let Q be the amount of heat flowing through the rod from the end H to C whose length is 2λ. $\therefore$ The heat conducted

$$Q \, \alpha \, \frac{A(T_1 - T_2)}{2\lambda} t \qquad \text{Or} \qquad Q = \frac{KA(T_1 - T_2)}{2\lambda} t$$

Where K is the coefficient of thermal conductivity, A is the area of cross section, t is the time for conduction and 2λ is the length of the rod.

$\therefore$ The Thermal conductivity per unit area per unit time is

$$K = \frac{2\lambda \, Q}{A(T_1 - T_2)t}$$

Let n be the number of available conduction electrons and v be the root mean square velocity of the electrons.

Let us assume that the available free electrons in the metal are having an equal probability to move in all six possible directions. Therefore an average of 1/6 nv electrons can travel in any one direction.

We know that the free electrons are assumed to be free moving gas molecules.

The average kinetic energy of an electron at hot end H of temperature $T_1 = \dfrac{3}{2} k_B T_1$

Similarly,

The average kinetic energy of an electron at cold end C of temperature $T_2 = \dfrac{3}{2} k_B T_2$

The number of electrons crossing the area at A per second $= \dfrac{1}{6} nv$

∴ The heat energy transferred per unit area per unit time from hot end H to cold end C is = Number of electrons x Average kinetic energy of electrons from H to C

$$= \dfrac{1}{6} nv \, \dfrac{3}{2} k_B T_1 \qquad = \dfrac{1}{4} nv k_B T_1$$

Similarly, the heat energy transferred across A per second from C to H

$$= \dfrac{1}{6} nv \, \dfrac{3}{2} k_B T_2 \qquad = \dfrac{1}{4} nv k_B T_2$$

∴ The resultant heat energy transferred from H to C across A per second,

$$Q = \dfrac{nv}{4} k_B \left(T_1 - T_2\right) \quad \text{------- (2)}$$

We know that, temperature gradient $\dfrac{dT}{dx} = \dfrac{\left(T_1 - T_2\right)}{2\lambda}$ ----- (3)

Substituting the values of Q and temperature gradient, in equation (1), we get

Thermal conductivity, $\qquad K = \dfrac{2\lambda \dfrac{nv}{4} k_B \left(T_1 - T_2\right)}{\left(T_1 - T_2\right)}$

$$K = \dfrac{1}{2} nv k_B \, \lambda \qquad \text{------ (4)}$$

We know from classical free electron theory, the electronic heat capacity of the metal is,

$$C_e = \dfrac{3}{2} R$$

Where R is gas constant and is equal to n k_B.   i.e. $R = n \, k_B$

So that $\qquad R = \dfrac{2}{3} C_e = n \, k_B \qquad$ equation (4) becomes

∴ Thermal conductivity, $\qquad K = \dfrac{1}{3} C_e \, v \, \lambda \qquad$ ----- (5)

Thermal conductivity of a metal is determined either using equation (4) or (5).

Wiedemann – Franz Law

The ratio between the thermal conductivity and electrical conductivity of a metal is directly proportional to the absolute temperature of the metal when the temperature is not too low.

$$\text{i.e., } \frac{K}{\sigma} \alpha \, T \qquad \text{Or} \qquad \frac{K}{\sigma} = L \, T$$

Where $L = K/\sigma T$ is a constant known as Lorentz number. The value of L is equal to 2.44×10^{-8} WΩK^{-2} at 293 K.

We know that the expression for

Thermal conductivity $\qquad\qquad K = \frac{1}{2} n v k_B \lambda \qquad$ ----- (1)

Electrical conductivity $\qquad\qquad \sigma = \frac{n e^2 \tau}{m} \qquad$ ------(2)

$$\therefore \quad \frac{K}{\sigma} = \frac{\frac{1}{2} n v k_B \lambda}{\frac{n e^2 \tau}{m}} = \frac{m v k_B \lambda}{2 e^2 \tau}$$

Substituting $\lambda = v \, \tau$ in the above equation, we get

$$\frac{K}{\sigma} = \frac{m v^2 k_B \tau}{2 e^2 \tau} = \frac{1}{2} m v^2 \frac{k_B}{e^2}$$

Since $\frac{1}{2} m v^2 = \frac{3}{2} k_B T$, we get

$$\frac{K}{\sigma} = \frac{3}{2} k_B T \frac{k_B}{e^2} = \frac{3}{2} \frac{k_B^2}{e^2} T$$

Therefore, $\qquad \frac{K}{\sigma T} = \frac{3}{2} \frac{k_B^2}{e^2} = L$

Substituting the value of k_B and e in the above equation, we get

$$L = \frac{3}{2} \frac{k_B^2}{e^2} = \frac{3}{2} \frac{\left(1.38 \times 10^{-23}\right)^2}{\left(1.6 \times 10^{-19}\right)^2} = 1.11 \times 10^{-8} \text{ W} \Omega \text{K}^{-2} \quad \text{-----(3)}$$

The value of Lorentz number is not matching with experimental value $\qquad$ (2.44 x 10^{-8} WΩK^{-2}), due to failure of classical theory.

According to quantum free electron theory, the expression for thermal conductivity is modified by considering the electronic specific heat as,

$$K = \frac{n\pi^2 k_B^2 T\tau}{3m} \qquad \text{------(4)}$$

Since

$$L = \frac{K}{\sigma T} = \frac{n\pi^2 k_B^2 T\tau}{3m} \times \frac{m}{ne^2 \tau T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

$$\therefore \ L = \frac{\pi^2 \left(1.38 \times 10^{-23}\right)^2}{3\left(1.6 \times 10^{-19}\right)^2} = 2.44 \times 10^{-8} \ \text{W}\Omega\text{K}^{-2} \qquad \text{-------(5)}$$

Equation (5) gives the correct value of Lorentz number and is in good agreement with the experimental value.

Thermal conductivity of a Bad conductor by Lee's method

AIM: To determine the thermal conductivity of bad conductors such as card board, ebonite, etc.

Apparatus:

1. Lee's disc apparatus
2. a brass disc and a metallic disc of large diameter compared to its thickness
3. sample of bad conductor in the form of the disc with same diameter
4. two mercury thermometers
5. stop watch
6. vernier
7. screw gauge and
8. a balance.

Experimental Set up:

The experimental set up is shown in Figure A. The brass disc *B* is hung from the stand with the help of three strings. On the brass disc, the bad conductor sample disc 'S' is placed and over that a metallic disc M is placed. On the metallic disc, a heating chamber, H with facility for steam-in and steam-out is placed.
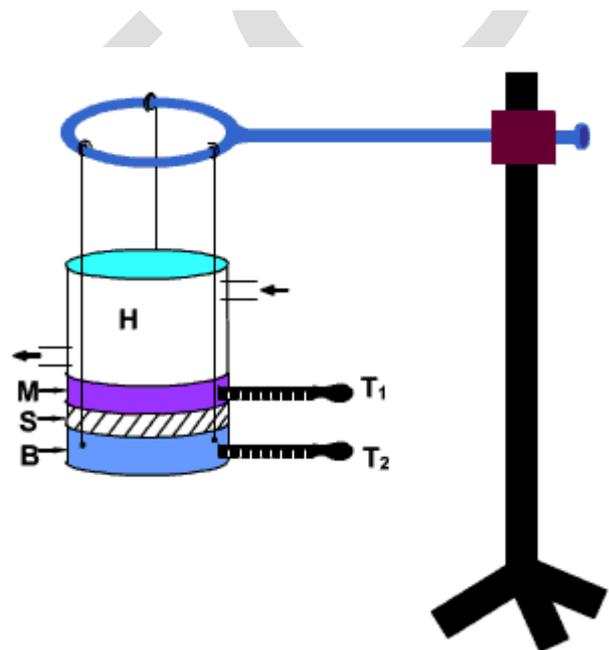
Fig. A

Theory:

Assuming that the heat losses to from the sides of the sample are negligible, the steady state rate of heat transfer (H) by conduction is given by: $H = kA\dfrac{(T_2 - T_1)}{x}$ .... (1), where the k is the thermal conductivity of the sample, A is the cross sectional area and $T_2 - T_1$ is the temperature difference across the sample thickness x (see figure 1).
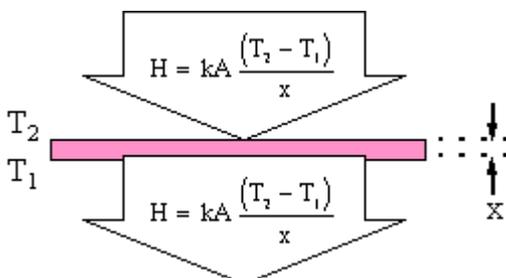
Figure 1

As the sample is an insulator, lagging at the sides will not significantly reduce the energy losses.

Therefore to keep these losses small the sample is a thin disk with a large cross sectional area $\left[A = \dfrac{\pi d^2}{4} \right]$

compared to the area exposed at the edge $\left[a = \pi dx \right]$. Keeping A large and x small produces a large rate of energy transfer across the sample. Keeping x small also means that the apparatus reaches a steady state (when temperatures T_1 and T_2 are constant) more quickly.
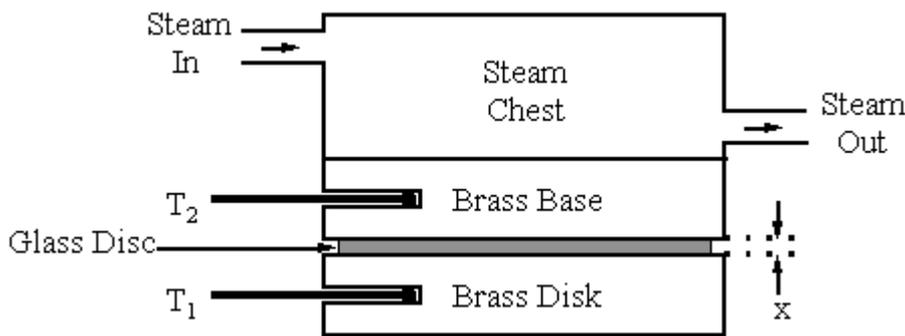

Figure 2

The thin sample is sandwiched between the brass disk and brass base of the steam chest (see figure 2). The temperature of the brass base (measured by thermometer T_2) is very close to the temperature of the top surface of the bad conductor disk because the thermal conductivity of brass is about one hundred times that of bad conductor. Similarly the temperature of the brass disk (measured by T_1) is very close to the temperature of the lower bad conductor surface. In this way the temperature difference across such a thin sample can be accurately measured.
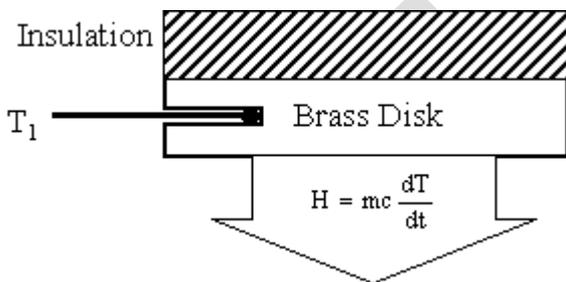

Figure 3

When the apparatus is in a steady state (temperatures T_1 and T_2 constant), the rate of heat conduction into the brass disk must be equal to the rate of heat loss due to cooling (by air convection) from the bottom of the brass disk. The rate of heat loss can be determined by measuring how fast the brass disk cools at the previous (steady state) temperature T_1 (with the top of the brass disk covered with insulation, see figure 3). If the disk cools down at a rate $\dfrac{dT}{dt}$ then the rate of heat loss is given by: $H = mc \dfrac{dT}{dt}$ ....(2), where m is the mass of the brass disk and c is the specific heat capacity of brass.

When a steady state is reached, let T_1 and T_2 be the temperatures of metallic disc M and brass disc B. So, the temperature difference between the two ends of bad conductor is ($T_1 - T_2$).

∴ The rate of heat conducted through the bad conductor is,

$$Q_1 = \frac{K A (T_1 - T_2)}{d}$$ .... (1)

where, *'d'* is thickness of the bad conductor and *'A'* is the area of cross section.
The rate of heat lost by the brass disc to the surrounding under steady state is,

$$Q_2 = m c \left(\frac{dT}{dt}\right)_{T_2}$$ .... (2)

Where m-mass of the brass disc, C is the heat capacity of brass disc and $\frac{dT}{dt}$ is its rate of cooling at T_2

From eqn (1) and (2),

$$K = \frac{m c d \left(\frac{dT}{dt}\right)_{T_2}}{A (T_1 - T_2)}$$ .... (3)

By measuring, $\left(\frac{dT}{dt}\right)_{T_2}$ and $(T_1 - T_2)$ using Lee's apparatus the thermal conductivity K can be determined.

Procedure:

(1) Measure the mass of the brass disc using a balance and take it as *m* kg.
(2) Measure the diameter and hence the radius of the sample, *S* using vernier callipers. Calculate the circular area of the disc, $A = \pi r^2$
(3) Measure the thickness of the sample *S* using a screw gauge and take it as *d*
(4) Arrange the brass disc, sample disc and metallic disc as shown in the Figure A. Insert the thermometers into the grooves of metallic disc and brass disc, which measure the temperatures T_1 and T_2 respectively.
(5) Place the heating chamber on the above assembly and suspend it as shown in Figure 1. Start the heater, by sending steam through the heating chamber.
(6) Monitor the temperatures T_1 and T_2 at a regular interval till they reach the steady state. Note the steady state temperatures T_1 and T_2
(7) The next part is to determine the rate of cooling of brass disc. Lift the heating chamber and remove the metallic plate *M* and sample disc *S,* then place the heating chamber directly on the brass disc, *B*.
(8) Allow the brass disc *B* to heat atleast about $10\,^0C$ above the steady state temperature T_2 measured in the first part of the experiment. Remove the heating chamber.

(9) Switch on the stop watch and measure the temperature of brass disc at an interval of 60 sec as it cools down. Allow the brass disc to cool down to at least $5\,^0C$ below the steady state temperature, T_2. The suggested table is as shown below.
(10) Plot a graph of temperature T of brass disc as a function of time. A typical plot is shown in Fig. B. Draw tangential line to the curve, corresponding to the temperature, T_2 and determine its slope. The slope is equivalent to $\left(\frac{dT}{dt}\right)_{T_2}$

(11) Calculate thermal conductivity, 'K' using equn (3) and by multiplying a correction factor

$$C_f = \frac{r + 2h}{2r + 2h}$$

Here, h is the thickness of the brass disk. The correction factor is introduced because the cooling measurement was not exactly the same environment of steady state measurement.
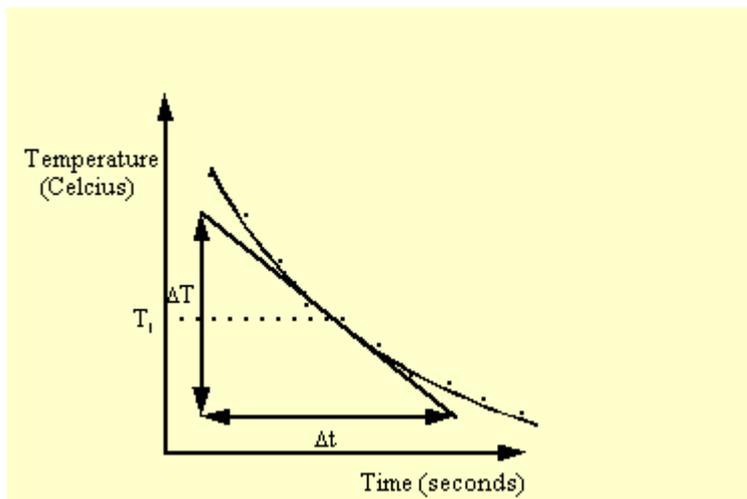
Figure B

Table : Cooling rate of Brass disc

Sl. No	Time t (min.)	Temperature of Brass disc T(^{0}C)
1.		
2.		
3.		
4.		
--		
--		

Error Analysis:

The fractional error in K is,

$$\frac{\Delta K}{K} = \frac{\Delta m}{m} + \frac{\Delta d}{d} + \frac{\Delta\left(\frac{dT}{dt}\right)}{\frac{dT}{dt}} + \frac{2\Delta r}{r} + \frac{\Delta(T_1 - T_2)}{T_1 - T_2}$$

Δm, Δd, $\Delta(dT/dt)$, Δr and $\Delta(T_1 - T_2)$ are the error in the measurements of mass, thickness, $\dfrac{dT}{dt}$, radius and $(T_1 - T_2)$.

Result :

The thermal conductivity of given bad conductor =

Thermal conductivity of good conductor by Forbes method

Aim: To measure the thermal conductivity of good conductors such as Aluminium, Copper, Brass, etc. by following Forbes method.

Apparatus:
(a) A long rod of uniform cross sectional area whose thermal conductivity '*K*' is to be measured, with grooves at an interval of 10 cm to mount the thermometers, **(b)** Mercury thermometer **(c)** a small sample length (10 cm) of same material (preferably cut from the same rod). **(d)** A heater or boiling water bath **(e)** stop watch .

Experimental Setup:
The experimental set up is shown in Fig. 1. One end of the experimental rod is connected to a Heating Chamber. There is a shield to avoid radiation and direct heating of other portion of the rod from the heater.
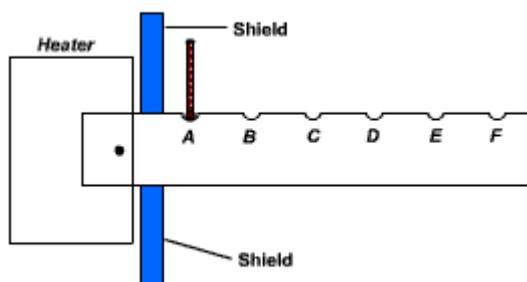

Fig.1. Experimental setup

Theory:

When a steady state is reached, the amount of heat conducted through a particular point say *B*, per second can be written as,

$$Q_1 = K A \left(\frac{dT}{dx} \right)_B \qquad \text{............... (1)}$$

where *K* is the thermal conductivity of the material, *A* is the area of cross-section of the material, $\left(\frac{dT}{dx} \right)_B$ is the change in temperature per unit length of the rod at *B*.

The amount of heat lost per second in a small length element 'Δx' is given by

$$\Delta Q_2 = \Delta m \ C \ \frac{\Delta T}{\Delta t}$$
$$= \rho A \Delta x \ C \ \frac{\Delta T}{\Delta t} \qquad \text{..........................(2)}$$

where Δm is the mass of the small length element, - is the heat capacity of the rod. $\Delta T / \Delta t$ is the rate of change in temperature over the length element, and, ρ is the density of the material.

The total heat lost from the point B to the cold end C of the rod is,

$$Q_2 = \rho \, C \, A \int\limits_{B}^{cold\,end} \frac{dT}{dt} dx$$

.... (3)

In a steady state condition, $Q_1 = Q_2$

$$K \left(\frac{dT}{dx} \right)_B = \rho \, C \int\limits_{B}^{end} \frac{dT}{dt} dx$$

.... (4)

Similarly, for another point of the rod, say E, we can write

$$K \left(\frac{dT}{dx} \right)_E = \rho \, C \int\limits_{E}^{end} \frac{dT}{dt} dx$$

.... (5)

from equn (4) and (5),

$$K \left(\frac{dT}{dx} \right)_B - K \left(\frac{dT}{dx} \right)_E = \rho \, C \left[\int\limits_{B}^{end} \frac{dT}{dt} dx - \int\limits_{E}^{end} \frac{dT}{dt} dx \right]$$

$$= \rho \, C \int\limits_{B}^{E} \frac{dT}{dt} dx$$

or Thermal conductivity,

$$K = \frac{\rho C \int\limits_{B}^{E} \frac{dT}{dt} dx}{\left(\frac{dT}{dx} \right)_B - \left(\frac{dT}{dx} \right)_E}$$

.... (6)

From eqn. (6), K can be calculated by measuring $\frac{dT}{dx}$ as a function of position and $\frac{dT}{dt}$ as a function of position. Instead of B and E any other pair of points can be chosen.

Procedure

1. In the experimental set up, heater is switched on and the rod is allowed to rise to steady state temperature. At this state the temperature at points *A, B, C, D*, etc remains constant without any variation with time.

2. Measure the temperatures at the points *A, B, C*, etc. and tabulate the reading. Draw the graph of $T(^0C)$ as a function of horizontal distance such as *O* to *A*, *O* to *B* etc. The typical graph would be as shown in Figure 2.

3. Find the slope of the curve at two points, such as B and E, by drawing tangential lines to the curve at points B and E.
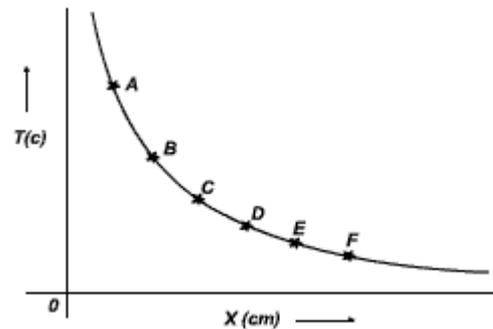
Figure 2

They are   taken as $\left(\dfrac{dT}{dx}\right)_B$ and $\left(\dfrac{dT}{dx}\right)_E$ respectively.

4. Heat the sample rod using a heater or boiling water bath for a sufficient time to reach a steady state. Take out the sample rod, hang it using a string and stand. Insert the thermo couple or thermometer into the groove as shown in Figure 3.
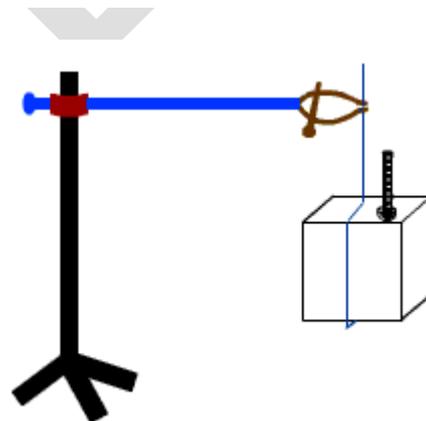

Figure 3

Table 1

Sl. No	Distance from the hot end	Position	Temperature T (^{0}C)
1			
2			
3			
4			
5			
6			

5. Measure the temperature as a function of time at regular interval, using a stop watch and the thermometer. Tabulate them as suggested in table2. Plot a graph of T versus time. The typical plot of T versus time is given in Figure 4

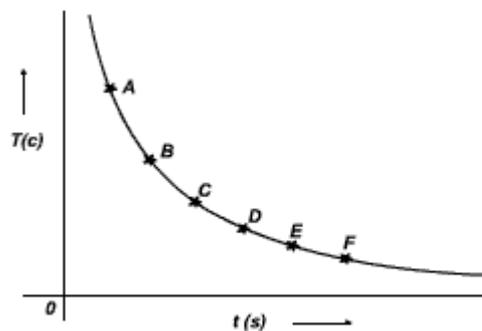6. By comparing Figure 2 and Figure 4 spot the points A, B, C, D, etc in Figure 4 and mark them.

7. Find the slopes $\dfrac{dT}{dt}$ at the points $A,\ B,\ C,\ D$ etc. from the Figure 4

Figure 4

8. Plot $\dfrac{dT}{dt}$ verses x. The typical graph is shown in Figure 5

Mark two points x and y on the graph corresponding to the position B and E..

9. Determine the area under the curve X, Y, i.e

   BXYE in Figure 5.

   Area $\text{BXYE} = \displaystyle\int_{B}^{E} \dfrac{dT}{dt}\, dx$ .... (7)

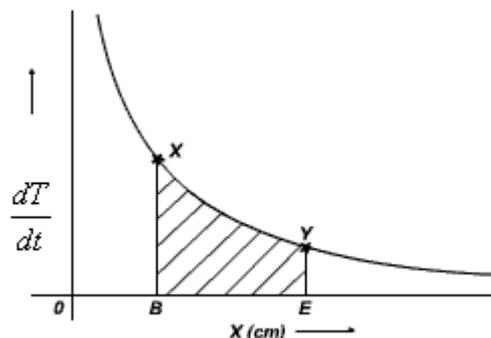**Figure 5**

10. Thermal conductivity K can be calculated using eq. (6) and (7).

    i.e. $K = \dfrac{\rho C\,(Area\ BXYE)}{\left(\dfrac{dT}{dx}\right)_{B} - \left(\dfrac{dT}{dx}\right)_{E}}$ ...... (8)

Note that instead of B and E, any two pair of points can be taken and accordingly the eq. (8) can be modified.

Table 2

Sl. No	Time	Temperature T (^{0}C)

Table 3

Sl. No	Position	Distance from the hot end	$\dfrac{dT}{dx}$

<u>Result :</u>
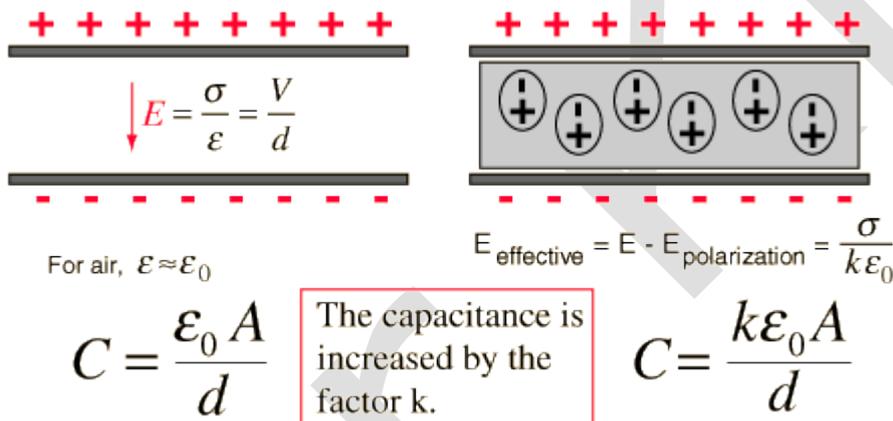
The thermal conductivity of given material = ' '

UNIT 3 – MATERIALS SCIENCE (DIELECTRICS & SEMICONDUCTORS)

Dielectric Materials:

A dielectric material (dielectric for short) is an electrical insulator that can be polarized by an applied electric field. When a dielectric is placed in an electric field, electric charges do not flow through the material as they do in a conductor, but only slightly shift from their average equilibrium positions causing dielectric polarization. Because of dielectric polarization, positive charges are displaced toward the field and negative charges shift in the opposite direction. This creates an internal electric field that reduces the overall field within the dielectric itself

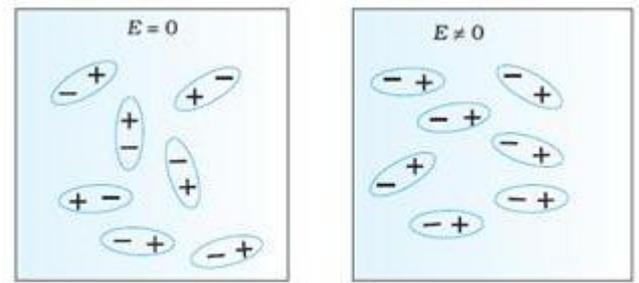**Parallel Plate with Dielectric:**

The capacitance of a set of charged parallel plates is increased by the insertion of a dielectric material. The capacitance is inversely proportional to the electric field between the plates, and the presence of the dielectric reduces the effective electric field. The dielectric is characterized by a dielectric constant k, and the capacitance is multiplied by that factor.

$$E = \frac{\sigma}{\varepsilon} = \frac{V}{d}$$

For air, $\varepsilon \approx \varepsilon_0$

$$C = \frac{\varepsilon_0 A}{d}$$

The capacitance is increased by the factor k.

$$E_{effective} = E - E_{polarization} = \frac{\sigma}{k\varepsilon_0}$$

$$C = \frac{k\varepsilon_0 A}{d}$$

When a dielectric is placed between charged plates, the polarization of the medium produces an electric field opposing the field of the charges on the plate. The dielectric constant k is defined to reflect the amount of reduction of effective electric field as shown below. The permittivity is a characteristic of space, and the relative permittivity or "dielectric constant" is a way to characterize the reduction in effective field because of the polarization of the dielectric. The capacitance of the parallel plate arrangement is increased by factor k.

$$E = \frac{\sigma}{\varepsilon_0}$$

σ = charge per unit area
ε_0 = permittivity of space
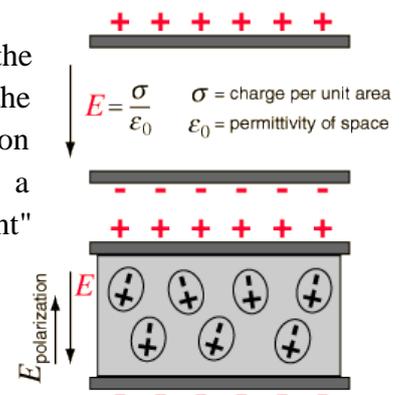
Polar Dielectrics: Polar dielectrics are those in which the possibility of center coinciding of the positive as well as negative charge is almost zero i.e. they don't coincide with each other. The reason behind this is their shape. They all are of asymmetric shape. Some of the examples of the polar dielectrics is NH_3, HCL, water etc.

Non Polar dielectrics: In case of non polar dielectrics the centres of both positive as well as negative charges coincide. Dipole moment of each molecule in non polar system is zero. All those molecules which belong to this category are symmetric in nature. Examples of non polar dielectrics are: methane , benzene etc.
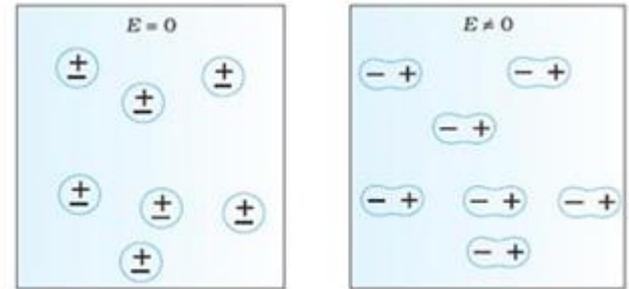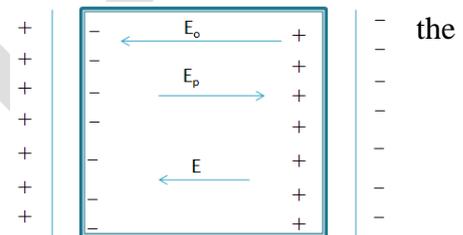
Polar molecules

Non-polar molecules

Expression for dielectric constant:

The electric field between the plates due to the charges +q, -q on the capacitor plates is

$E_o = \sigma/\varepsilon_o = q/A\varepsilon_o$ ----------(1)

in a direction left to right as shown in the figure

From the definition of dielectric constant we can write the resultant field in terms of dielectric constant as

$E = E_o/k = q/A\varepsilon_o k$ ----------(2)

The potential difference between the plates is given by

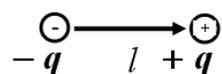$V = Ed = qd/A\varepsilon_o k$ ----------(3)

Capacitance of the capacitor is given by

$C = q/V = q/[qd/A\varepsilon_o k] = A\varepsilon_o k/d = C_o k$

$\mathbf{k = C/C_o}$

Electric dipole, dipole moment and polarization

A pair of equal and opposite charges whose distance of separation is small – electric dipole

$$\ominus \xrightarrow{} \oplus$$
$$-q \quad l \quad +q$$

Product of the magnitude of one of the charges and the distance of separation between them – dipole moment

$$\mathbf{\mu = ql}$$

Where μ - dipole moment (unit – coulomb-meter)

q- magnitude of the charge

l- distance of separation of charges

Polarization (P):

It can be defined as vibration confined to single direction or alignment confined to one direction also it is the dipole moment per unit volume

Definition:

The displacement of charges in the atom or molecules of a dielectric under the action of an applied field leading to the development of dipole moment is called polarization or electric polarization

The charges appearing separated are called polarized charges.

$P = \varepsilon_o(\varepsilon_r - 1)E$ unit of P-coulomb/meter^2

Polarizability (α):

When an atom or molecule is subject to electric field the atom or molecule acquire dipole moment. i.e. $\mu \propto E$

Or Dipole moment of the atom or molecule is $\mu = \alpha E$

Where α is the proportionality constant called Polarizability of the atom or molecule

Polarizability is the property of the individual atom or molecule

Types of Polarization

There are different mechanisms through which electrical polarization can occur in dielectric materials they are

1. Electronic polarization

2. Ionic polarization

3. Orientational polarization

4. Space charge polarization
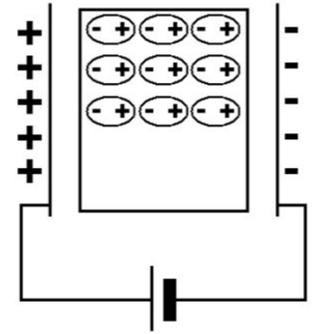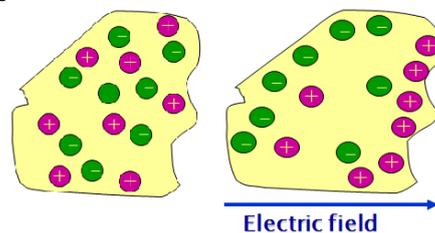
Electronic polarization

The displacement of nucleus and electrons in the atom under the influence of external electric field. As electrons are very light they have a rapid response to the field changes; they may even follow the field at optical frequencies. It occurs in monoatomic gases and is independent of temperature.

$$\alpha_e = \frac{\varepsilon_0(\varepsilon_r - 1)}{N}$$

N is the number of atoms/unit volume
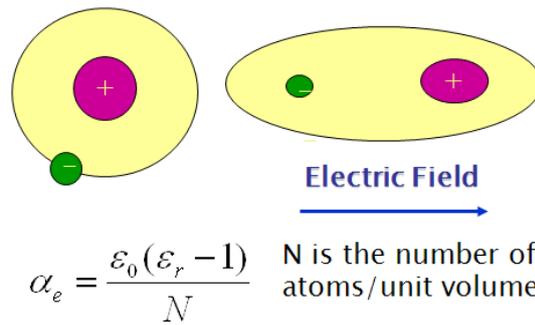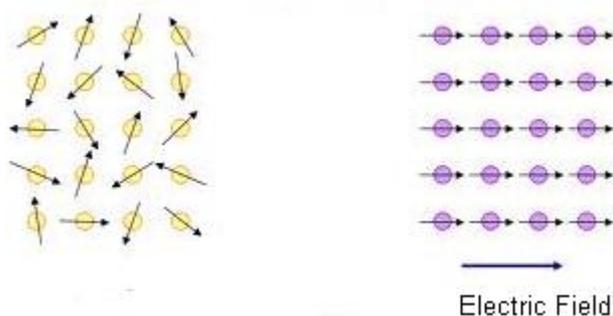
Ionic polarization

Ionic polarization occurs only in those dielectrics which contains ionic bonds. Example: NaCl

In ionic lattice, the positive ions are displaced in the direction of an applied field while the negative ions are displaced in the opposite direction, giving a resultant dipole moment to the whole body and is independent of temperature

Orientational polarization

Occurs in those dielectrics which possess permanent dipole moment (Polar dielectrics). It is dependent on temperature.

Space charge polarization

Occurs in multiphase dielectric materials or heterogeneous dielectric materials. Space charge polarization is also called as interfacial polarization or Migrational polarization. The Migrational polarization takes longer time and is therefore occurs at low frequency

The total polarizability ,α, is given by

$$\alpha = \alpha_e + \alpha_i + \alpha_o$$

Frequency dependence of dielectric constant :
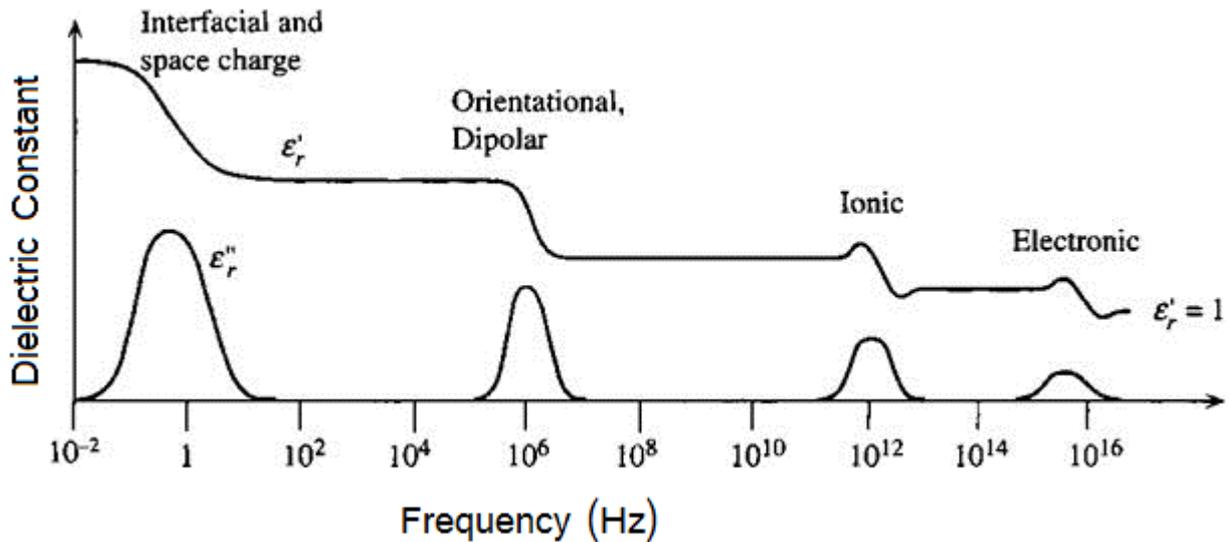
If the static electric field is applied to a dielectric material then, the dipoles tend to align parallel to the field. However, in the presence of an alternating electric field the dipoles follow the changing field directions.

At low frequencies, the dipoles tend to aligns with the electric field easily. As the frequency of the applied electric field increases, the dipoles alignment tends to lag behind the field. This results in an effective decrease in the polarization of the material at higher frequencies. The ability of the dipoles to follow the applied alternating field depends on the mechanisms by which the dipoles are produced.

Space charge polarization involves the movement of interfacial charges in the dielectric medium and hence is the slowest process. Its contribution is normally observed in static (or dc) fields and disappears at very low frequency. This shows up as a decrease in the dielectric constant of the material in the low frequency regime.

Orientation polarization involves the rotation of molecules and is maximum at about 10^6 Hz which is radio frequency. At frequencies greater than 10^6 Hz, the inertia of the molecules is so high that the dipoles due to this type of polarization does not any more respond to the applied electric field and hence the contribution from this type of polarization also disappears.

Ionic polarization involving displacement of ions has considerable contribution up to frequency 10^{12} Hz which is microwave frequency. Beyond this frequency the dipoles loses its ability to respond to the applied field and hence ionic polarization vanishes.

Electronic polarization which is the fastest mechanism of polarization as it involves the motion of electron cloud, is observed even up to 10^{18} Hz which is infrared frequency. Assuming that all the four types of polarization are possible in a dielectric medium, the variation of total polarization with the frequency of the applied electric field may be as shown in figure

For every type of polarization, there exists a minimum time for reorientation (dipole reversal) and is called the relaxation time. Its reciprocal is the relaxation frequency. If τ_e, τ_i and τ_0 are the relaxation times for electronic, ionic and orientation polarizations, then $\tau_e < \tau_i < \tau_0$.

Expression for polarization P :

Consider a parallel plate capacitor with plates between which an electric field E_o exist, if 'σ' is the charge per unit area on the plates, then from Gauss law we have

$$E_o = \frac{\sigma}{\varepsilon_o} \text{--------------(1)}$$

After the introduction of slab in between the plates the field developed inside is E_i. The field due to polarization will be in a direction opposite to that of E_o.

∴The resultant field 'E' in the material can be written as

$$E = E_o - E_i \text{-----------------(2)}$$

If σ_p is the charge/unit area on the slab surfaces then by following equation (1) we write

$$E_i = \frac{\sigma_P}{\varepsilon_o} \text{---------------(3)}$$

From equation (1) (2) and (3)

$$E_i = \frac{\sigma}{\varepsilon_o} - \frac{\sigma_P}{\varepsilon_o}$$

Or $\qquad\qquad \varepsilon_o E = \sigma - \sigma_P \text{----------------(4)}$

Since magnitude of polarization P =charge/unit area

$$P = \sigma_p$$

Also by Gauss law, we know that

$$D = \sigma$$

Where $D \rightarrow$ electric flux density

Equation (4) can be written as $\varepsilon_o E = D - P$

Or $\qquad\qquad D = \varepsilon_o E + P \text{----------------(5)}$

But we know that

$$D = \varepsilon_o \varepsilon_r E$$

∴ equation (5) $\rightarrow \varepsilon_o \varepsilon_r E = \varepsilon_o E + P$

or $\qquad\qquad P = \varepsilon_o (\varepsilon_r - 1)E$

or $\qquad\qquad P = \varepsilon_o x E$

where $\qquad\qquad \chi = (\varepsilon_r - 1)$ is the dielectric susceptibility of the material.

Derivation of electronic polarizability (α_e)

     The polarization 'P' of a non-polar gas is given by $P = N \alpha_e E$

Where α_e is called the electronic polarizability

     Consider a monochromatic dielectric material as shown. Let the charge on the nucleus is 'Ze' and let this be surrounded by an electronic cloud of '– Ze' in a shere of radius 'R' as shown.

Nucleus   Original position   Displaced position

Sphere of elec....... ....rge
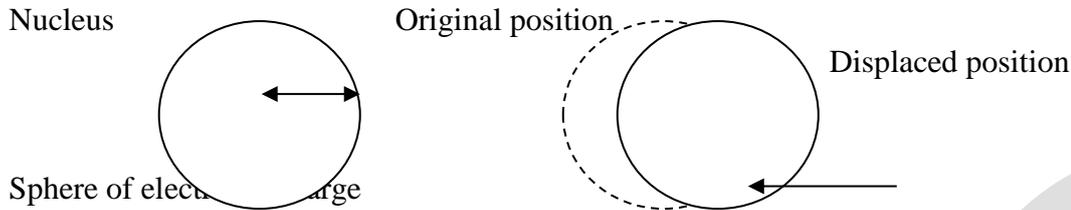
The charge density 'ρ' is given by

$$\rho = \frac{ch\arg e}{volume} = \frac{-Ze}{\frac{4}{3}\pi R^3}$$

$$\rho = \frac{-3Ze}{4\pi R^3} \qquad ----(1)$$

Let an external electric field 'E be applied to the atom.

The nucleus and the electron experience Lorentz force = ZeE in opposite directions. Thus the nucleus and electron cloud are pulled apert. But because of Coulomb force the displacement will be very small. Let it be 'x'.

Lorentz force = - ZeE

Coulomb force = $\dfrac{Ze \times ch\arg e\ enclosed\ in\ the\ sphere\ of\ radius\ x}{4\pi\varepsilon_0 R^3}$

$$= \frac{Ze \times \left(\frac{4}{3}\pi x^3 \rho\right)}{4\pi\varepsilon_0 x^2}$$

Therefore, Coulomb force $= \dfrac{Ze \times \left(\frac{4}{3}\pi x^3 \left[\frac{-3Ze}{4\pi R^3}\right]\right)}{4\pi\varepsilon_0 x^2}$

$$= \frac{Ze \times \left(\frac{-Zex^3}{R^3}\right)}{4\pi\varepsilon_0 x^2}$$

Therefore, Coulomb force $= \dfrac{-Z^2 e^2 x}{4\pi\varepsilon_0 R^3}$

At equilibrium Lorentz force = Coulomb force

$$- \text{ZeE} = \frac{-Z^2 e^2 x}{4\pi\varepsilon_0 R^3}$$

Therefore $x = \dfrac{4\pi\varepsilon_0 R^3}{Ze} E$

Because of the displacement, dipole moments are produced.
Therefore the dipole moment $\mu = Z e x$

Therefore $\mu = Z e \dfrac{4\pi\varepsilon_0 R^3}{Ze} E = 4\pi\varepsilon_0 R^3 E$ ----(2)

By definition $\mu = \alpha_e E$ ----(3)

Comparing equations (1), (2) and (3)

$$\alpha_e = 4\pi\varepsilon_0 R^3$$

This gives the expression for electronic polarizability.

By definition $P = N \mu = N \alpha_e E$

But, $P = \varepsilon_o(\varepsilon_r - 1)E$

$N \alpha_e E = \varepsilon_o(\varepsilon_r - 1)E$

$\alpha_e = \dfrac{\varepsilon_o(\varepsilon_r - 1)}{N}$

The electronic polarizability can also be given by the above expression. Here N is the number of atoms / unit volume. The Unit of α_e is F-m^2.

Expression for dielectric loss (or loss tangent)

Let a dielectric material be imagined to have been placed between the plates of a capacitor subjected to an alternating electric field. As a result the dipoles of the material got engaged in switching action the movement of which will be opposed by the internal free form. The action of frictional forces could be treated as equivalent to the presence of a resistance accompanying the capacitor.
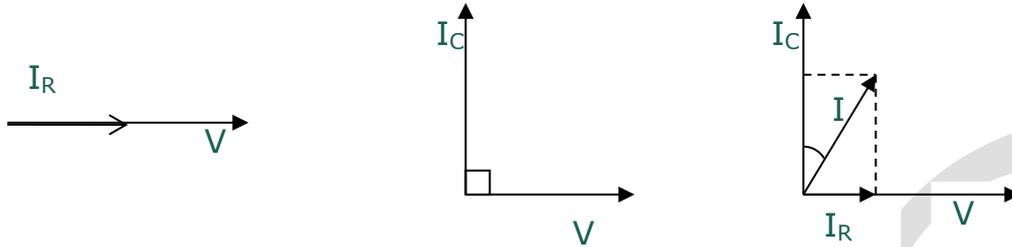
IR is the phase with V, and I_e leads by V by 90°. The resultant of the I_C and I_R is I.. The angle between I and I_C is denoted by δ and is called the dielectric loss angle.

Now the dielectric loss is due to the factor of Joule heating given by the product VI_R.

$$\text{Dielectric loss} = VI_R = V \times I \cos(90 - \delta)$$
$$= VI \sin \delta$$

but $I_C = I \cos\delta$

$$\Rightarrow I = \frac{I_C}{\cos \delta}$$

∴ Dielectric loss $= V. \dfrac{I_C}{\cos \delta} .\sin \delta$

$$= V.I_C \tan \delta$$

But $I_C = \dfrac{V}{X_C}$ where X_C is the reactance of the capacitor given by

$$X_C = \frac{1}{2\pi fc}$$

∴ $I_C = V(2\pi fc)$

∴ Dielectric loss $= V^2(2\pi fc) \tan \delta$

Large tanδ value indicates higher dielectric loss. It is also referred to as tangent loss.

Internal fields in liquids and solids

The internal field is the electric field that acts at the site of any given atom of a solid or liquid dielectric subject to an external electric field and is the resultant of the applied field and the field due to all the surrounding dipoles"

Expression for the internal field in the case of liquid or solid

Consider a dielectric which is kept in a external uniform electric field strength E

In the dielectric, an array of atomic dipoles aligns parallel to the direction of the applied electric field.
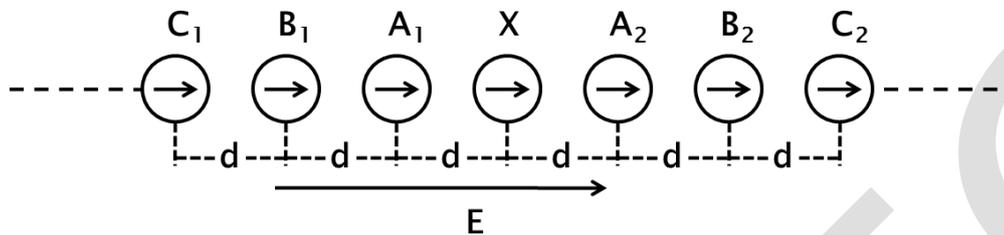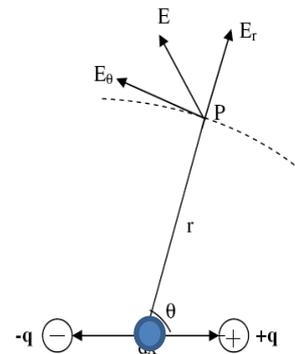

d- is the inter atomic distance

μ - is the atomic dipole moment

The electric field component at a point P due to an electric dipole is expressed in polar form as

$$E_r = \frac{\mu \cos\theta}{2\pi\varepsilon_0 r^3} \qquad E_\theta = \frac{\mu \sin\theta}{4\pi\varepsilon_0 r^3}$$

The electric field at X due to the dipole A1 is given by

$$E_{XA_1} = E_r + E_\theta$$

$$E_{XA_1} = -\frac{\mu}{2\pi\varepsilon_0 d^3} \qquad E_\theta = 0 \; (\theta = 180^0 \, \& \, r = -d)$$

The electric field at X due to the dipole A_2 is given by

$$E_{XA_2} = \frac{\mu}{2\pi\varepsilon_0 d^3} \qquad E_\theta = 0$$

The field E_1 at X due to both the dipoles A_1 and A_2 is given by

$$E_1 = E_{XA_1} + E_{XA_2}$$

$$E_1 = \frac{\mu}{2\pi\varepsilon_0 d^3} + \frac{\mu}{2\pi\varepsilon_0 d^3} = \frac{\mu}{\pi\varepsilon_0 d^3}$$

Similarly, the field E_2 at X due to both B_1 and B_2 dipole which are located at a distance of 2d from X is given by

$$E_2 = \frac{\mu}{2\pi\varepsilon_0(2d)^3} + \frac{\mu}{2\pi\varepsilon_0(2d)^3} = \frac{\mu}{\pi\varepsilon_0(2d)^3}$$

Similarly, the field at X due to both C1 and C2 is given by

$$E_3 = \frac{\mu}{2\pi\varepsilon_0(3d)^3} + \frac{\mu}{2\pi\varepsilon_0(3d)^3} = \frac{\mu}{\pi\varepsilon_0(3d)^3}$$

The total field at X due to all the dipoles in the linear array is

$$E_T = E_1 + E_2 + E_3 + ...$$

$$E_T = \frac{\mu}{\pi\varepsilon_0 d^3} + \frac{\mu}{\pi\varepsilon_0(2d)^3} + \frac{\mu}{\pi\varepsilon_0(3d)^3} + ...$$

$$E_T = \frac{\mu}{\pi\varepsilon_0 d^3}\left[1 + \frac{1}{2^3} + \frac{1}{3^3} + ...\right]$$

$$E_T = \frac{\mu}{\pi\varepsilon_0 d^3}\sum_{n=1}^{\infty}\frac{1}{n^3} \quad \text{where n=1,2,3..}\infty$$

But, $\quad \sum_{n=1}^{\infty}\frac{1}{n^3} = 1.2$

Therefore, $\quad E_T = \frac{1.2\mu}{\pi\varepsilon_0 d^3}$

Therefore the total internal field at X is given by $E_i = E + E_T$

i.e $\quad E_i = E + \frac{1.2\mu}{\pi\varepsilon_0 d^3}$

If αe is the electronic Polarizability for the dipole, then $\mu = \alpha_e E_i$

Or $\quad E_i = E + \frac{1.2\alpha_e E_i}{\pi\varepsilon_0 d^3}$

Or $\quad E_i = \frac{E}{1 - \frac{1.2\alpha_e}{\pi\varepsilon_0 d^3}}$ is the expression for the internal field

But in three dimension al array, the general equation for internal field is expressed as

$$E_i = E + \left(\frac{\gamma}{\varepsilon_0}\right)P$$

Where P is the polarization and γ is a proportionality constant called internal constant

For cubic lattice $\Upsilon = 1/3$

$$E_i = E + \frac{P}{3\varepsilon_0}$$ is called Lorentz equation

Clausius- Mossotti Equation

Consider a elemental solid dielectric material of dielectric constant ε_r

Let N is the number of atoms/unit volume of the material

μ-is the atomic dipole moment

Dipole moment/unit volume = Nμ

Let E_i be the internal field, α_e is the electronic Polarizability of the atom

$$\mu = \alpha_e E_i$$

Therefore,   Dipole moment/unit volue = $N\alpha_e E_i$

$$P = N\alpha_e E_i$$

Therefore, $$E_i = \frac{P}{N\alpha_e}$$

But $$P = \varepsilon_0(\varepsilon_r - 1)E$$ where E is the applied field

Rearranging we get $$E = \frac{P}{\varepsilon_0(\varepsilon_r - 1)}$$

Expression for the internal field is given by $E_i = E + \left(\frac{\gamma}{\varepsilon_0}\right)P$

Substitute for E_i and E we get $$\frac{P}{N\alpha_e} = \frac{P}{\varepsilon_0(\varepsilon_r - 1)} + \left(\frac{\gamma}{\varepsilon_0}\right)P$$

$$\frac{1}{N\alpha_e} = \frac{1}{\varepsilon_0}\left[\frac{1}{(\varepsilon_r - 1)} + \gamma\right]$$

Consider the internal field in the material to be Lorentz field

i.e γ=1/3

$$\frac{1}{N\alpha_e} = \frac{1}{\varepsilon_0}\left[\frac{1}{(\varepsilon_r - 1)} + \frac{1}{3}\right] = \frac{1}{\varepsilon_0}\left[\frac{3 + \varepsilon_r - 1}{3(\varepsilon_r - 1)}\right] \qquad \frac{\varepsilon_0 \text{ or}}{N\alpha_e} = \left[\frac{(\varepsilon_r + 2)}{3(\varepsilon_r - 1)}\right]$$

Rearranging we get $$\frac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \frac{N\alpha_e}{3\varepsilon_0}$$

The above equation is known as Claussius-Mossotti equation

Extrinsic semiconductor

Fermi level in extrinsic semiconductor

In extrinsic semiconductor, the number of electrons in the conduction band and the number of holes in the valence band are not equal. Hence, the probability of occupation of energy levels in conduction band and valence band are not equal. Therefore, the Fermi level for the extrinsic semiconductor lies close to the conduction or valence band.

Fermi level in n-type semiconductor

In n-type semiconductor pentavalent impurity is added. Each pentavalent impurity donates a free electron. The addition of pentavalent impurity creates large number of free electrons in the conduction band.
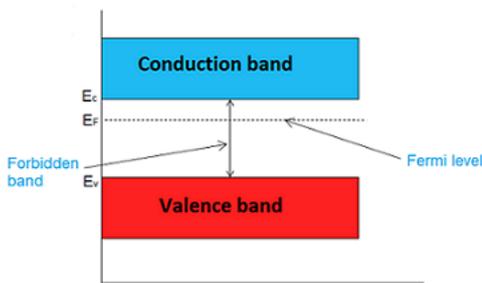
At room temperature, the number of electrons in the conduction band is greater than the number of holes in the valence band. **Hence, the probability of occupation of energy levels by the electrons in the conduction band is greater than the probability of occupation of energy levels by the holes in the valence band**. This probability of occupation of energy levels is represented in terms of Fermi level. Therefore, the Fermi level in the n-type semiconductor lies close to the conduction band.

The Fermi level for n-type semiconductor is given as

$$E_F = E_C - K_B T \log \frac{N_C}{N_D}$$

Where E_F is the fermi level, E_C is the conduction band, K_B is the Boltzmann constant.

T is the absolute temperature; N_C is the effective density of states in the conduction band.

N_D is the concentration of donor atoms.

Fermi level in p-type semiconductor:

In p-type semiconductor trivalent impurity is added. Each trivalent impurity creates a hole in the valence band and ready to accept an electron. The addition of trivalent impurity creates large number of holes in the valence band.
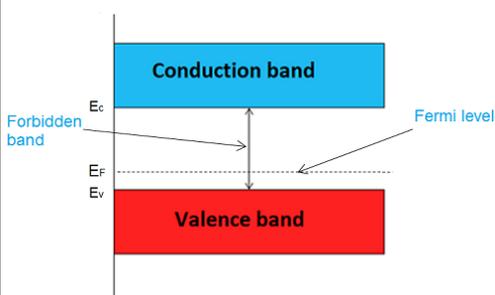
At room temperature, the number of holes in the valence band is greater than the number of electrons in the conduction band. **Hence, the probability of occupation of energy levels by the holes in the valence band is greater than the probability of occupation of energy levels by the electrons in the conduction band.** This probability of occupation of energy levels is represented in terms of Fermi level. Therefore, the Fermi level in the p-type semiconductor lies close to the valence band.

The Fermi level for p-type semiconductor is given as $E_F = E_V + K_B T \log \frac{N_V}{N_A}$

Where N_V is the effective density of states in the valence band.

N_A is the concentration of acceptor atoms.

Expression for concentration of electrons in conduction band:

For a semiconductor in a conduction band, some lower energy states are filled with electrons at room temperature. The concentration of electrons in conduction band is given by

$$n = \int N(E)f(E)dE \quad \text{----------------(1)}$$

Where

N(E) = No. of electrons/unit energy/unit volume and f(E) = Fermi factor

We have

$$N(E) = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} E^{1/2} \quad \text{----------------(2)}$$

$$f(E) = \frac{1}{1+\exp\left(\frac{E-E_f}{k_BT}\right)} \quad \text{----------------(3)}$$

When $(E - E_f) > k_BT$

$$f(E) = \frac{1}{\exp\left(\frac{E-E_f}{k_bT}\right)} = \exp\left[-\left(\frac{E-E_f}{k_BT}\right)\right] \quad \text{----------------(4)}$$

Hence eqn(1) becomes

$$n = \int_{E_C}^{E_C+\varphi} \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} (E - E_C)^{1/2} \exp\left[-\left(\frac{E-E_f}{k_BT}\right)\right] dE$$

Here $E^{1/2}$ has been replaced by $(E-E_c)^{1/2}$ since Ec is lower energy level in conduction band and Φ is the work function of the metal. The combination of Ec + Φ turns out to be huge and we can replace it by ∞.

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \int_{E_C}^{\infty}(E - E_C)^{1/2} \exp\left[-\left(\frac{E-E_f}{k_BT}\right)\right] dE \quad \text{----------------(5)}$$

Evaluating the above integral by taking E = Ec +x and dE = dx and limit of the integration as 0 to ∞ **(assuming the lowest energy almost to be equal to zero).**

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \int_0^{\infty} (x)^{1/2} \exp\left(\frac{E_f - E_c - x}{k_BT}\right) dx$$

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \int_0^{\infty} (x)^{1/2} \exp\left(\frac{E_f - E_c}{k_BT}\right) \exp\left(\frac{-x}{k_BT}\right) dx$$

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \exp\left(\frac{E_f - E_c}{k_BT}\right) \int_0^{\infty} (x)^{1/2} \exp\left(\frac{-x}{k_BT}\right) dx$$

Let $y = \frac{x}{k_BT}$ then $dy = \frac{dx}{k_BT}$

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \exp\left(\frac{E_f-E_c}{k_BT}\right) (k_BT)^{\frac{3}{2}} \int_0^{\infty}(y)^{1/2} \exp(-y)\, dy \quad \text{----------------(6)}$$

Using gamma integral function we can write $\int_0^{\infty}(y)^{1/2} \exp(-y)\, dy = \frac{\pi^{1/2}}{2}$

$$n = \left(\frac{4\pi}{h^3}\right)(2m_e^*)^{3/2} \ \exp\left(\frac{E_f - E_c}{k_B T}\right)(k_B T)^{\frac{3}{2}}\left(\frac{\pi^{1/2}}{2}\right)$$

$$\boldsymbol{n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_f - E_c}{k_B T}\right) = N_c \exp\left(\frac{E_f - E_c}{k_B T}\right)} \text{---------------(7)}$$

Where $\boldsymbol{N_c = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}}$ and equation (7) represents concentration of electrons in conduction band

Expression for concentration of holes in valence band:

The concentration of holes in valence band can be calculated as follows

$$n = \int N(E)[1 - f(E)] \, dE \quad \text{---------------(1)}$$

By substituting the values for N(E) & f(E) and solving the integral as we did for the concentration of electrons in conduction band we can arrive at the following equation

$$\boldsymbol{n = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_v - E_f}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_f}{k_B T}\right)} \text{---------------(2)}$$

Where $\boldsymbol{N_v = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2}}$ *represents the concentration of holes in valence band*

and equation (2) represents concentration of holes in valence band

Expression for intrinsic carrier concentration:

In an intrinsic semiconductor, the concentration of holes and electrons are equal, i.e. n = p. The product of hole and electron concentrations for a given material is constant at a given temperature. If impurity is added to increase n, there will be corresponding decrease in p so that the product n x p remains constant and is sometimes called law of mass action. Therefore in an intrinsic semiconductor

$$n \times p = n_i \times p_i = n_i^2$$

$$n_i^2 = \left[2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_f - E_c}{k_B T}\right)\right]\left[2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_v - E_f}{k_B T}\right)\right]$$

$$n_i^2 = 4\left(\frac{2\pi k_B T}{h^2}\right)^3 (m_h^* m_e^*)^{3/2} \exp\left[-\left(\frac{E_c - E_v}{k_B T}\right)\right]$$

Substituting $(E_c - E_v) = E_g$ and the values of constants we get

$$n_i^2 = 4\left(\frac{2\pi \times 1.38 \times 10^{-23}}{(6.634 \times 10^{-34})^2}\right)^3 (m_h^* m_e^*)^{3/2} T^3 \exp\left[-\left(\frac{E_g}{k_B T}\right)\right]$$

$$n_i^2 = 4\left(\frac{2\pi \times 1.38 \times 10^{-23} \times 9.1 \times 10^{-31}}{(6.634 \times 10^{-34})^2}\right)^3 \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/2} T^3 \exp\left[-\left(\frac{E_g}{k_B T}\right)\right]$$

$$n_i^2 = 2.322 \times 10^{43} \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/2} T^3 \exp\left[-\left(\frac{E_g}{k_B T}\right)\right]$$

$$n_i = 2\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/4} \exp\left[-\left(\frac{E_g}{2 k_B T}\right)\right]$$

$$n_i = A_o T^{3/2} exp\left[-\left(\frac{E_g}{2k_B T}\right)\right]$$

Where $A_o = A^{1/2} = 4.819 \times 10^{21} \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/4}$

Fermi level in an intrinsic semiconductor:

In an intrinsic semiconductor, the concentrations of electrons and holes are equal. Therefore we can write

$$N_c \exp\left(\frac{E_f - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_f}{k_B T}\right)$$

$$\frac{N_c}{N_v} = \exp\left[-\left(\frac{E_f - E_c}{k_B T}\right)\right] \exp\left(\frac{E_v - E_f}{k_B T}\right)$$

$$\frac{N_c}{N_v} = \exp\left[\left(\frac{E_v + E_c - 2E_f}{k_B T}\right)\right]$$

$$ln\left[\frac{N_c}{N_v}\right] = \frac{E_v + E_c - 2E_f}{k_B T}$$

$$E_v + E_c - 2E_f = k_B T \, ln\left[\frac{N_c}{N_v}\right]$$

$$E_f = \frac{E_v + E_c}{2} - \frac{k_B T}{2} \, ln\left[\frac{N_c}{N_v}\right]$$

If the effective masses of the holes and electrons are equal, then

$$E_f = \frac{E_v + E_c}{2}$$

Hence it is clear from the above equation that for an intrinsic semiconductor, the Fermi level lies at the middle of the energy gap, when the effective masses of the holes and electrons are equal.

Expression for conductivity of semiconductors:

The conductivity of a metal can be written as

$\sigma = ne\mu$ -------------------------- (1)

Where n = concentration of electrons ; μ = mobility of electrons

In a semiconductor, both electrons & holes are charge carriers. Therefor eqn (1) can be written as

$\sigma = ne\mu_e + pe\mu_h$ -------------------------- (2)

Where n & p= concentrations of electrons & holes ; μ_e & μ_h = mobility of electrons & holes

For an intrinsic semiconductor, the concentrations of electrons & holes are equal, hence eqn. (2) can be written as

$\sigma = n_i e(\mu_e + \mu_h)$ -------------------------- (3)

In a p-type semiconductor, since p >> n eqn. (2) can be written as

$\sigma = pe\mu_h$ -------------------------- (3)

In an n-type semiconductor, since n >> p eqn. (2) can be written as

$\sigma = ne\mu_e$ -------------------------- (4)

Substituting the value for n_i in eqn. (3) we get

$\sigma = 2\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/4} \exp\left[-\left(\frac{E_g}{2k_B T}\right)\right] e(\mu_e + \mu_h)$ ----------------(5)

Eqn. (5) can be written as

$\sigma = A \exp\left[-\left(\frac{E_g}{2k_B T}\right)\right]$ ---------------- (6)

Where $A = 2\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \left(\frac{m_h^* m_e^*}{m^2}\right)^{3/4} e(\mu_e + \mu_h)$ -------------- (7)

Hence eqn. (6) can be rewritten as

$\frac{1}{\rho} = A \exp\left[-\left(\frac{E_g}{2k_B T}\right)\right] = \frac{l}{Ra}$ ---------------- (8)

$R = \frac{l}{Aa}\exp\left[\frac{E_g}{k_B T}\right] = C \exp\left[\frac{E_g}{2k_B T}\right]$ ---------------- (9)

Here C = l/Aa, where a = area of cross section ; l = length of the specimen. Taking natural log on both sides of eqn. (9) we get

ln R = ln C + E$_g$/2k$_B$T ---------------- (10)

Eqn.(10) is similar to equation of straight line y = mx + c,
where y = ln R, x = 1/T, m = E_g/2k$_B$ and c = ln C . If a plot is drawn between _**ln R verses 1/T**_ . The value of E_g can be determined from the slope of the straight line. Hence E_g = 2k$_B$ x slope.
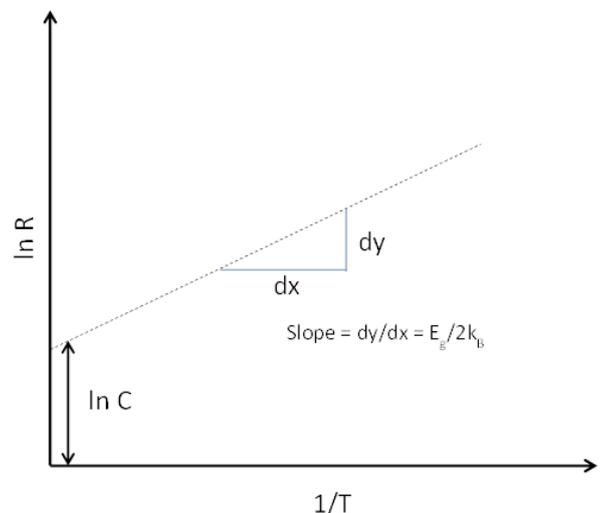
Hall Effect :

In a conductor, the flow of electric current is the movement of charges due to the presence of an electric field. If a magnetic field is applied in a direction perpendicular to the direction of motion of the charges, the moving charges accumulate such that opposite charges lie on opposite faces of the conductor. This distribution of charges produces a potential difference across the material that opposes the migration of further charge. This creates a steady electrical potential as long as the charges are flowing in the material and the magnetic field is on. This is the Hall effect.
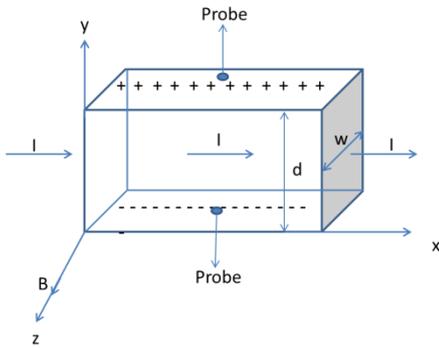
Consider a rectangular slab of a semiconductor material in which a current I is flowing in the positive x-direction. Let the semiconducting material be of n-type, which means that the charge carriers are electrons. Let a magnetic field B be applied along the z-direction as shown in the figure. Under the influence of the magnetic field, the electrons experience the Lorentz force F_L given by

$$F_L = -Bev \text{ ------------ (1)}$$

Applying the Flemming's left hand rule, we see that the force is exerted on the electrons in the negative y-direction. The electrons are therefore deflected downwards. As a result, the density of the electrons increases in the lower end of the material, due to which its bottom edge becomes negatively charged. On the other hand, the loss of electrons from the upper end causes the top edge of the metrical to become positively charged. Hence a potential V_H, called the Hall voltage appears between the upper and lower surfaces of the semiconductor material which establishes an electric field E_H called the Hall field across the conductor in the negative y-direction. The field E_H, exerts an upward force F_H on the electrons given by

$$F_H = -eE_H \text{ ------------ (2)}$$

Now as the deflection of electrons continues in the downward direction due to the Lorentz force FL, it also contributes to the growth of Hall field. As a result , the force FH which acts on the electron in the upward direction also increases. These two opposing forces reach equilibrium at which stage,

$$F_L = F_H$$

Using eqns. (1) & (2), above equation becomes

$-Bev = -eE_H$ or $E_H = Bv$ ------------ (3)

If d is the distance between the upper and lower surfaces of the slab, then,

$E_H = V_H/d$ or $V_H = E_H d = Bvd$ ------------ (4)

Let w be the thickness of the material in the z-direction

Its area of cross section normal to the direction of I is = wd.

The current density $J = I/wd$ ------------ (5)

But, we know that $J = nev = \rho v$ ------------ (6)

Therefore, $\rho v = I/wd$ or $v = I/wd\rho$ ------------ (7)

Comparing equations (4) & (7) we get   **$V_H = BI/new$**

Hall coefficient (R_H) :

For a given semiconductor, the Hall field E_H depends upon the current density J and the applied field B.

$E_H \propto JB$

$E_H = R_H JB$, where R_H is called the Hall Coefficient

Therefore,

$R_H = E_H / JB = Bv / nevB = 1/ne$

$R_H = 1/ne$

Note:

1. Positive value of **R_H** indicates that the charge carriers are holes.
2. Negative value of **R_H** indicates that the charge carriers are electrons.

Application of Hall Effect

1. Hall Effect is used to find whether a semiconductor is N-type or P-type.
2. Hall Effect is used to find carrier concentration.
3. Hall Effect is used to calculate the mobility of charge carriers (free electrons and holes).
4. Hall Effect is used to measure conductivity.
5. Hall Effect is used to measure a.c. power and the strength of magnetic field.
6. Hall Effect is used in an instrument called Hall Effect multiplier which gives the output proportional to the product of two input signals.

***** End *****

UNIT 4 - LASERS AND OPTICAL FIBERS

Introduction on LASER

- **L**ight **A**mplification by **S**timulated **E**mission of **R**adiation is **LASER**. A laser is a generator of *highly monochromatic, coherent, intense light*. The production of laser is the consequence of interaction of radiation with matter, which occurs under appropriate conditions leading to the transition of the system from one energy level to another.

- The transition of an atom or molecule from one energy level to another occurs in a jump & is called quantum transitions. Quantum transition may be induced by the various causes. In particular, they can occur when the atoms interact with optical radiation.

- The system of energy levels of atoms governs the behavior of electrons performing the transition in atoms.

- Unlike other sources of light, the laser produces radiation with highly regular light field, outstanding in its coherence, monochromaticity and directivity.

Interaction of radiation with matter

Interactions of radiation with matter can take place through three possible ways. They are

(1) Induced Absorption:

Let the energy of the lower level be E_1 and that of the upper level be E_2. Assume that the atom is in lower level and a photon of energy $h\upsilon = E_2 - E_1$ travels nearer the atom. The atom can absorb this photon and rise from the level E_1 to E_2 thus making a transition upon the absorption of a quantum of light. This is called induced or stimulated absorption and can be represented as

$$atom + photon = atom*$$


(2) Spontaneous Emission:

When an atom is in the level E_2 makes transition to E_1 by spontaneously emitting a photon of energy $E_2 - E_1$ without any stimulus, then the process is called Spontaneous emission. In this case,

$$atom* = atom + photon$$
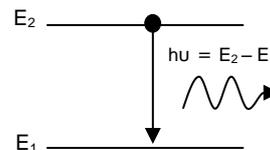
Due to spontaneous emission, the photons are emitted in all possible directions. There is no phase relationship between the photons. Thus, the emitted light is incoherent. The number of spontaneous transitions taking place in a system depends only on the number of atoms N_2 in the excited state E_2.

(3) Stimulated Emission:

The emission of photons by an atom under the influence of a passing photon of just right frequency due to which the atom makes a transition from a higher energy state to a lower energy state is called stimulated emission. A photon of energy $E_2 - E_1$ induces the excited atom to make downward transition releasing the energy in the form of photon. Thus, the interaction of a photon with an excited atom triggers the exited atom to drop to the lower energy state emitting a photon. The phenomenon of forced emission of photons is known as stimulated emission a photon emitted during stimulated emission has the same energy as the incident photon. It is emitted in the same direction and as the same phase as the incident photon thus the photons are coherent. If these two coherent photons then interact with two more excited state atoms, four coherent photons are produced and so on. Therefore the stimulated process leads to photo amplification. The process is represented by

<p align="center">Atom* + Photon = Atom + 2 photons</p>
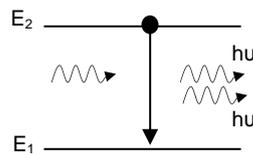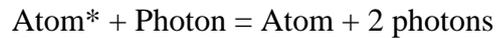
The stimulated transition depends on both the energy density of incident radiation and the number of atoms N_2 available in the excited state E_2 for de excitation.

Conditions, requisites & properties of laser

(i) Conditions for Laser

Presence of metastable states: An atom can remain in the excited state for a limited time of about 10^{-8}s. However, there exist such excited states in which the lifetime is greater than 10^{-8}s. These states are called as metastable states.

Population inversion: For lasing action to occur there should be more number of atoms in the higher state than the lower state. Over a period of time atomic density in the higher level decreases. The process of achieving back higher atomic density in the higher level is known as population inversion.

(ii) Requisites of a Laser system

Energy Source (Excitation Source) : Which will rise the system to an excited state.

Active medium: Which when excited achieves population inversion. It may be a solid, Liquid or gas.

*Optical Cavity***:** Consisting of two mirrors facing each other. The active medium is enclosed in this cavity. One of the mirrors is 100% reflective and the other is partially transparent to let the some of the radiation to pass through. The optical cavity is made use of to make the stimulated emission possible in more number of atoms in the active medium. This naturally increases the intensity of the laser beam.

Einstein's coefficients and expression for energy density of photons at a given frequency and temperature.

Einstein's coefficients are transition probabilities, which tell us about the extent of stimulated & spontaneous emission and induced absorption.

Let A_{21} = Spontaneous emission transition probability / unit time
$E(\upsilon)$ = Energy density of the atomic field
E_1 & E_2 = Two energy levels occupied by N_1 & N_2 atoms
$B_{12} E(\upsilon)$ = Absorption transition probability/unit time
$B_{21} E(\upsilon)$ = stimulated emission transition probability/unit time

The no. of atoms that fall from level E_2 to E_1 / unit time = $[A_{21} + B_{21}E(\upsilon)]N_2$
The no. of atoms that raise from level E_1 to E_2 / unit time = $B_{12}E(\upsilon)N_1$
Therefore net rate of change of atoms in the level E_2 / unit time is
$[dN_2/dt] = \{B_{12}E(\upsilon)N_1 - [A_{21} + B_{21}E(\upsilon)]N_2\}$ ---------------------- (1)
Under equilibrium conditions, the net rate of change of atoms in any level must be zero. So
$[dN_2/dt] = 0$ ----------------------(2)
Comparing eqns.(1) & (2)
$B_{12}E(\upsilon)N_1 = [A_{21} + B_{21}E(\upsilon)]N_2$
$N_2/N_1 = \{B_{12}E(\upsilon) / [A_{21} + B_{21}E(\upsilon)]\}$ ----------------------(3)

According to Boltzmann, the atomic population at different energy levels at a given temperature T is given by
$N_2/N_1 = \exp[-h\upsilon/k_BT]$ ----------------------(4)
Comparing eqns. (3) & (4)
$B_{12}E(\upsilon) / [A_{21} + B_{21}E(\upsilon)] = \exp[-h\upsilon/k_BT]$
$[B_{12} \exp(h\upsilon/k_BT) - B_{21}]E(\upsilon) = A_{21}$ (where $k_B = 1.38\times10^{-23}$ J/K)

$\boxed{E(\upsilon) = (A_{21}/ B_{12}) / [\exp(h\upsilon/k_BT) – (B_{21}/ B_{12})]}$ ----------------------(5)

This is the expression for the energy density of the photons at a given frequency & temperature
Planck's formula for the energy density of radiation at a given temperature T is given by

$E(\upsilon) = (8\pi h\upsilon^3/c^3) / [\exp(h\upsilon/k_BT) – 1]$ ----------------------(6)
Comparing eqns. (5) & (6)

$\boxed{A_{21}/ B_{12} = 8\pi h\upsilon^3/c^3}$ **and** $\boxed{B_{21}/ B_{12} = 1}$

Note:
(1) eqn. (5) can be written as
    $[A_{21}/ B_{12} E(\upsilon)] = [\exp(h\upsilon/k_BT) – 1]$
    If $h\upsilon > kT$ then $A_{21}/ B_{12} E(\upsilon)$ is +ve and large. Then spontaneous emission is much more probable
    than stimulated emission.
(2) If $h\upsilon < kT$ then $A_{21}/ B_{12} E(\upsilon)$ is +ve and small. Then stimulated emission may become
    Important
(3) The ratio $A_{21}/ B_{12} \propto \upsilon^3$. This shows that the probability of spontaneous emission increases
    rapidly with the energy difference between two states

Construction and working of He-Ne laser

Helium – Neon gas laser:

The active lasing species in this laser is the neon atoms. Neon atoms are excited by the transfer of energy from excited He atoms which in turn are excited by collisions with the electrons. Thus, population inversion involves

a) Electron impact (of He) or collision of first kind
b) Excitation transfer (of Ne from He) or collision f second kind

Construction:

It consists of fused quartz tube, the ends of which are sealed with a transparent material and are called windows. These windows are inclined at an angle known as Brewster's angle in order to get polarized laser out put. The tube contains two electrodes at either side. A power supply (D.C) is connected across the electrodes. Two external plain mirrors are mounted on either side of the tube. One of them is fully silvered so that it is 100% reflective but the other is partially transparent. A mixture containing He at a pressure of 1mm of Hg and Ne at a pressure of 0.1mm of Hg and in the ratio 10:1 is filled in the tube. This mixture acts as an active medium.
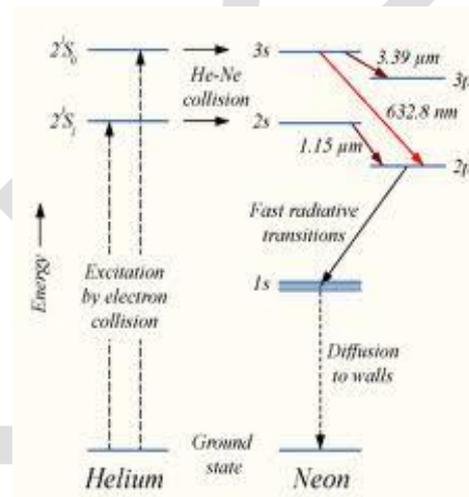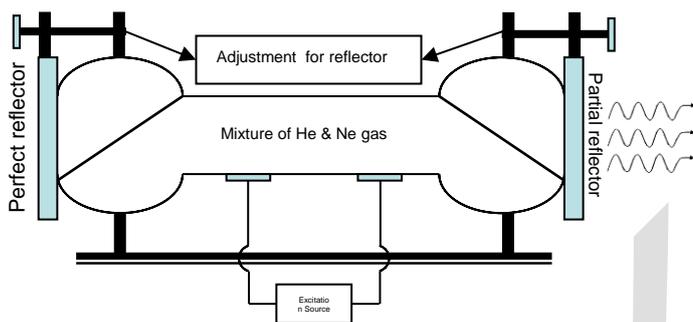
Working:

When the DC discharge voltage is applied across the electrodes, fast moving electrons are produced. These electrons collide with more abundant helium atoms in the mixture. As a result of this collision, the helium atoms are excited from the ground level to the higher metastable states. This kind of collision is called collision of first kind and can be represented as

$$He + e^- \rightarrow He^*$$
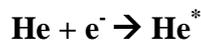
Since the excited energy levels of He atoms are nearly same as that of Ne atoms, the Ne atoms in the ground stage are able to receive the energy due to the collision with excited He atoms. This kind of collision is called collision of second kind, and can be represented as

$$He^* + Ne \rightarrow Ne^* + He$$
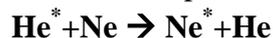
As a result of collision of second kind, the energy levels 3S and 2S of Neon are well populated. Hence population inversion builds up between the energy levels **3S and 3P, 3S and 2P, 2S and 2P**. The laser transition takes place continuously between the levels 3S and 3P, yielding a laser light of wavelength 3.39 micrometer, **3S and 2P** transition yielding a laser light of wavelength **6328 Å.** Transition between **2S and 2P yields a laser light of wavelength 1.15 micrometer**, hence Helium Neon gas laser is a continuous laser. Out of many laser transitions which are possible in the active medium, a laser beam of desired wavelength can be trapped by adjusting the distance between the mirrors while the other radiations can be suppressed. On the other hand a methane chamber can be used to absorb IR radiations. Hence the laser cavity is called resonant cavity for that radiation.

Construction and working of semiconductor laser

A semiconductor laser is a specially fabricated pn junction device (both the p and n regions are highly doped) which emits coherent light when it is forward biased. It is made from Gallium Arsenide (GaAs). They are of very small size (0.1 mm long), efficient, portable and operate at low power. These are widely used in Optical fiber communications, in CD players, CD-ROM Drives, optical reading, laser printing etc.

p and n regions are made from same semiconductor material (GaAs). A p type region is formed on the n type by doping zinc atoms. The diode chip is about 500 micrometer long and 100 micrometer wide and thick. The top and bottom faces have metal contacts to pass the current. The front and rear faces are polished to constitute the resonator.

Active medium:

The active medium in GaAs is GaAS. But it is also commonly said that depletion region is the active medium in semiconductor laser. The thickness of the depletion layer is usually very small (0.1 μm).

Pumping Source: Forward biasing is used as pumping source. The p-n junction is made forward biased that is p side is connected to positive terminal of the battery and n side to negative. Under the influence of forward biased electric field, conduction electrons will be injected from n side into junction area, while holes will enter will enter the junction from the p side. Thus, there will again be recombination of holes and electrons in depletion region

and thus depletion region becomes thinner. If E_{fc} is the quasi conduction Fermi level and if E_{fv} is the quasi Fermi valence level then the condition for lasing action is $E_{fc} - E_{fv} > E_g$.

Optical resonator system: The two faces of semiconductor which are perpendicular to junction plane make a resonant cavity. The top and bottom faces of diode, which are parallel to junction plane are metallised so as to make external connections. The front and back faces are roughned to suppress the oscillations in unwanted direction.

Achievement of population inversion: When p-n junction diode is forward biased, then there will be injection of electrons into the conduction band along n-side and production of more holes in valence band along p-side of the junction. Thus, there will be more number of electrons in conduction band
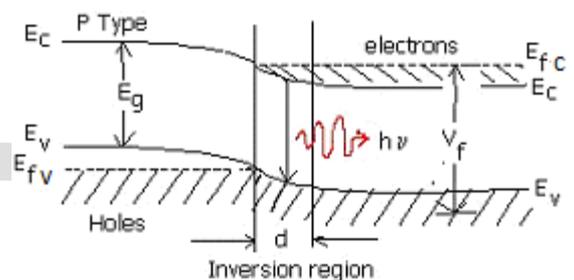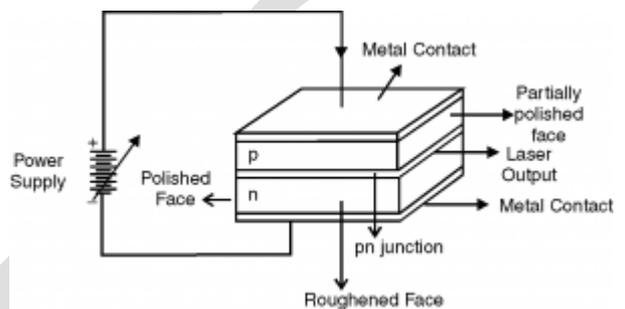
Applications of laser

★ *Measurement of Pollutants in Atmosphere:*
Atmospheric optics uses lasers for the remote probing of the atmosphere, including the measurement to traces of pollutant gases, temperature, water vapour concentration, sometimes at ranges greater than 8 to 15 km away.

The pollutants in the atmosphere include carbon monoxide, nitrous oxide, sulphur dioxide, Freon, ethylene, vinyl chloride (the cancer causing agent from plastic industries) and other matter.

The laser technique consists of a laser source, a transreceiver optical system, a signal processing electronic unit and retro reflector. The principle involves projecting a laser beam, through the atmosphere. The area where the pollutants are to be measured. The system employs a pulsed laser as a source of light energy. The measurement is based on the spectral absorption of the laser beam. Since different gases in atmosphere absorb laser energy at different wavelengths, the amount of absorption by each wavelength indicates the amount of pollutant in the atmosphere. Light that is back scattered by the congestion of matter is detected by a photo detector. The reflected laser beam undergoes attenuation due to spectral absorption by the pollutants in the atmosphere. The distance of the scattering matter is calculated from the time the laser pulse takes to go to the matter and return back to the system. The attenuated beam received at the photo detector and the beam energy is integrated and compared with reference laser energy source, the difference in the energy called error signal is analyzed and converted into a direct readout by the computer. The reading indicates the concentration and the distribution of pollutants in different vertical sections.

★ *Laser welding*
The spot to be welded is focused by a laser beam. Due to the generation of heat, the material melts over a tiny area on which the laser beam is focused. The impurities in the material float up on the surface of the material and upon cooling the material becomes homogeneous solid structure which makes the stronger joint.

★ *Laser Drilling*
The spot to be drilled is focused by a laser beam. Drilling is done with high power pulsed lasers. The light pulses will be of the order of 10-4s to 10-3s duration. The principle of laser drilling is mainly to heat the metal to its boiling point and vapourise it or remove it by high pressure vapour. When high power pulsed lasers are projected onto the metal spot, a vapour keyhole surrounded with molten metal is formed. With continued heating by laser beam, the metal vapourises and atoms ionize. The metal vapour then interacts with light beam and thereby the electrons get accelerated by electromagnetic radiation. This further heats the metal vapour, increasing the number of ions, forming plasma. Plasma absorbs laser light and emits blackbody radiation. Since the plasma interactions in the keyhole generate detonation waves, combined with the high power pressure, the molten metal gets ejected from the keyhole, thereby forming drilling operation.

★ *Laser Cutting*
Lasers are found to be very effective in cutting different types of material. The material to be removed in laser cutting can be accomplished by melting and blowing out the molten metal. For blowing out the molten metal, a very high velocity gas jet of some inert gas is used. This process is known as **Gas assisted laser beam machining**.

Holography :

The light waves reflected by an object are characterized by their amplitude and phase. In conventional photography, the photographic plate records only the intensity and not the phase. Hence, it loses the 3D nature of the object. An ordinary photograph represents a 2D recording of a 3D scene. This inherent limitation in conventional photography is eliminated in holography. In holography, the photographic plate records the intensity and phase distribution of the electromagnetic wave scattered from an object. The principle of holography involves two steps:

(i)   Recording of the image.
(ii)   Reconstruction of the image.

(i)   Recording of the image:

During the recording process, the scattered waves from the object superimpose on the reference wave. These two waves interfere in the plane of the recording medium and produce interference pattern which are characteristic of the object. The recording medium records the intensity distribution in the interference pattern which has also recorded the phase of the electromagnetic wave scattered from the object. The recorded wave is called the hologram. The hologram has little resemblance to the object and it has in it a coded form of the object wave.
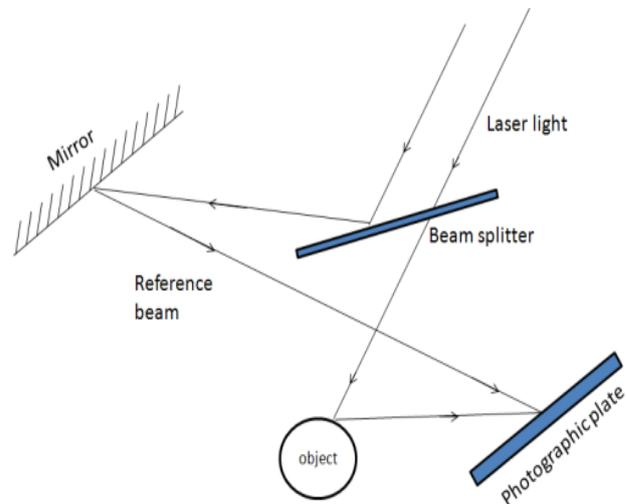
(ii)   Reconstruction of the image:

In this process, the hologram is illuminated with a reference beam whose position is the same as that of the recording. This beam is called reconstruction beam. When hologram is illuminated by the reconstruction beam, two waves are produced. One wave appears to diverge from the object and provides the virtual image of the object. The second wave the converges to a second image which is real and thus can be recorded on a screen or photographed.
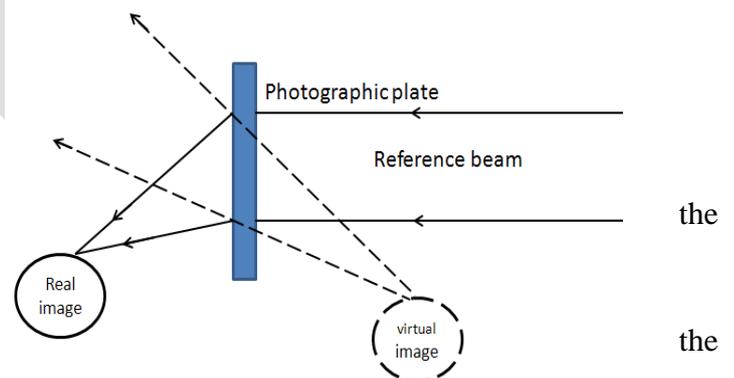
Applications:

- Used for character recognition i.e. to identify finger prints, postal addresses, etc.
- Used in data storage devices. To produce gratings.

**Principle of ray propagation in an optical fiber :**

Optical fibers are wires of either glass of plastics and are used in modern communication systems. The optical fiber consists of a central core, medium of higher refractive index n_1, and an outer cladding of slightly lesser refractive index n_2. The Optical fiber is protected from the external corrosive atmosphere and handling with an outer polyurethane jacket.

Light propagates in a optical fiber by phenomena of Total Internal reflection at the core cladding interface. If the angle of incidence at core cladding interface is greater than the critical angle of incidence then the ray of light would be totally reflected back into the optical fiber's core. The ray propagates through the fiber through reflections at the core cladding interfaces.
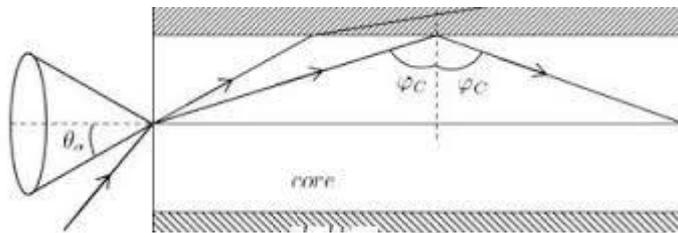
The angle of incidence θ_0 at the core end face has to be less than a critical value called as the angle of acceptance. The cylindrical symmetry of the optical fiber corresponds to a conical shape for the rays with an acceptance angle θ_0. Hence, it also called as the acceptance cone half angle.

Condition for ray propagation in an optical fiber :
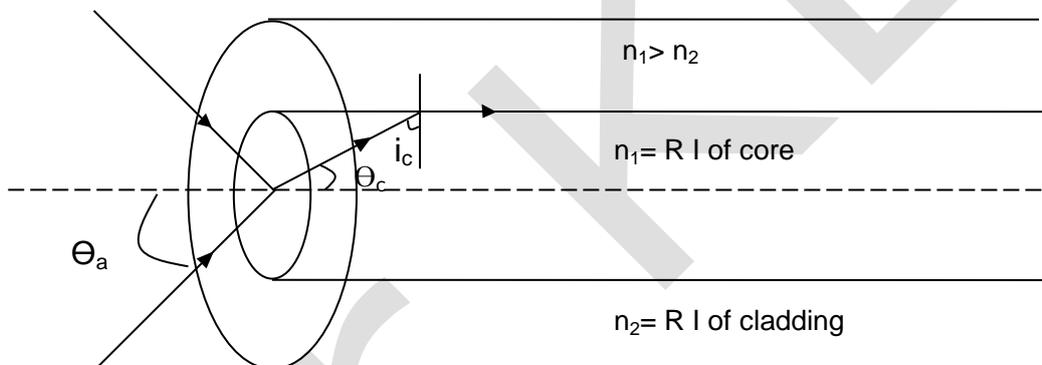
A ray of light incident at an angle of incidence θ_0 on the end face of the fiber undergoes refraction. The angle of refraction being θ_1 . Applying Snell's law at the end face of the core we have

$$n_0 \sin \theta_0 = n_1 \sin \theta_1$$

$$\sin \theta_1 = \frac{n_0}{n_1} Sin \theta_0 \cdots \cdots \quad (1)$$

The ray travels in the core and undergoes refraction at the core cladding interface. The angle of incidence at the interface is θ_2 (equal to 90- θ_1). If this angle is equal to the critical angle for Total internal refraction then the ray travels along the core cladding interface and the angle of refraction is 90^0.

Applying Snell's law at the core cladding interface

$$n_1 \sin(90 - \theta_1) = n_2 \sin 90$$

$$\therefore \quad \cos\theta_1 = \frac{n_2}{n_1} \quad \text{-----} \quad (2)$$

From equations 1 and 2 we have

$$\frac{n_0}{n_1} Sin\,\theta_0 = \sin\theta_1 = \sqrt{(1-\cos^2\theta_1)} = \sqrt{1-\left(\frac{n_2}{n_1}\right)^2} = \frac{\sqrt{n_1^2-n_2^2}}{n_1}$$

$$\sin\theta_0 = \frac{\sqrt{n_1^2-n_2^2}}{n_0} \quad \ldots \quad (3)$$

Thus a ray of light has to be incident at an angle less than or equal to the acceptance angle as given by equation 3 for the ray to propagate through the fiber. If the optical fiber is placed in air then

$$\sin\theta_0 = \sqrt{n_1^2-n_2^2}$$

This is also referred to as the Numerical Aperture (NA) of the optical fiber and determines the maximum angle of incidence for a given combination of core and cladding refractive indices.

$$Numerical \quad Aperture \quad = \quad \sin\theta_0 = \quad \sqrt{n_1^2-n_2^2}$$

The Numerical aperture of an optical fiber measures the ability of the fiber to gather light incident on it. It also is an index of the fiber's capability to carry multiple modes of communication.

**Types of optical fibers and modes of propagation :**

Optical fibers are classified according to their ability to propagate an optical signal effectively through the fiber and the number of modes supported by the fiber. In practice three types of fibers are in use

- Single mode step index fiber
- Multi mode step index fiber
- Graded Index multimode fibers.

Single mode fiber

In a single mode fiber only a single mode of propagation is allowed. In these types of fibers the diameter of the core is about 8μm to 10μm and a cladding diameter of about 125 μm. The optical signal is injected along the axis of the fiber and travels along the axis of the fiber. Single mode fibers have lower attenuation losses compared to the multimode fibers.
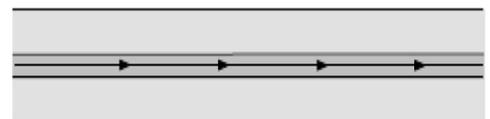
Single mode fibers require precision connectors for coupling between fiber and equipments. The Single mode fibers use precision laser light sources for optical signals. Manufacturing costs of single mode fibers are very high. These factors make the use of single mode fibers expensive. However, the reliability of transmission and low losses in the fiber make them attractive for high reliability transmissions.
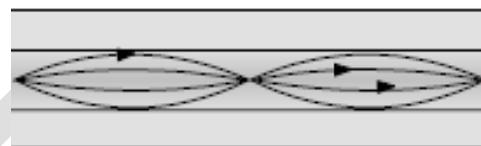
Multi mode step index fibers

Multimode fibers have a core diameter of about 50μm and a cladding diameter of about 250 μm. Since the V number of the fiber is much greater than 2.405 the number modes that can be propagated through the fiber can be about 400. The different modes are incident at

different angles at the endface of the fiber and traverse increasing path lengths with increasing angle of incidence. This increased path lengths are traversed with the same velocity and hence the different signals arrive at different time intervals. This phenomena is called the inter modal dispersion of signals in a multi mode fiber.
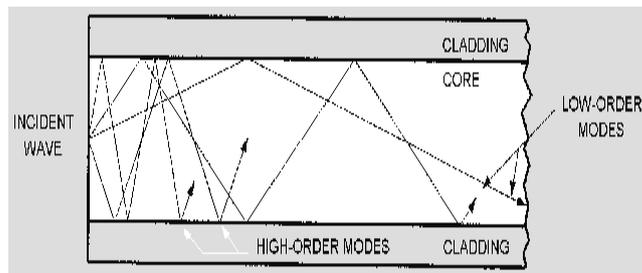
The light source in the case of step index multimode fibers can be either LEDs or LASERS. Multimode fibers find extensive application in commercial optical communication systems.

Graded Index multimode fibers (GRIN)

Graded index multimode fibers are similar to Multimode fibers in construction. However in these fibers the problem of multimodal dispersion of the Step index fiber is overcome by varying the refractive index of the core. The refractive index of the core

region decreases in a designed profile as the distance from the center of the core. Signals traveling through the lower refractive index regions travel with increased velocities. Thus signal traveling through the axis and the outer regions effectively arrive the same time, eliminating the problems of inter modal dispersion.

The GRIN multimode fiber can propagate upto 800 modes. Though expensive it is commonly used in high reliability communication systems.
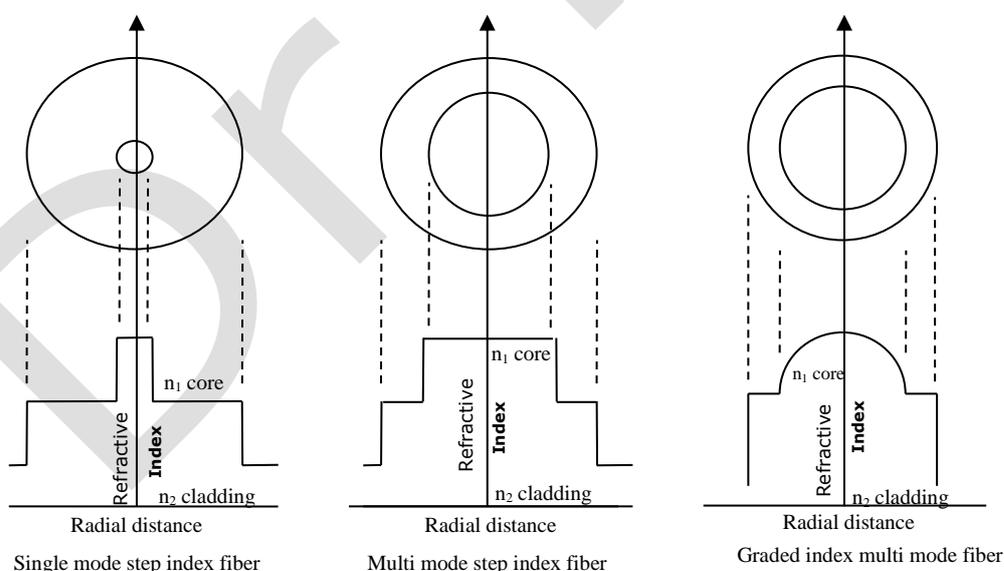
Refractive index profiles of different types of optical fibers

Attenuation in optical fibers

The attenuation of an optical fiber measures the amount of light lost between input and output. When a ray of light propagates through the optical fiber, energy is lost by.   The loss of energy in the fiber is mostly attributed to three different mechanisms.

[1] Absorption   [2] Scattering   [3] Radiation losses

Absorption

All materials absorb some amount of light energy incident on it. The absorption depends on the composition of the material and the wavelength of light incident on it. Most of the glasses absorb strongly in the ultraviolet and minimum in the infrared.

Intrinsic absorption

Intrinsic absorption arises out of the electronic configuration and the bond formation of the basic materials of the optical fiber. The absorption loss exhibited by the material in the highest purity is attributed to the intrinsic absorption of the material. Intrinsic absorption in the ultraviolet regions are contributed to the electronic transitions and that at the infra-red tail is attributed to the vibration of the atomic bonds.

Extrinsic absorption

Absorption losses due to external impurities are termed as extrinsic absorption. Impurities such as iron, nickel, and chromium included in the core material either in the raw material or during the fiber processing contribute strongly to losses due to absorption. Extrinsic absorption also occurs when hydroxyl ions (OH^-) are introduced into the fiber. Absorption losses contribute to approx. 3-4 percent of the total losses in a fiber. With improved technology and high purity raw materials, the loss due to absorption can be minimized to a large extent.

Scattering

Loss due to scattering of light occurs when atoms or other particles whose sizes are less than $1/10^{th}$ of λ to the wavelength of the light known as Rayleigh scattering. The scattering can also occur due to density fluctuations in the fiber and the size of these regions is comparable to the wavelength of light. Loss caused by Rayleigh scattering is proportional to the fourth power of the wavelength ($1/\lambda^4$). As the wavelength increases the loss caused by Rayleigh scattering decreases. The Rayleigh scattering is a inherent feature of Optical fiber losses and cannot be controlled in the manufacturing of the fibers. Rayleigh's scattering account for 94% of the power loss in an optical fiber.

Radiation loss :

Bending the fiber also causes attenuation. Bending loss is classified according to the bend radius of curvature: micro bend loss or macro bend loss.

Macro bends are bends having a large radius of curvature relative to the fiber diameter. During installation, if fibers are bent too sharply the ray of light is refracted out of the fiber is the angle of

incidence at the bend is less than the critical angle. This results in loss of power.
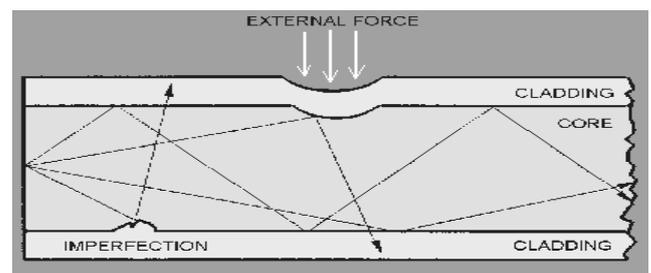
Micro bend losses are caused by small discontinuities or imperfections in the fiber. Uneven coating applications and improper cabling procedures increase micro bend loss. External forces are also a source

of micro bends. An external force deforms the cabled jacket surrounding the fiber but causes only a small bend in the fiber. Micro bends change the path that propagating modes take. **Micro bend loss** increases attenuation because low-order modes become coupled with high-order modes that are naturally lossy.

Micro bend and macro bend losses are very important loss mechanisms, but can be controlled by ensuring that the radius of the bends are greater than the value specified by the manufacturer.

These attenuation phenomena in an optical fiber define three regions or windows of preferred operation. The first window is centered at 850 nm. The second window is centered at 1300 nm. The third window is centered at 1550 nm. Fiber optic systems operate at wavelengths defined by one of these windows.
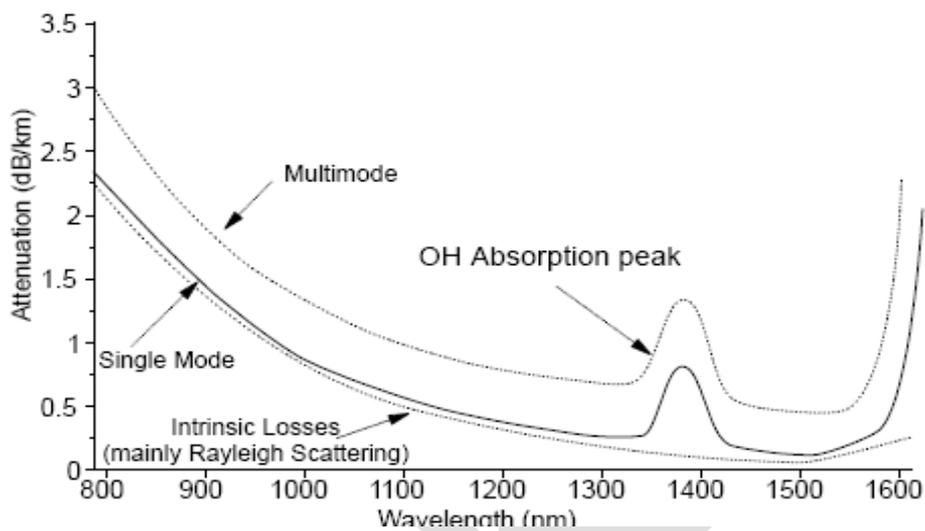
Normalized frequency or V number of an optical fiber:

Electromagnetic waves bound to an optical fiber are described by the fiber's normalized frequency. The normalized frequency determines the number of modes supported in a fiber. Normalized frequency is a dimensionless quantity. Normalized frequency is also related to the fiber's cutoff wavelength. Normalized frequency (V) is given by

$$V = \frac{\pi d \sqrt{\left(n_1^2 - n_2^2\right)}}{\lambda}$$

where n_1 is the core index of refraction, n_2 is the cladding index of refraction, *a* is the core diameter, and λ is the wavelength of light in air.

The number of modes that can be propagated in an optical fiber is given by

$$N \approx \frac{V^2}{2} \qquad \text{when } V \gg 1$$

When V is ≤ 2.405 only a single mode at the specified wavelength is propagated through the fiber. In multimode fibers the V number is quite large and can propagate about 400 independent modes depending on the wavelength and the characteristics of the optical fiber.

Advantages of optical fibers:

- **Noise Immunity**

  Optical fibers are used in environments where electromagnetic interference is prominent and unavoidable. While cables are normally contained in protective sheaths and often run inside conduit, there is no need to physically isolate fiber optic cables from electrical cables. This makes cable routing simpler.

- **Electrical Isolation**

  The problem of ground loop noise and common mode potential differences is eliminated by the use of fiber optic cables. Field signals, generated by devices floating at high potentials, can be coupled to other equipment at much lower potentials without the risk of damage. This is particularly desirable in industrial applications.

- **Safe for Use in Hazardous Areas**

  Fiber optic links can be used to couple signals into areas with potentially explosive atmospheres without a risk to delivering or storing sufficient energy to ignite an explosion. This makes fiber optic technology particularly useful when designing intrinsically safe systems.

- **Wide Bandwidth**

  Fiber optic cables can carry very wide bandwidth signals, well into the GHz range. Many individual, lower bandwidth signals can be multiplexed onto the same cable. In commercial systems fiber optic cable often carries a mixture of signal types, including voice, video and data all on the same fiber.

- **Low Signal Attenuation**

  Optical fibers do exhibit some attenuation due to absorption and scattering. However, this attenuation is relatively independent of frequency, a factor that is significant in copper cables.

- **Light Weight, Small Diameter**
  Because many signals can be multiplexed onto one fiber, cables tend to be smaller and lighter. This makes installation easier.

- **No Crosstalk**
  Since fibers do not pick up electromagnetic interference, signals on adjacent cables are not coupled together.

- **Inherent Signal Security**
  Optical fibers cannot be 'tapped' and hence signal security is very high as compared to copper wires.

Expression for attenuation coefficient of an optical fiber.

According to Lambert's law, the rate of decrease of intensity of light with distance travelled in a homogeneous medium is proportional to the initial intensity
i.e. $-[dP/dL]$ proportional to P   where P = Initial intensity, L = Length travelled

$-[dP/dL] = \alpha P$ where α = attenuation coefficient

$-[dP/P] = -\alpha \, dL$

$$\int \frac{dP}{P} = -\propto \int dL$$

Let P_{in} = Initial intensity with which light is launched ; P_{out} = Light intensity received as output

$$\int_{Pin}^{Pout} \frac{dP}{P} = -\propto \int_0^L dL \quad \text{or} \quad \log\left[\frac{P_{out}}{P_{in}}\right] = -\propto L$$

$$\propto = \frac{-1}{L}\log\left[\frac{P_{out}}{P_{in}}\right] \; Bel/km \quad \text{or} \quad \propto = \frac{-10}{L}\log\left[\frac{P_{out}}{P_{in}}\right] \; dB/km$$

UNIT 5 - THEORY OF OSCILLATIONS

Theory of free vibrations:

Periodic Motion

When the motion of an object continually repeats itself it is called periodic motion. The object can be repeatedly moving back and forth or it could be moving in a circular orbit or rotation.

Since the law of inertia states that an object moves in a straight line unless acted upon by a force, periodic motion requires some sort of force to create this special type of motion.

Characteristics of periodic motion are

- the velocity of the object,

- the period of motion and

- the amplitude of the motion.

Periodic motion is seen in various waveforms and is used in clocks and other devices.
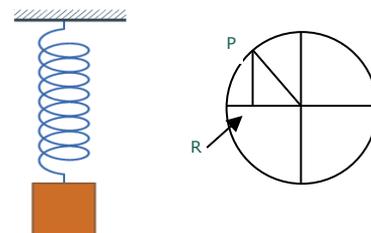
Simple harmonic motion

Simple harmonic motion (SHM) is the motion of a simple harmonic oscillator. A body in simple harmonic motion experiences a single force which is given by Hooke's law, which states that the force is directly proportional to the displacement x and points in the opposite direction.

The simple harmonic motion is periodic; the body oscillates about an equilibrium position in a sinusoidal pattern. Each oscillation is identical, and thus the period, frequency and amplitude of the motion are constant.

Examples: the simple harmonic motion is exhibited by a variety of physical systems. Following are two examples.

1. Mass on a spring   2. Uniform circular motion

Mass on a spring: A mass m attached to a spring with spring constant k exhibits simple harmonic motion in space.

Uniform circular motion: Simple harmonic motion in some cases can be considered as the one dimensional projection of uniform circular motion. If an object moves with an angular velocity Ω around a circle of radius r centered at the origin of x-y plane, then its motion along each coordinate is simple harmonic motion with amplitude r and angular frequency ω.

As mentioned above for a particle executing simple harmonic motion, the force is directly proportional to the displacement x and acts in an opposite direction. i.e.

$F \alpha - x$

From Newton' second law $F = \dfrac{dp}{dt} = m\dfrac{dv}{dt} = m\dfrac{d^2x}{dt^2}$

Combining the above two equations we can write

$$m\dfrac{d^2x}{dt^2} \alpha - x \Rightarrow m\dfrac{d^2x}{dt^2} = -Kx, \Rightarrow \dfrac{d^2x}{dt^2} = -\dfrac{k}{m}x$$

where K is force per unit displacement (spring constant).

Let $\omega^2 = \dfrac{K}{m}$ then we can write,

$$\dfrac{d^2x}{dt^2} + \omega^2 x = 0$$

A solution of this equation is of the form, $x = A\cos\omega t + B\sin\omega t$ which can be verified immediately.

$x = A\cos\omega t + B\sin\omega t$

$\Rightarrow \dfrac{dx}{dt} = -A\omega\sin\omega t + B\omega\cos\omega t$

$\Rightarrow \dfrac{d^2x}{dt^2} = -A\omega^2\cos\omega t - B\omega^2\sin\omega t$

$= \omega^2\left[A\cos\omega t + B\sin\omega t\right] = -\omega^2 x$

$$\dfrac{d^2x}{dt^2} + \omega^2 x = 0$$

which verifies the solution.

$\omega = \sqrt{\dfrac{k}{m}}$ is called angular frequency.

Let us set $A = a\cos\theta$ and $B = -a\sin\theta$ then $\tan\theta = -\dfrac{B}{A}$ and

$A^2 + B^2 = a^2\cos^2\theta + a^2\sin^2\theta$

thus $a^2 = A^2 + B^2$ then

$x = a\cos\theta\cos\omega t - a\sin\theta\sin\omega t$
$= a\cos(\omega t + \theta)$

A, B, a and θ are arbitrary. x and $\dfrac{dx}{dt}$ recur when ωt increases by 2π. Consequently, the maximum displacement is a-which is the amplitude of oscillation.

The time period T is given by $T = \dfrac{2\pi}{\omega} = 2\pi\sqrt{\dfrac{m}{K}}$ which is independent of a (isochronous motion).

The velocity $v = \dfrac{dx}{dt} = -a\omega \sin(\omega t + \theta)$

and the acceleration $a = \dfrac{d^2 x}{dt^2} = -a\omega^2 \cos(\omega t + \theta) = -\omega^2 x.$

Energy considerations in simple harmonic motion

In simple harmonic motion without dissipative forces, the total mechanical energy is conserved (E=T+U is constant). We will study this in case of a simple harmonic motion in which the displacement is

$x = x_m \cos(\omega t + \phi)$.

The potential energy at any instant is given by

$U = \dfrac{1}{2} Kx^2 = \dfrac{1}{2} Kx_m^2 \cos^2(\varpi t + \phi)$.

The potential energy therefore oscillates with time and has a maximum value of $\dfrac{1}{2} Kx_m^2$. During motion, the potential energy oscillates between 0 and this value and is graphically shown in the figure below.
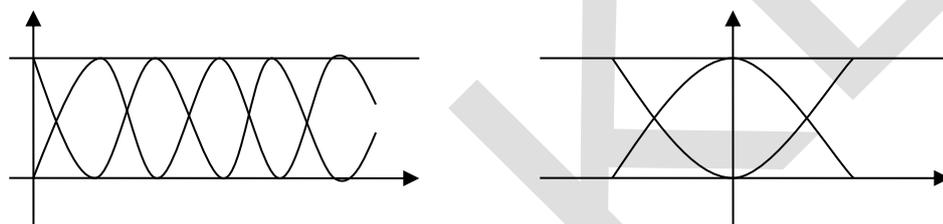
The kinetic energy at any instant is $\dfrac{1}{2} mv^2$. Since

$v = \dfrac{dx}{dt} = -\varpi x_m \sin(\varpi t + \phi)$, we get

$T = \dfrac{1}{2} mv^2 = \dfrac{1}{2} m\varpi^2 x_m^2 \sin^2(\varpi t + \phi) = \dfrac{1}{2} Kx_m^2 \sin^2(\varpi t + \phi)$

The kinetic energy also oscillates with time and has a maximum value of $\dfrac{1}{2} Kx_m^2$. During the motion, the kinetic energy oscillates between 0 and this value. The total mechanical energy is constant.

$E = T + U = \dfrac{1}{2} Kx_m^2$.

At maximum displacement, $U = \dfrac{1}{2} Kx_m^2$, T=0 and at equilibrium position, U=0, $T = \dfrac{1}{2} Kx_m^2$. At any other position, the sum is always equal to $\dfrac{1}{2} Kx_m^2$. It can be shown that the average kinetic energy for motion

during one period is exactly equal to average potential energy and each of these average quantities is half the total energy i.e. $\frac{1}{4}Kx^2$.

We can generalize the total energy

$$T + U = \frac{1}{2}mv^2 + \frac{1}{2}Kx^2 = \frac{1}{2}Kx_m^2$$

$$\Rightarrow v^2 = \frac{K}{m}(x_m^2 - x^2)$$

$$\Rightarrow v = \frac{dx}{dt} = \pm\sqrt{\frac{K}{m}(x_m^2 - x^2)}$$

$$\Rightarrow v = \pm\sqrt{\omega^2(x_m^2 - x^2)}$$

$$\Rightarrow v = \pm\omega\sqrt{(x_m^2 - x^2)}$$

v is maximum when x=0, v is minimum when $x=x_m$.

Electrical oscillations: Energy considerations

Let us consider an electric circuit shown in figure 1a with a charged capacitor, a switch and an ideal inductor (no resistance). At the instant when the circuit is closed, the capacitor starts to discharge through the inductor. At a little later time, the capacitor has completely discharged and the potential difference between its terminals (and those of the inductor also) has decreased to zero (figure 1b). The current in the inductor has meanwhile established a magnetic field in the space around it. This magnetic field now decreases, inducing an emf in the inductor in the same direction as the current. The current therefore persists, although with diminishing magnitude, until the magnetic field has disappeared and the capacitor has been charged in the opposite sense to its initial polarity as in figure 1c. The process now repeats itself in the reversed direction and in the absence of energy losses the charges on the capacitor will surge back and forth indefinitely. This process is called electrical oscillation.
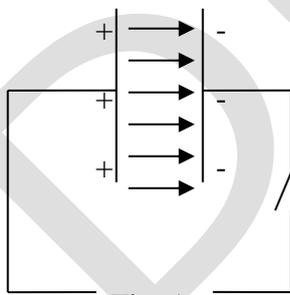

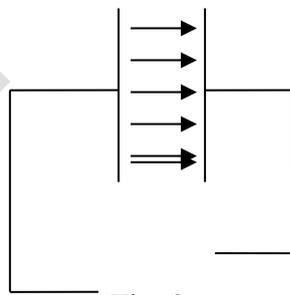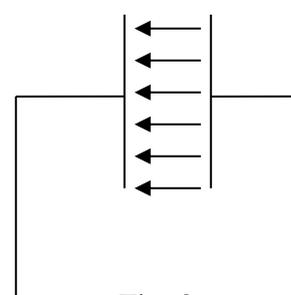Fig. 1   Fig. 2   Fig. 3

We can write, $V_{ab} = \frac{q}{C} = L\frac{di}{dt}$ which gives us $\left(\because i = \frac{dq}{dt}\right)$

$$L\frac{di}{dt} + \frac{q}{C} = 0 \Rightarrow \frac{d^2q}{dt^2} + \frac{1}{LC}q = 0$$

This is the differential equation of simple harmonic motion. The solution is

$$q = Q\cos 2\pi ft$$

where $f = \dfrac{1}{2\pi}\sqrt{\dfrac{1}{LC}}$ and Q is the initial charge on the capacitor. The charge thus oscillates just analogous to the oscillation of a mass suspended from the spring. The frequency f is called the natural frequency of the circuit.

From the energy point of view, the oscillations of an electrical circuit consist of a transfer of energy back and forth from the electric field of the capacitor to the magnetic field of the inductor. In the process, the total energy associated with the circuit remains constant. Again, this is analogous to the transfer of energy in a mechanical system from kinetic to potential and vice versa.

The energy of the capacitor at any instant is $\dfrac{1}{2}Cv^2$, that of inductor is $\dfrac{1}{2}Li^2$. Thus

$$\frac{1}{2}Cv^2 + \frac{1}{2}Li^2 = \frac{1}{2}CV_m^2 = \frac{1}{2}LI_m^2 = \text{constnat}$$

where v and i are the instantaneous, V_m and I_m are the maximum potential difference and the current respectively.

Theory of Damped Vibrations:

In our discussion of oscillator, we have assumed that no frictional force act on the motion of the oscillator. If this assumption holds strictly, a pendulum or a mass on spring will oscillate indefinitely. In all oscillating system, the amplitude of the oscillator gradually decreases to zero as a result of friction. The motion is now said to be damped by friction and is sometimes called damped harmonic motion. The friction arises mostly from air resistance or internal forces.

Equation of motion; Expression for amplitude

The damped oscillating system of mass 'm' is subjected to

(a) a restoring force which is proportional to displacement 'x', directed opposite. This is written as – kx, where 'k' is force constant.

(b) a frictional force proportional to velocity, but directed opposite. This is written as – r. dx/dt, where 'r' is frictional force per unit velocity.

We can now write the equation of motion for a damped oscillator,

$$F = ma = -kx - r\frac{dx}{dt}$$

Or $\qquad m\dfrac{d^2x}{dt^2} + kx + r\dfrac{dx}{dt} = 0$

$$\frac{d^2x}{dt^2} + \frac{r}{m}\frac{dx}{dt} + \frac{k}{m}x = 0 \qquad \text{---(1)}$$

This equation can be written as

$$\frac{d^2x}{dt^2} + 2b\frac{dx}{dt} + \omega^2 x = 0 \qquad \text{where } r/m = 2b \text{ and } k/m = \omega^2$$

Equation (1) is second order differential equation, we can now assume a solution as

$$x = A\,e^{\alpha t} \qquad \text{--- (2)}$$

Where 'A' and 'α' are constants to be determined.

From equation (2) we get,

$$\frac{dx}{dt} = A\,\alpha\,e^{\alpha t} \quad \text{and} \quad \frac{d^2x}{dt^2} = A\,\alpha^2\,e^{\alpha t}$$

Then equation (1) becomes

$$A\,\alpha^2\,e^{\alpha t} + 2bA\,\alpha\,e^{\alpha t} + \omega^2 A\,\alpha\,e^{\alpha t} = 0$$

Dividing by $A\,e^{\alpha t}$, we obtain

$$\alpha^2 + 2b\,\alpha + \omega^2 = 0$$

This is a quadratic equation and the roots are $\qquad\qquad\qquad ax^2+bx+c=0$

$$A = -b \pm \sqrt{b^2 - \omega^2} \qquad\qquad \text{roots are } x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Using this in equation (1), we get

$$x = A\,e^{\left(-b \pm \sqrt{b^2 - \omega^2}\right)t}$$

In general, $\qquad x = A_1\,e^{\left(-b + \sqrt{b^2 - \omega^2}\right)t} + A_2\,e^{\left(-b - \sqrt{b^2 - \omega^2}\right)t}$ --- (3)

Equation (3) is the general solution for the motion of a damped harmonic oscillator. (expression for decaying amplitude).

Three cases of damping:

The expression for amplitude of a harmonic oscillator is given by

$$x = A_1\,e^{\left(-b + \sqrt{b^2 - \omega^2}\right)t} + A_2\,e^{\left(-b - \sqrt{b^2 - \omega^2}\right)t} \qquad\qquad \text{----- (1)}$$

Where A_1 and A_2 are arbitrary constants and $2b = r/m$ and $\omega^2 = k/m$

Where m => mass of the oscillating body

    r => frictional force per unit velocity,   k => force constant

Depending upon the value of 'b' and 'ω' three distinct cases of damping are possible.

Case (1): When $b^2 > \omega^2$, $\sqrt{b^2 - \omega^2}$ is real and grater than 'b'. Both exponential terms in equation (1) are negative. Therefore the displacement 'x' has two terms bothe decreasing exponentially to zero without performing oscillation. The rate of decrease of displacement is governed by the term $(-b + \sqrt{b^2 - \omega^2})t$, as the other term reduces much rapidly. This type of motion is called *overdamped* or *deadbeat*. This type of motion is shown by a pendulum moving in a thick oil or by dead beat moving coil galvanometer.
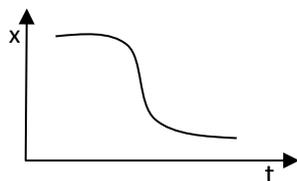
Case (2): When $b^2 = \omega^2$, if we substitute in equation (1),

$x = A_1 e^{-bt} + A_2 e^{-bt}$ does not satisfy equation of motion for the damped harmonic oscillator. $\therefore$ let us assume $\sqrt{b^2 - \omega^2} = h$ (a small quantity $\longrightarrow$ 0)

Then equation (1) becomes,

$x = A_1 e^{(-b+h)t} + A_2 e^{(-b-h)t}$

$x = e^{-bt}\left(A_1 e^{ht} + A_2 e^{-ht}\right)$

$x = e^{-bt}\left(A_1 \left[1 + ht + ...\right] + A_2 \left[1 - ht + ...\right]\right)$

$x = e^{-bt}\left[(A_1 + A_2) + ht(A_1 - A_2) + ...\right]$

$x = e^{-bt}\left[p + qt\right]$

Where $p = (A_1 + A_2)$ and $q = (A_1 - A_2)h$

As 't' increases (p+qt) increases, but e^{-bt} decreases. Therefore, 'x' initially increases and then decreases and approaches zero as 't' increases. In this case, exponential term is (-bt), while in case 1, it was more than (-bt). Therefore here the particle tends to acquire equilibrium much faster than the previous case. This case is called *critically damped* motion. This is exhibited by many pointer instruments like voltmeter, ammeter etc., in which the pointer moves to correct position and comes to rest immediately without any oscillation.

Case (3): When $b^2 < \omega^2$, then $\sqrt{b^2 - \omega^2}$ becomes imaginary. Let us write $\sqrt{b^2 - \omega^2} = i\sqrt{\omega^2 - b^2} = i\beta$, where $\beta = \sqrt{\omega^2 - b^2}$. Then equation (1) becomes,

$$x = A_1 e^{(-b+i\beta)t} + A_2 e^{(-b-i\beta)t}$$

$$x = e^{-bt}\left(A_1 e^{i\beta t} + A_2 e^{-i\beta t}\right)$$

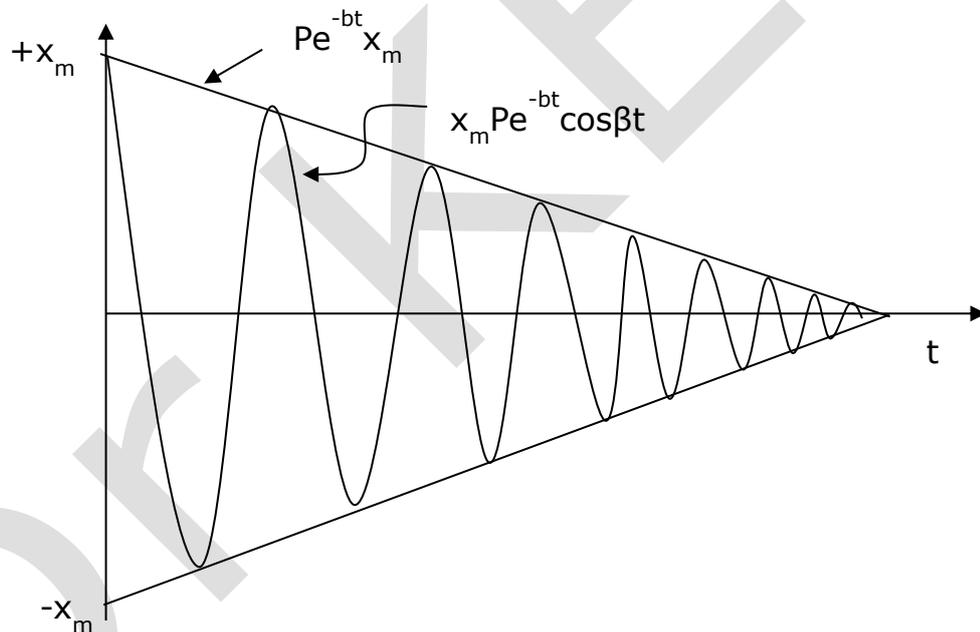$$x = e^{-bt}\left[A_1(\cos\beta t + i\sin\beta t) + A_2(\cos\beta t - i\sin\beta t)\right]$$

$$x = e^{-bt}\left[(A_1 + A_2)\cos\beta t + i(A_1 - A_2)\sin\beta t\right]$$

$$x = e^{-bt}\left[p\cos\phi\,\cos\beta t + p\sin\phi\,\sin\beta t\right]$$

Where $p\cos\phi = (A_1 + A_2)$ and $p\sin\phi = i(A_1 - A_2)$

$$x = p e^{-bt}\left[\cos(\beta t - \phi)\right]$$

This equation represents the simple harmonic motion with amplitude pe^{-bt} and time period T = $\dfrac{2\pi}{\beta} = \dfrac{2\pi}{\sqrt{\omega^2 - b^2}}$

The amplitude of the motion continuously decreases due to the factor e^{-bt} called damping factor. Because the value $\left|\cos\left(\left(\sqrt{\omega^2 - b^2}\right)t - \phi\right)\right|$ varies between +1 and -1, the amplitude varies between e^{-bt} and - e^{-bt}. The decay of the amplitude depends on damping coefficient 'b'. The figure below represents this motion. The examples of this type of motion are the motion of a pendulum in air, the motion of the coil of a ballistic galvanometer and the electrical oscillations of an LCR circuit.

Logarithmic decrement:

Logarithmic decrement measures the rate at which the amplitude of damped oscillation dies away. The amplitude of harmonic oscillator is given by,

$x = p e^{-bt}$, where b is damping coefficient.

Let $x = x_0$ at $t = 0$ and at $t = T, 2T, 3T, …..$, x be represented as $x_1, x_2, x_3, ….$, respectively, where T is period of oscillation. Then,

$x_0 = p$; $x_1 = pe^{-bT}$; $x_2 = pe^{-2bT}$; $x_3 = pe^{-3bT}$; …..

Now, we get $\dfrac{x_0}{x_1} = \dfrac{x_1}{x_2} = \dfrac{x_2}{x_3} = ... = e^{bT} = e^{\lambda}$ Where $bT = \lambda$

'λ' is known as logarithmic decrement.

Therefore, $\lambda = \ln\left(\dfrac{x_0}{x_1}\right) = \ln\left(\dfrac{x_1}{x_2}\right) = \ln\left(\dfrac{x_2}{x_3}\right) = ...$

Logarithmic decrement is the logarithm of ration of successive amplitudes of vibration.

Relaxation time:

It is defined as the time taken for the total mechanical energy to decay to (1/e) of its original value.

The mechanical energy of a damped harmonic oscillator is given by,

$E = ½ kx^2 = ½ p^2 k e^{-2bt}$

Let $E = E_0$ at $t = 0$ $\therefore E_0 = ½ p^2 k$

Now $E = E_0 e^{-2bt}$

Let 'τ' be the relaxation time, i.e., at $t = \tau$, $E = E_0/e$, using this in above relation

$E_0/e = E_0 e^{-2b\tau}$

$e^{-1} = e^{-2b\tau}$ => $2b\tau = 1$ or **$\tau = 1/2b$**

Finally we get $E = E_0 e^{-t/\tau}$

Quality factor:

It is defined as '2π' times the ratio of the energy stored in the system to the energy lost per period.

$Q = 2\pi \dfrac{\text{energy stored in the system}}{\text{energy lost per period}}$

$Q = 2\pi \dfrac{E}{PT}$ Where P is power dissipated and T is the period

Since P can be written as $\qquad$ $P = E/\tau$, we get

$$Q = 2\pi\frac{E}{\dfrac{E}{\tau}T} = 2\pi\frac{\tau}{T} = \omega\tau \qquad \text{Where '} \omega = 2\pi/T \text{' is the angular frequency.}$$

$\therefore$ Higher Q => higher τ => low damping $\quad$ (since $\tau = 1/2b$)

In case of low damping $\omega = \omega_0$ and in terms of 'k' and 'm'

$$\omega_0 = \sqrt{\frac{k}{m}} \qquad \text{Also } \tau = \frac{1}{2b}$$

Then $Q = \dfrac{1}{2b}\sqrt{\dfrac{k}{m}}$

Low damping => high Q

Theory of Forced vibrations:

Forced vibrations are the vibrations in which a body vibrates with a frequently other than its natural frequency under the influence of an external periodic force.

Ex: (1) Vibration of bridge under the influence of marching soldiers.

        (2) Tuning fork exposed to periodic force of a sound wave.

Following are the forces acting on the particle.

        i] A restoring of force proportional to displacement acting in opposite direction, given by –kx, k being force constant.

        ii] A frictional force proportional to velocity directed in opposite, given by - $r\frac{dx}{dt}$, r being frictional force per unit velocity.

        iii] An external periodic force represented by Fcospt, where 'F' is the maximum value of this force and 'p/2π' is its frequency

∴ The forces acting are thus,

$$m\frac{d^2x}{dt^2} + kx + r\frac{dx}{dt} = Fcospt$$

Or $\frac{d^2x}{dt^2} + \frac{r}{m}\frac{dx}{dt} + \frac{k}{m}x = \frac{F}{m}cospt$

→ $\frac{d^2x}{dt^2} + 2b\frac{dx}{dt} + \omega^2 x = f\cos pt$ ------ (1)

Where $\frac{r}{m} = 2b$, $\frac{k}{m} = \omega^2$ and $\frac{F}{m} = f$

Equ (1) is the differential equation of the particle oscillating under an applied force.

In case of this motion, when the steady state is setup, the particle vibrates with frequency of the applied force and not with its natural frequency.

We can assume a solution of the type,

x = A cos (pt − ϕ) -------(2)

Differentiating (2) and we, have,

$\frac{dx}{dt} = -AP \sin(pt - \phi)$

and $\frac{d^2x}{dt^2} = -AP^2 \cos(pt - \phi)$

using these derivatives in equ (1) we obtain

-Ap² cos (pt-ϕ) - 2b AP sin (pt- ϕ) + ω² A cos (pt-ϕ) = f cos [(pt − ϕ) + ϕ] sin ϕ

Now, equating co-efficient

$-Ap^2 + \omega^2 A = f \cos \phi$ and $2bAp = f \sin \phi$

Or $A(\omega^2 - p^2) = f \cos \phi$ and $2bAP = f \sin \phi$ -------(3) & (4)

Squaring.

$A^2(\omega^2 - p^2)^2 = f^2 \cos^2\phi$ and $4b^2 A^2 P^2 = f^2 \sin^2 \phi$

Adding,

$$A^2(\omega^2 - p^2)^2 + 4b^2 A^2 P^2 = f^2$$

$$\rightarrow \quad A^2[(\omega^2 - p^2)^2 + 4b^2 P^2] = f^2$$

And $\quad A = \dfrac{f}{\sqrt{(\omega^2 - p^2)^2 + 4b^2 p^2}} = \dfrac{F/m}{\sqrt{(\omega^2 - p^2)^2 + 4b^2 p^2}}$

$$A = \dfrac{F}{p\sqrt{4b^2 m^2 + m^2\left(\dfrac{\omega^2}{p^2} - 1\right)^2}} \quad\text{--------(5)}$$

$$A = \dfrac{F}{PZ} \quad\text{-------(5A)}$$

Where $\quad Z = \sqrt{4b^2 m^2 + m^2\left(\dfrac{\omega^2}{p^2} - 1\right)^2}$

is called the mechanical impedance of the system.

Dividing (4) by (3), we get

$$\text{Tan } \phi = \dfrac{2bAP}{A(\omega^2 - p^2)} = \dfrac{2bP}{(\omega^2 - p^2)}$$

$$\text{Or } \phi = \tan^{-1}\left(\dfrac{2bP}{(\omega^2 - p^2)}\right) \quad\text{---------(6)}$$

Equation (5) gives the amplitude of forced vibrations and equations (6) gives its phase.

The general solution:

We know that the equation of motion for a damped harmonic oscillator is

$$\dfrac{d^2 x}{dt^2} + 2b\dfrac{dx}{dt} + \omega^2 x = 0$$

and its solution is $x = Ae^{-bt}\cos\left[\left(\sqrt{\omega^2 - p^2}\right)t - \phi\right]$

Now, we can write the complete solution of forced oscillator as

$$x = Ae^{-bt} \cos\left[\left(\sqrt{\omega^2 - p^2}\right)t - \phi\right] + \frac{F}{m\sqrt{\left(\omega^2 - p^2\right)^2 + 4b^2p^2}} \cos[pt - \phi]$$

Inspecting (4), we can think of motion to be composed of two components. The first term represents a damped vibration decaying at a rate determined by 'b', which is same as that of the system when no force is acting.

The second term represents a simple harmonic vibration ie, $2\pi\big/p$ differing in phase ϕ from the force. Initially these two vibrations may be expected to produce beats whose frequency is the difference of two frequencies, i.e., $p\big/2\pi \sim \omega^1\big/2\pi$. The lesser the natural damping of the system, the more marked and prolonged are the beats. One can actually recognize these beats. However, in time free vibration is damped out and only the forced vibration is left so that the steady state corresponds to forced vibration with amplitude.

$$A = \frac{f}{\sqrt{\left(\omega^2 - p^2\right)^2 + 4b^2p^2}} \quad \text{and Phase angle} \quad \phi = \tan^{-1}\left(\frac{2bP}{(\omega^2 - p^2)}\right)$$

Depending on the relative values of 'p' and 'w', the following three cases are possible.

Case 1: when driving frequency is low i.e $p << \omega$. then

$$A = \frac{f}{\sqrt{\left(\omega^2 - p^2\right)^2 + 4b^2p^2}} \approx \frac{f}{\omega^2} = \text{constant} = \frac{F/m}{k/m} = \frac{F}{m}$$

And $\phi = \tan^{-1}\left(\frac{2bP}{(\omega^2 - p^2)}\right) = \tan^{-1}(0) = 0$

i] Amplitude is independent of frequency of force.

ii] Amplitude depends on the magnitude of applied force and the force constant k

iii] The force and displacements are in phase.

Case 2: when $p = \omega$, i.e, the frequency of the force is equal to the frequency of the body.

Now the amplitude of vibration is given by

$$A = \frac{f}{2bp} = \frac{F/m}{2\frac{r}{2m}\omega} = \frac{F}{r\omega} \qquad\qquad (F = f/m, 2b = \frac{r}{m} \text{ \& } p = \omega)$$

Also, $\phi = \tan^{-1}\left(\frac{bp}{0}\right) = \tan^{-1}(\infty) = \pi\big/2$

i] The amplitude of vibration depends on damping force and for small damping forces, the amplitude of vibration is quite large.

ii] The displacement lags behind the force by phase of $\pi/2$.

Case 3: When $p >> \omega$, the frequency of force is of greater than the natural frequency 'ω' of the body.

$$A = \frac{f}{\sqrt{p^2 + 4b^2p^2}} \approx \frac{f}{p^2} = \frac{F}{mp^2}$$

And $\quad \phi = \tan^{-1}\left(\frac{2bp}{\omega^2 - p^2}\right) = \tan^{-1}\left(\frac{-2b}{p}\right) \approx \tan^{-1}(-0) = \pi$

      i] the amplitude goes of decreasing

ii] phase difference approaches π.

Resonance :

      The phenomenon of making a body vibrate with its natural frequency under the influence of another vibrating body with the same frequency is called resonance.

Examples of Resonance:

1. If we bring a vibrating turning fork near another stationary tuning fork of the same natural frequency as that as the vibrating tuning fork, we find that the stationary fork starts vibrating.

2. Soldiers crossing a suspension bridge are advised not to cross in steps. The steps can make the bridge to oscillate in resonance & eventually may lead to collapse.

3. All mechanical structures- such as buildings, bridges and airplanes- have one or more natural resonant frequencies. It can be dangerous to subject the structure to one of these frequencies.

4. A classic example of resonance occurred in the Tacoma narrows Bridge in Washington state in 1940. The wind blowing through Tacoma Narrows broke up into vertices. This provided puffs of wind that shook the bridge at a frequency that matched one of its natural frequencies. The result was a gentle vertical rolling motion. About 5 months after the bridge opened, the gentle rolling oscillations became violent torsional oscillations, which soon caused the collapse of the bridge.

Expression for maximum amplitude or condition for amplitude resonance:

The amplitude of forced oscillation is given by

$$A = \frac{f}{\sqrt{\left(\omega^2 - p^2\right)^2 + 4b^2p^2}} \text{-------- (1)}$$

      Equation (1) shows that the amplitude varies with the frequency of the force 'P'. For a particular 'p', the amplitude becomes maximum. This phenomenon is known as amplitude resonance. The amplitude is maximum when the denominator $\sqrt{\left(\omega^2 - p^2\right)^2 + 4b^2p^2}$ is minimum.

The condition for minimum value is $\dfrac{d}{dp}\left[\left(\omega^2 - p^2\right)^2 + 4b^2p^2\right] = 0$

$$2\left(\omega^2 - p^2\right)(-2p) + 4b^2 2p = 0$$

$$-4\left(\omega^2 - p^2\right)p + 8b^2p = 0 \qquad\qquad (\div \text{ by } 4p)$$

$$\left(\omega^2 - p^2\right) = 2b^2$$

$$p = \sqrt{\left(\omega^2 - 2b^2\right)} \text{ --- (2)}$$

Equ (2) gives the condition for maximum amplitude of forced vibration.

i) The amplitude is maximum when the frequency of impressed force becomes $\dfrac{\sqrt{\left(\omega^2 - 2b^2\right)}}{2\pi}$ is the resonant frequency

ii) Natural frequency of the system is $\dfrac{\omega}{2\pi}$

iii) Damped frequency of the system is $\dfrac{\sqrt{\left(\omega^2 - b^2\right)}}{2\pi}$

Now using condition (2) in equ (1), we get

$$A_{max} = \frac{f}{\left\{\left[\omega^2 - \omega^2 + 2b^2\right]^2 + 4b^2\left(\omega^2 - 2b^2\right)\right\}^{1/2}}$$

$$A_{max} = \frac{f}{\left\{4b^4 + 4b^2\omega^2 - 8b^4\right\}^{1/2}}$$

$$A_{max} = \frac{f}{\left\{4b^2\omega^2 - 4b^4\right\}^{1/2}}$$

$$A_{max} = \frac{f}{\left\{4b^2\left(\omega^2 - b^2\right)\right\}^{1/2}}$$

$$A_{max} = \frac{f}{2b\sqrt{\left(\omega^2 - b^2\right)}}$$

$$A_{max} = \frac{f}{2b\sqrt{\left(\omega^2 - 2b^2 + b^2\right)}}$$

$$A_{max} = \frac{f}{2b\sqrt{\left(\omega^2 - \left(\omega^2 - p^2\right) + b^2\right)}} \qquad (\because 2b^2 = \omega^2 - p^2)$$

$$A_{max} = \frac{f}{2b\sqrt{\left(p^2 + b^2\right)}}$$

For low damping, b is small

$$\therefore A_{max} = \frac{f}{2b\sqrt{p^2}} \quad = \quad \frac{f}{2bp} \qquad \text{Showing that, } A_{max} \to \infty, \text{ as } b \to 0$$

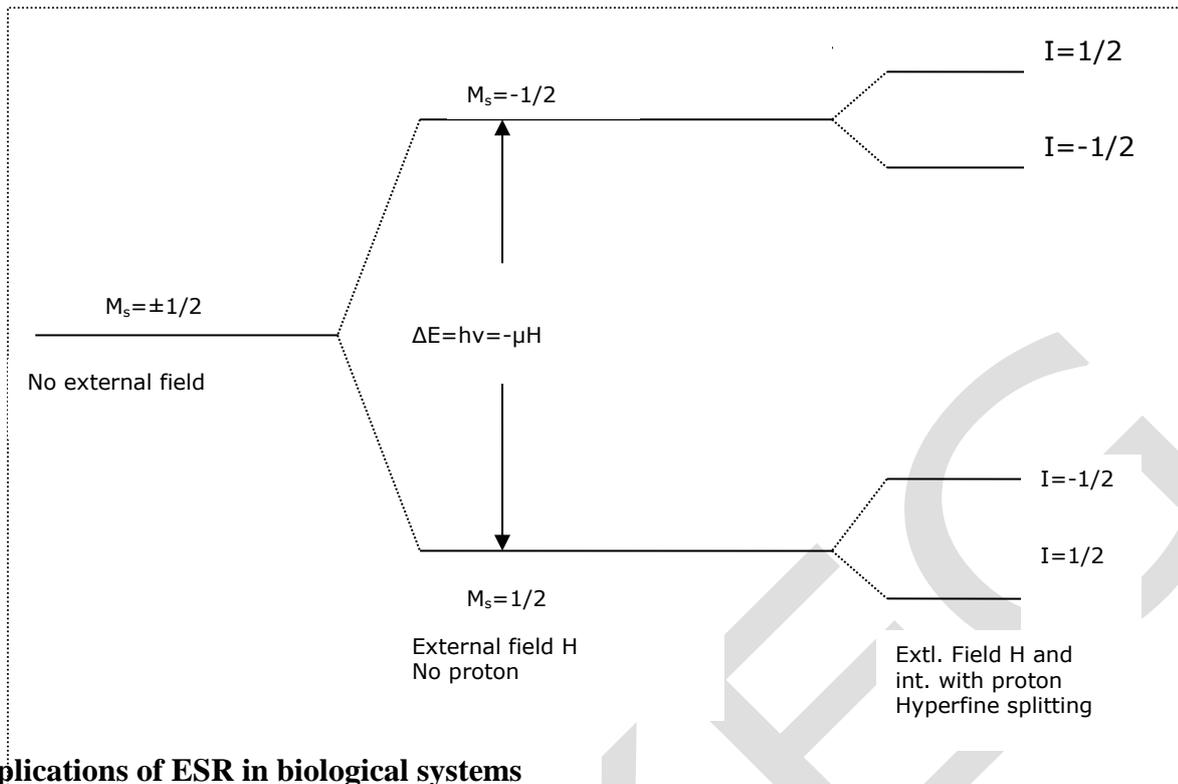**Electron Spin Resonance (ESR) Spectroscopy**

Principle: Electron is a charged particle with orbital and spin motions. It behaves like a tiny magnet. When an external magnetic field is applied to spinning electrons, the magnetic field produced by the electrons interacts with the external magnetic field. This is the basis of ESR.

- o ESR also called EPR (Electron Paramagnetic Resonance) deals with transitions between magnetic energy levels of electron with unpaired spins. The magnetic energy splitting is caused by Zeemann effect.

- o The transition between these split energy levels is caused by radiation in the microwave region of the spectrum.

- o The presence of unpaired electrons in the sample is an essential condition for ESR.

- o Unpaired electrons are present in free radicals, triplet electron states, transition metals, and rare Earth ions.

- o In biological systems unpaired electrons occur in transition metal complexes and short lived intermediates.

- o When a sample exhibiting Zeemann effect is irradiated by photons in a direction perpendicular to the magnetic field, the magnetic dipole transition takes place between split energy levels when $\Delta E = h\nu$. This is ESR absorption.

- o Hyperfine splitting arises due to interaction with nucleus.

Origin of an ESR signal

- o Every electron has a magnetic moment and spin quantum number $s = 1/2$, with magnetic components $m_s = +1/2$ and $m_s = -1/2$. In the presence of an external magnetic field with strength B_0, the electron's magnetic moment aligns itself either parallel ($m_s = -1/2$) or antiparallel ($m_s = +1/2$) to the field, each alignment having a specific energy (the Zeeman effect). The parallel alignment corresponds to the lower energy state, and the separation between it and the upper state is $\Delta E = g_e\,\mu_B\,B_0$, where g_e is the electron's so-called g-factor. This equation implies that the splitting of the energy levels is directly proportional to the magnetic field strength.

- o An unpaired electron can move between the two energy levels by either absorbing or emitting electromagnetic radiation of energy $\varepsilon = h\nu$ such that the resonance condition, $\varepsilon = \Delta E$, is obeyed. Substituting in $\varepsilon = h\nu$ and $\Delta E = g_e\mu_B B_0$ leads to the fundamental equation of EPR spectroscopy: $h\nu = g_e\mu_B B_0$. Experimentally, this equation permits a large combination of frequency and magnetic field values, but the great majority of EPR measurements are made with microwaves in the 9000 – 10000 MHz (9 – 10 GHz) region, with fields corresponding to about 3500 G (0.35 T).

Energy Level Diagram in ESR

$M_s=-1/2$

$I=1/2$

$I=-1/2$

$M_s=\pm1/2$

No external field

$\Delta E=h\nu=-\mu H$

$I=-1/2$

$I=1/2$

$M_s=1/2$

External field H
No proton

Extl. Field H and
int. with proton
Hyperfine splitting

Applications of ESR in biological systems

o Study of transition metal complexes. E.g. Cu- Fe- proteins.

o In clinical diagnostics, e. g. muscular dystrophy

o Spin labeled ESR is applied in radiation biology.

ESR Instrumentation
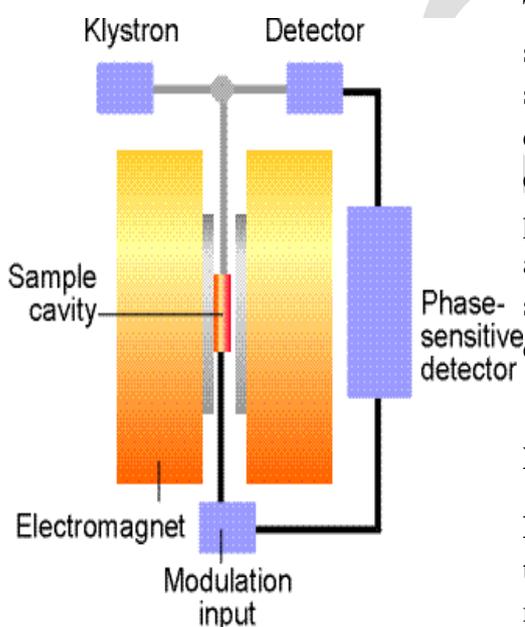
The ESR spectrometer consists of an electromagnet with power supplies to generate and modulate a uniform magnetic field of several thousand Gauss, as well as the components that generate and detect microwave power. A static magnetic field is provided by an electromagnet. The microwave system consists of a microwave power supply which uses a klystron. The samples to be investigated are mounted in the middle of the cavity. There are varieties of schemes for detecting resonant EPR transitions. Most popular is the detection of absorption of the microwave power.

Nuclear Magnetic Resonance (NMR)

Principle: Nucleus is a charged entity with spin. It behaves like a tiny magnet. When an external magnetic field is applied to spinning nucleus, the magnetic field produced by the nucleus interacts with the external magnetic field. This is the basis of NMR.

o Principle: similar to ESR.

o Nucleus has a net spin. Even mass no. I=0. e.g. C^{12}, O^{16}, S^{32} etc.

- Odd mass no. I=1/2 integral. H^1, Na^{23}, etc.

- Even mass no. but odd charge no. have spin=integral. E.g. D^2

- Atomic nuclei such as H^1, C^{13} which have nuclear spin exhibit magnetic properties. In an external field they behave as tiny magnets and energy levels get separated.

- When radiation of suitable radio frequency is incident, the transitions occur.

- Chemical Shift: When a neutral atom is in an external magnetic field, the nucleus is shielded by the electrons. This shielding gives rise to chemical shift.

- The nuclei of an element in different chemical environment gives rise to distinct spectral lines (chemical shifts), which is an important aspect in structural studies by NMR.

- Chemical shifts of nuclei are measured with respect to a standard reference frequency. The reference compound is so chosen that it has a single absorption frequency occurring in region far away from the signals and the compound should be chemically inert.

- Common reference compound: tetramethylsilane (TMS)

Energy Level Diagram in NMR

m1=1/2
α-state

No external field

$\Delta E = h\nu = -\mu H$

m2=-1/2
β-state

External field H
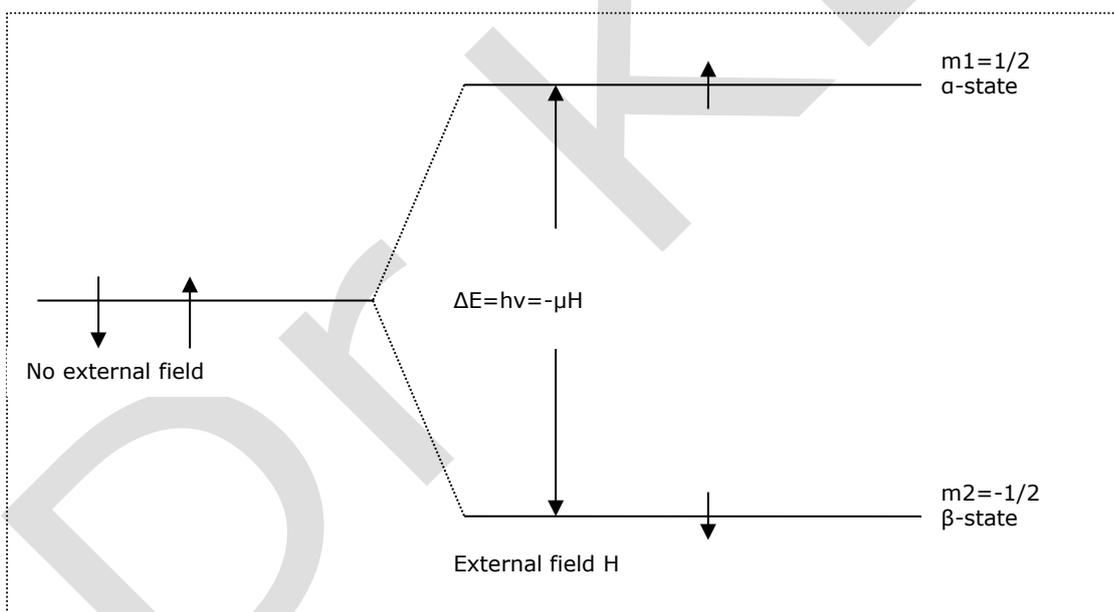
NMR Applications:

- Biomedical NMR: cellular metabolic process at molecular level, biochemical energetics of living organisms and NMR imaging (MRI).

Spin Flip

o If rf energy having a frequency matching the Larmor frequency is introduced at a right angle to the external field (e.g. along the x-axis), the precessing nucleus will absorb energy and the magnetic moment will flip to its I = -1/2 state. This excitation is shown in the following diagram. Note that frequencies in radians per second may be converted to Hz by dividing by 2π.
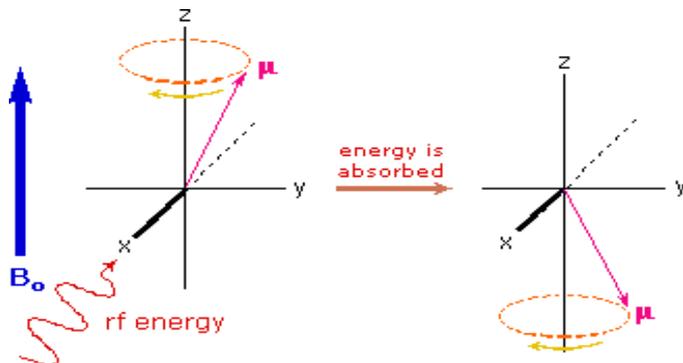
NMR Instrumentation

• An NMR machine is basically a big and expensive FM radio.
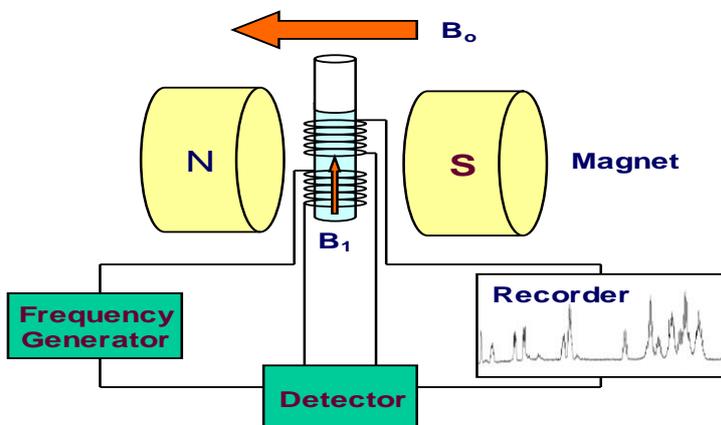
• *Magnet* - Normally superconducting. Some electromagnets and permanent magnets are still used.

• *Frequency generator* - Creates the alternating current (at ω_o) that induces **B₁**. Continuous wave or pulsed.

• *Detector* - Subtracts the base frequency (a constant frequency very close to ω_o) to the output frequency. It is lower frequency and much easier to deal with.

• *Recorder* - XY plotter, oscilloscope, computer, etc., etc.

---------------- **The End** ---------------