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### Review of electric and magnetic fields

#### Electric Fields

Electric fields are felt due to the presence of electric charges. It is obvious that electric charges can be isolated. Fundamentally electric charges can be of the positive or the negative charge type.

The fundamental unit of electric charge is the charge of the electron which has a magnitude of  $1.602 \times 10^{-19} C$

Though an atom is neutral, an electron can be removed from the influence of the nucleus by providing enough energy in the form of thermal energies. The atom is then an ion with a unit positive charge and the electron is a unit of negative charge.

Electric charges can be isolated and separated. The presence of positive or negative charges are felt by the presence of an electric field. The quantity of the charge at any point would decide the strength of the electric field. The presence of the charge can be quantified by the electric potential which is the work done in bringing unit positive charge from infinity to the point at a distance  $x$ .

The electric potential at any point  $x$  from the charge

$$V_x = \frac{Q}{4\pi\epsilon_0} \times \frac{1}{x}$$

The electric potential is inversely proportional to the distance of the test charge from the point charge. If the charge is positive, external work has to be done in moving the positive charge and if the charge is negative the field does the work to move the positive charge.

The electric field due to a point charge

$$E_x = \frac{Q}{4\pi\epsilon_0} \times \frac{1}{x^2}$$

The electric field is inversely proportional to the square of the distance of the test charge from the point charge in reference.

The electric field in terms of the electric potential

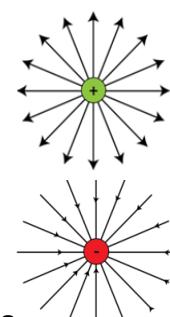
$$E_x = -\frac{dV_x}{dx}$$

The presence of an electric field can be visualized in terms of the flux lines which indicate the direction of the force felt by the unit positive charge along the line.

In the case of the presence of a positive charge, the lines of force are directed radially outwards, the direction of repulsion of the test charge.

In the case of the presence of a negative charge, the lines of force are directed radially inwards, the direction of attraction of the test charge.

The flux of electric field lines is a measure of the electric field at a point and hence a measure of the amount of charge present at the point.



#### Magnetic fields

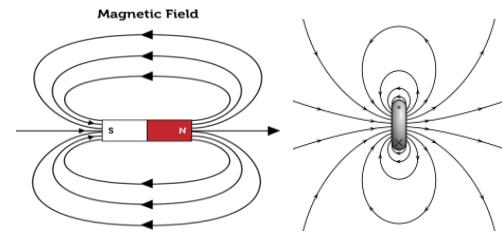
Interestingly magnetic fields are generally due to a dipole – a north and south pole which cannot be isolated from each other.

Though theoretically a magnetic monopole can exist, no experimental results are available to confirm the same as of date.

Just as in the case of electric fields the magnetic field at any point is inversely proportional to the square of the distance from the magnetic dipole, and the magnetic potential is inversely proportional to the distance of the reference point from the given dipole.

The magnetic field lines are continuous (closed loops) from the north pole and the south pole external to the material and the field lines are continuous in the material as well. The flux of magnetic field lines is indicative of the strength of the magnetic field at any point.

We are also familiar with magnetic fields created by a current carrying solenoid. The direction of the current through the solenoid defines which end of the solenoid behaves as a north pole or a south pole.



The common observation is that there is a strong interplay between electric fields and magnetic fields when they are time dependent quantities.

The Ampere's law - the current through a straight conductor creates a magnetic field around the wire and the Faraday's law of electromagnetic induction – of an induced current in a closed coil placed in a time varying magnetic fields are strong evidences for the two forces, electric and magnetic

### **1. Maxwell's equations in a medium**

Maxwell summarized the existing ideas of electric and magnetic fields and their inter-related phenomena into four equations (in 1860) which are known as the Maxwell's equation. This also paved the way for describing radiation as an electromagnetic wave.

[A review of the operations with the  $\nabla$  operator (nabla operator)]

The  $\vec{\nabla}$  operator is a partial differential mathematical operator given by  $\nabla = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$  where  $\hat{i}$ ,  $\hat{j}$ , and  $\hat{k}$  are the unit vectors in the three orthogonal directions.

The operator  $\nabla = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$  when operates on a scalar quantity gives rise to a vector.

The simple multiplication of  $\nabla$  with a scalar field  $A$  written as  $\nabla A$  is the **gradient** of the field and gives the direction of the highest rate of change of the field

For example, the  $\nabla$  operator operating on an electric potential gives the electric field at the point

$$\nabla V = \hat{i} \frac{\partial V_x}{\partial x} + \hat{j} \frac{\partial V_y}{\partial y} + \hat{k} \frac{\partial V_z}{\partial z} = \hat{i} E_x + \hat{j} E_y + \hat{k} E_z = \vec{E}$$

The dot product of the  $\nabla$  operator with another vector field results in a scalar quantity which is referred to as the **divergence** of the defined field or the rate of change of the field in the three orthogonal directions.  $\nabla \cdot \vec{A} = \left( \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) \cdot \hat{i} A_x + \hat{j} A_y + \hat{k} A_z = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$

The cross product of  $\nabla$  operator with a vector field gives the **curl of the field** and results in a vector which is perpendicular to both  $\nabla$  and the given vector.

$$\nabla \times \vec{A} = \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{bmatrix} = \hat{i} \left( \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) - \hat{j} \left( \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) + \hat{k} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right)$$

Another important identity with the  $\vec{\nabla}$  operator is the curl of the curl of a vector is equal to the gradient of the divergence of the field minus the **Laplacian** operating on the vector ie.,

$$\nabla \times \nabla \times \vec{E} = \nabla (\nabla \cdot \vec{E}) - \nabla^2 \vec{E}$$

where  $\nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  is the scalar Laplacian operator.]

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### **Gauss's law for electric fields**

Divergence of the electric field is due to a system of charges enclosed by a surface is given by the charge density divided by  $\epsilon_0$

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \quad (\text{Gauss' law for electric fields})$$

### **Gauss's law for magnetic fields**

Divergence of the magnetic field is uniformly zero.

$$\nabla \cdot \vec{B} = 0 \quad (\text{Gauss' law for magnetic fields})$$

This implies the absence of magnetic monopoles.

### **Faraday's law of electromagnetic induction**

The curl of the electric field is equal to the rate of change of the magnetic field which is the standard Faraday's law of electromagnetic induction.  $\nabla \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}$

### **Ampere - Maxwell circuital law (Ampere's law modified by Maxwell)**

The curl of the magnetic field is given by the current density through the closed loop and the displacement current

$$\nabla \times \vec{B} = \mu_0 \vec{J} + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

This equation is an extension of the Ampere's law. The second term represents the concept of displacement current associated with time varying electric fields which is Maxwell's contribution.

### **Maxwell's equations in free space**

In the case of free space (which does not have sources of charges and currents) then the Maxwell's equations reduce to

$$\nabla \cdot \vec{E} = 0 \quad \dots \quad (1)$$

$$\nabla \cdot \vec{B} = 0 \quad \dots \quad (2)$$

$$\nabla \times \vec{E} = - \frac{\partial \vec{B}}{\partial t} \quad \dots \quad (3)$$

$$\nabla \times \vec{B} = +\mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} \quad \dots \quad (4)$$

Taking the curl of curl of the electric field the equation can be written as

$$\nabla \times (\nabla \times \vec{E}) = \nabla \times \left( - \frac{\partial \vec{B}}{\partial t} \right) \quad \text{this reduces to}$$

$$\nabla \times (\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = \left( - \frac{\partial \nabla \times \vec{B}}{\partial t} \right)$$

Since  $\nabla \cdot \vec{E} = 0$  this reduces to  $-\nabla^2 \vec{E} = \left( -\frac{\partial \vec{B}}{\partial t} \right)$

Substituting for curl of B the above equation simplifies to  $\nabla^2 \vec{E} = \left( \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} \right)$ .

But  $\nabla^2 \vec{E} = \left( \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} \right)$  is the general form of a wave equation. Maxwell observed  $\mu_0 \epsilon_0 = \frac{1}{c^2}$  and the equation reduces to concluded that the wave equation should be an electric field in free space travelling at the speed of light  $c = \sqrt{\frac{1}{\mu_0 \epsilon_0}}$

In a very similar way, starting from the curl of the curl of the magnetic field the analysis yields

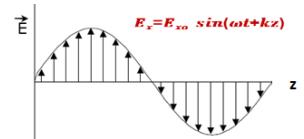
$\nabla^2 \vec{B} = \left( \frac{1}{c^2} \frac{\partial^2 \vec{B}}{\partial t^2} \right)$ . This describes a transverse magnetic field vector travelling at the speed of light.

The electric and magnetic waves must therefore be representing light and hence Maxwell proposed that light could be treated as electromagnetic waves, where the electric and magnetic vectors are mutually perpendicular and perpendicular to the direction of propagation of the radiation.

Consider a 1D electric wave  $E_x$  associated with radiation propagating in the Z direction which can be represented as

$$E_x = E_{xo} \sin(\omega t + kz)$$

This implies that the electric field vector has only an x component and the other two components  $E_y$  and  $E_z$  are zero.



Hence the associated magnetic component of the EM wave can be evaluated using the Maxwell's third equation namely  $\nabla \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}$

Evaluating the curl of the electric field  $\nabla \times \vec{E} = \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_x & 0 & 0 \end{bmatrix} = \hat{i} \times 0 + \hat{j} * \frac{\partial E_x}{\partial z} + \hat{k} * 0 = \hat{j} \frac{\partial}{\partial z} [E_{xo} \cos(\omega t + kz)] = \hat{j} * k * E_{xo} \sin(\omega t + kz)$

this implies that  $-\frac{\partial \vec{B}}{\partial t} = \hat{j} * k * E_{xo} \sin(\omega t + kz)$

Integrating the above equation with respect to time t we get

$$B = \hat{j} * k * E_{xo} \cos(\omega t + kz) * \left( \frac{1}{\omega} \right) = \hat{j} * E_{xo} \cos(\omega t + kz) * \left( \frac{1}{\frac{\omega}{k}} \right) = \hat{j} * E_x * \frac{1}{c}$$

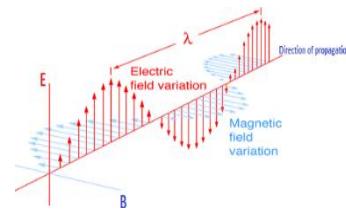
since  $c = \omega/k$  is the velocity of the radiations. We note that the magnetic component of the EM wave has only the Y component and the magnitude of the wave is  $\frac{1}{c}$  times the magnitude of the electric component of the wave.

Thus, we conclude that the EM waves have coupled electric and magnetic field components which are mutually perpendicular to each other and both are perpendicular to the direction of propagation of radiation.

### Energy of EM waves

Classically the energy of waves is equivalent to its intensity which is square of the amplitude of the waves.

The energy associated with an Electric field per unit volume of free space is  $E_n = \frac{1}{2} \epsilon_0 E^2$  where  $E$  is the electric field.



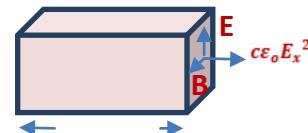
The energy content of the electric component of the wave  $= \frac{1}{2} \epsilon_0 E_x^2 = \frac{1}{2} \epsilon_0 E_{xo}^2 \cos^2(\omega t + kz)$

The energy content of the magnetic component of the wave  $= \frac{1}{2} \frac{B_y^2}{\mu_0} = \frac{1}{2} \frac{E_x^2}{c^2 \mu_0} = \frac{1}{2} \epsilon_0 E_x^2$

Hence the total energy content of the wave is the sum of the two components  $= \epsilon_0 E_x^2$ .

### **Poynting Vector**

EM waves carry energy in the direction perpendicular to the  $E$  and  $B$  field variations and is described by the Poynting vector



$$S \equiv \frac{1}{\mu_0} E \times B = c \cdot \epsilon_0 E^2$$

$E_x$  is however a time varying component and hence to determine the average energy of the wave transmitted per unit time through unit area can be found out as

$$\begin{aligned} \text{Average Energy } < S > &= \frac{c \epsilon_0}{T} \int_0^T E_x^2 dt = \frac{c \epsilon_0}{T} \int_0^T E_{xo}^2 \cos^2(\omega t + kz) dt \\ &= \frac{1}{2} \epsilon_0 c E_{xo}^2 = \frac{1}{2} c \frac{B_{yo}^2}{\mu_0} = \frac{1}{2} \frac{E_{xo} B_{yo}}{\mu_0} \end{aligned}$$

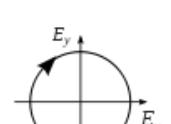
This implies that the average energy content of EM waves to be proportional to the square of the amplitude of the electric or magnetic vector and is independent of the frequency of the waves. Thus, the classical picture of the EM waves as carriers of energy gives a picture of frequency independence. For this reason, some of the observed phenomena of interaction of light with matter could not be consistently explained in spite of the fact that all other observed phenomena of radiation could be explained by the Maxwell's EM wave theory.

### Polarization states of EM waves

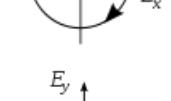
Light is a transverse electromagnetic wave, but natural light is generally unpolarized, all planes of propagation being equally probable.



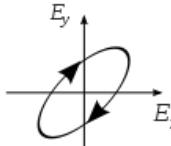
Light in the form of a plane wave in space is said to be linearly polarized. The addition of a horizontally linearly polarized wave and a vertically polarized wave of the same amplitude in the same phase result in a linearly polarized at a 45° angle



If an electromagnetic wave is the result of the superposition of two plane waves of equal amplitude but differing in phase by 90°, then the light is said to be circularly polarized.



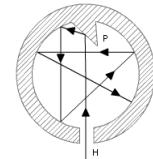
If two plane waves of differing amplitude are related in phase by 90°, or if the relative phase is other than 90° then the light is said to be elliptically polarized.



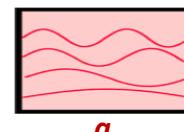
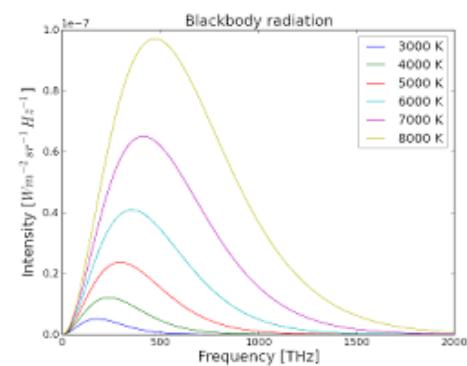
## 2. Black body radiation in equilibrium

Classically the interaction of radiation with matter with radiation is manifested in the way materials absorb radiations, emitted characteristic wavelengths which gives the color of the material.

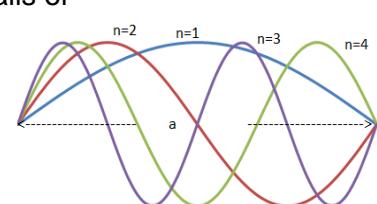
Gustav Robert Kirchhoff studied the absorption properties of materials and found materials which absorb all incident rays. If such a material is heated, then it would emit all wavelengths of radiation as it absorbed. Such a material is defined as a black body.



A black body is also modeled as a cavity which does not allow any incident radiation to escape due to multiple reflections inside the cavity. This cavity when heated radiates emit radiation of every possible frequency at a rate which increases with temperature of the body. The amount of radiant energy does not increase monotonically with time but is limited by the rate at which the radiation is also absorbed by the cavity. The amount of energy emitted at a frequency is limited by the thermodynamic equilibrium of the absorption and emission processes. It was also observed that the radiation density in an equilibrium state depends only on the temperature of the walls of the cavity and does not depend on the material or structure of the wall. The distribution as well as the characteristic maximum wavelength shifts to the lower wavelength side.



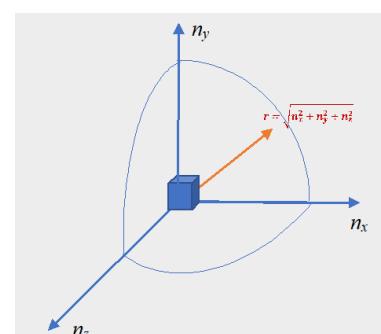
The emission from the blackbody at different temperatures can be modeled as due to emissions from harmonic oscillators on the surface of the walls of the cavity. Due to physical dimension of the cavity being large and the number of harmonic oscillators on the surface of the cavity is also large, a large range of wavelengths can be emitted. The emission from the cavity is limited to those radiations which can form standing waves in the cavity. Consider a cubical cavity of side  $a$ . The wavelengths of the oscillations that can resonate in the cavity has to satisfy the condition  $a = n \frac{\lambda}{2}$ .



Or the frequencies that can sustain in the cavity is given by  $\nu = \frac{c}{\lambda} = n \left( \frac{c}{2a} \right)$

The additional no. of frequencies  $d\nu$  when  $n$  changes to  $dn$  is  $d\nu = dn \left( \frac{c}{2a} \right)$

In a three-dimensional cavity the number of frequency states that can resonate in the cavity is estimated as  $\nu = r \left( \frac{c}{2a} \right)$  where



$r = \sqrt{n_x^2 + n_y^2 + n_z^2}$  is the radius of a surface in  $n$  space for allowed values of  $n_x$ ,  $n_y$  and  $n_z$ . This surface is an octant of a sphere of radius  $r$ . The volume of this octant is a measure of the number of frequency states in the cavity up to the allowed  $n_x$ ,  $n_y$  and  $n_z$

The additional no. of frequencies  $d\nu$  when  $r$  changes to  $dr$  is  $d\nu = dr \left( \frac{c}{2a} \right)$

The energy density of radiations can be estimated if the number oscillators and their average energy can be estimated. In the case of a cavity of volume  $V$  we can estimate the number of oscillators with frequencies between  $\nu$  and  $\nu + \delta\nu$  as  $dN = \frac{8\pi V}{c^3} \nu^2 d\nu$ .

Thus the density of frequency states (number of states per unit volume) with frequencies between  $\nu$  and  $\nu + \delta\nu$  as  $dN = \frac{8\pi}{c^3} \nu^2 d\nu$

The Boltzmann distribution function describing the probability of a large number of oscillators with energy  $E$  in thermal equilibrium at temperature  $T$  is given by  $P(E) = \frac{e^{-E/kT}}{kT}$ .

Rayleigh and Jeans estimated the average energy of the oscillators using the Boltzmann distribution function as  $\langle E \rangle = \frac{\int E * P(E) dE}{\int P(E) dE}$

This integral for  $E$  varying from 0 to infinity gives the equi-partition of energy  $\langle E \rangle = k_B T$ .

Thus, the energy density (energy per unit volume) of radiations with frequencies between  $\nu$  and  $\nu + \delta\nu$  can be estimated as

$$\rho(\nu) d\nu = \langle E \rangle * dN = \frac{8\pi}{c^3} \nu^2 d\nu k_B T.$$

This predicts that the intensity of radiations of a given frequency should increase as  $\nu^2$  and at very high frequencies the intensities must be infinite at any temperature  $T$ . This is the Rayleigh Jeans law which is in contradiction with the experimental observations and termed as the ultraviolet catastrophe.

A solution to this problem was provided by Max Planck in 1900 when he proposed that the energy of the harmonic oscillator are restricted to multiples of the fundamental natural frequency  $\nu$  times a constant ( $h = 6.6 \times 10^{-34} J s$ ) ie.,  $E = nh\nu$ . Thus, the radiations are from a collection of harmonic oscillators of different frequencies and the energy of the radiations from the oscillators has to be packets of  $h\nu$ . Hence the average energy has to determine as a summation of the probabilities of

$$\text{the energy of the individual oscillators to the total probability as } \langle E \rangle = \frac{\sum E * P(E) dE}{\sum P(E) dE} = \frac{\sum nh\nu \frac{e^{-nh\nu/kT}}{kT} dE}{\sum \frac{e^{-nh\nu/kT}}{kT} dE}$$

With this concept of energy of the radiations the average energy of the oscillators can be evaluated as  $\langle E \rangle = \frac{h\nu * e^{-h\nu/kT}}{1 - e^{-h\nu/kT}}$  and the energy density of radiations can be evaluated as

$$\rho(\nu) d\nu = \langle E \rangle dN = \frac{8\pi}{c^3} \nu^2 d\nu \frac{h\nu}{e^{h\nu/kT} - 1} = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1} d\nu$$

The decrease in the intensity at higher frequencies (smaller wavelengths) can be attributed to the fact that the excitation of the oscillators to the higher energy states is less probable at lower temperatures. At higher temperatures, the thermal energy  $kT$  enables oscillations at higher frequency  $n\nu$ . This expression gives excellent co-relation with experimental results which was a milestone. At very low frequencies this expression reduces to the Rayleigh Jeans expression.

Thus, Max Planck had unknowingly laid the foundation for quantization of energy states of a system though not in the currently understood terminologies.

## Atomic Spectra

Atoms of different elements have distinct spectra and therefore atomic spectroscopy allows for the identification and quantization of a sample's elemental composition.

Robert Bunsen and Gustav Kirchhoff discovered new elements by observing their emission spectra. Atomic absorption lines are observed in the solar spectrum and referred to as Fraunhofer lines after their discoverer. The existence of discrete line emission spectra or the absence of discrete lines in an absorption spectrum puzzled scientists since the atomic model had not evolved at the time of these observations.

Classical physics tried to model the emission from atoms as that due to the orbiting electron, since an accelerated charge should emit electromagnetic radiation --- light. However according to this model, the electron should be continually losing energy and fall into the atom in an extremely small time interval.

(The explanation of the line spectrum of atoms in terms of transition between energy states of an atom evolved after the quantum model of the atom evolved.)

**Photo electric effect** – an experiment in which radiation (electromagnetic waves) interact with matter where emission of electron from the metal when radiation of wavelengths lesser than a cutoff wavelength. The electron emission was instantaneous and the kinetic energy of the emitted electrons depended only on the wavelength of the incident radiation and not on the intensity.

These results could not be explained on the basis of the classical EM wave theory. The classical theory suggests that electrons accumulate of energy from the incident waves on continuous irradiation and when the energy of the electrons is more than the work function of the material it is emitted from the metal after a delayed time. According to the classical theory the kinetic energy of the electrons emitted should be dependent on the intensity of the radiation and independent of the wavelength. All these explanations were in contradiction to the experimental results.

Einstein explained the effect considering light to behave as particles called Photons and the interaction of the photons with the electrons in the metal can result in transfer of energy to the electron. If the energy gained by the electron is greater than the work function of the metal, then the electron can be emitted and the kinetic energy of the photo electron would depend on the energy of the incident photon. This was a classic example of radiation displaying a particle nature when the interaction is at atomic / sub atomic particles.

## Dual nature of radiation

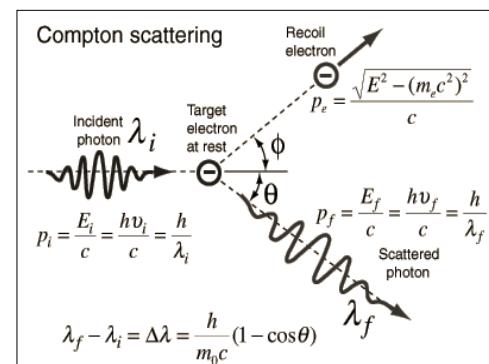
Radiation is part of the electromagnetic spectrum and can be described as electromagnetic waves. Electromagnetic waves are construed as mutually perpendicular sinusoidal electric and magnetic fields and perpendicular to the direction of propagation of the waves. The classical concept assumed that the energy content of the wave is proportional to the square of the amplitude of the waves. The wavelength (and hence the frequency) are not of any consequence with regard to the energy of the wave. Conventional wave theory of radiation explains the phenomena of reflection, refraction, interference, diffraction and polarization of light. Interference and diffraction though stand out as an exclusive wave property.

The Photo electric effect was explained by Einstein as a particle - particle interaction. This paved the way for the concept of the dual nature of radiations. The particle nature of radiations could be evident when radiation interacted with matter at the atomic / subatomic level.

## Compton effect :

Arthur H Compton while studying the scattering of X rays by materials observed that in addition to the emission of an electron, the scattered beam has a different wavelength as compared to the incident wavelength.

The scattering of X rays (the high energy end of the electromagnetic spectrum) if treated classically would not explain the origin of X rays of higher wavelength.



Compton treated the problem as a particle - particle collision in which photons of momentum  $p_i = \frac{h}{\lambda_i}$  are scattered with an electron at rest. This results in a transfer of momentum and energy to the electron which is scattered. The photon loses energy and momentum which results in a gain in momentum and energy for the electrons. The scattered X-ray photon has reduced energy which results in an increase in the wavelength.

The analysis of the conservation of energy and momentum conservation before and after the collision (taking into consideration the relativistic effects for the energy and momentum of the electron) gives the increase in the wavelength of the scattered photon.

If  $\lambda_i$  is the wavelength of the incident X-ray photon, the momentum of the photon is  $p_i = \frac{h}{\lambda_i}$  and the energy of the photon is  $E_i = \frac{hc}{\lambda_i}$ . Since the electron is at rest the initial momentum of the electron is zero and the energy of the electron is the rest mass energy  $m_0 c^2$ .

After the collision, the wavelength of the scattered X ray is  $\lambda_f$  and the momentum  $p_f = \frac{h}{\lambda_f}$ . The energy of the scattered X ray is  $E_f = \frac{hc}{\lambda_f}$ .

The momentum of the scattered electron is  $p_e$  and the energy is  $E_e = \sqrt{p_e^2 c^2 + m_0^2 c^4}$

The energy conservation equation is  $p_i c + m_0 c^2 = p_f c + \sqrt{p_e^2 c^2 + m_0^2 c^4}$

From this expression we get  $p_e^2 = p_i^2 + p_f^2 - 2p_i p_f + 2m_0 c(p_i - p_f)$  ...(i)

Since the X ray and the electron are scattered in different directions, the momentum conservation equation has to be treated as conservation of the momentum of the particles before and after collisions in the direction of incidence and in a perpendicular direction.

Momentum conservation along the incident direction is  $p_i + 0 = p_f \cos\theta + p_e \cos\phi$ .

Hence  $p_e \cos\phi = p_i - p_f \cos\theta$  ..(ii)

Momentum conservation in a perpendicular direction is  $0 = p_f \sin\theta - p_e \sin\phi$

Or  $p_e \sin\phi = p_f \sin\theta$  ... (iii)

Squaring and adding equation (ii) and (iii) we

$$p_e^2 = p_i^2 + p_f^2 - 2p_i p_f \cos\theta \dots \text{(iv)}$$

Comparing equations (i) and (iv) we obtain  $-2p_i p_f + 2m_0 c(p_i - p_f) = -2p_i p_f \cos\theta$  which can be simplified to  $\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c} (1 - \cos\theta)$

The change in the wavelength  $\Delta\lambda = \lambda_f - \lambda_i$  is known as the Compton Shift.

It is obvious that the Compton shift  $\Delta\lambda$  is

- independent of the incident wavelength of X rays
- independent of the type of the scattering material
- depends only on the angle of scattering of the X rays

The term  $\frac{h}{m_e c}$  is termed as the Compton wavelength  $\lambda_c$  and is a constant  $= 2.42 \times 10^{-12}$  m.

**Relativistic concepts of energy and momentum of particles**

*Einstein's concepts of relativistic particles (particles moving with speeds comparable to the speed of light) are*

- A particle at rest it has a rest mass energy given by  $E = m_0 c^2$ .
- A particle moving with a velocity  $v$  will have a mass given by  $m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$
- If  $p$  is the momentum of the particle then the kinetic energy of the particle is given by  $pc$
- The total energy of the particle is given by  $E = \sqrt{p^2 c^2 + m_0^2 c^4}$

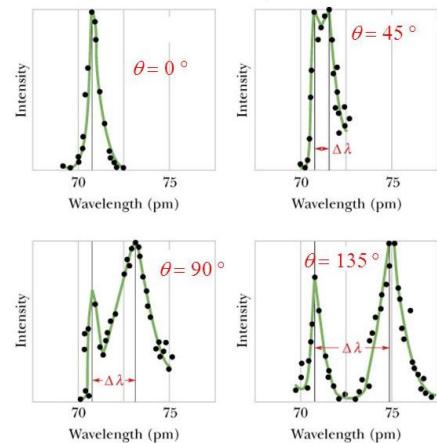
At  $\theta=0^\circ$  we notice there is no shift in the wavelength or there is no interaction of the X rays with the electrons.

At  $\theta=90^\circ$  the shift  $\Delta\lambda = \lambda_c$

At  $\theta=180^\circ$  the collision is a head on collision and the shift in the wavelength is maximum  $\Delta\lambda = 2\lambda_c$ . Thus we conclude that maximum momentum and hence energy transfer happens when the incident X ray is back scattered.

At other angles the predicted shift were in agreement with the experimental observations.

Thus, the Compton Effect was another instance of the particle nature of radiation.



The two experiments of interaction of radiation with matter at sub atomic levels (Photo electric effect and the Compton effect) led to the conclusion that radiation exhibit a dual nature - show the normal wave characteristics and a particle at times of interaction of radiation with matter.

### Dual nature of matter

Louis de Broglie (analyzing the results of the dual nature of radiation) put forward the hypothesis that matter (form of energy) when in motion can display wave characteristics and the wavelength associated with the moving particle  $\lambda = \frac{h}{mv}$  where  $mv$  is the momentum of the particle.

Common heavier particles have a wavelength that is beyond the measurement capabilities with the best of techniques available. For example, the wavelength of a carbon atom moving with a velocity of 100m per second could possess a wavelength of the order of  $10^{-10}$ m. This has to be measured with an experiment characteristic of waves such as diffraction or interference.

The wavelength of the associated waves has to be in the measurable range of an interference or diffraction experiment to prove the existence of matter waves.

This concept was experimentally verified by Davisson and Germer who observed unusual scattering characteristics for electrons scattered by a Ni crystal when the accelerating potential of the electrons was 54V and angle of scattering  $50^\circ$ .

The de Broglie wavelength of electrons accelerated by 54V can be estimated to be  $1.67 \times 10^{-10}$ m. If the electron wave possesses such a wavelength, it should be possible to diffract the waves with a known crystal.

If the scattering has to be explained as a diffraction phenomenon (characteristics of waves) following Bragg's law, then  $2d \sin \theta = n\lambda$  where  $d$  is the interplanar distance of the Ni crystal,  $\theta$  the glancing angle (angle between the incident ray and the surface of the crystal) and  $\lambda$  is the wavelength of the "waves".

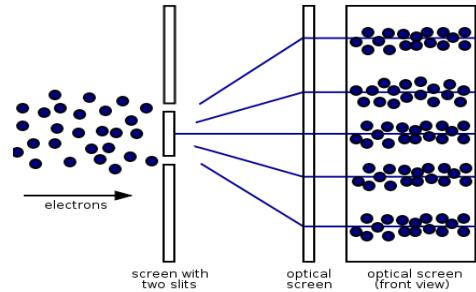
This yields a wavelength which is close to the value obtained using de Broglie's hypothesis (matter waves). Since diffraction is characteristic of waves, it was concluded that electrons undergo diffraction under the set experimental conditions.

Thus, it is concluded that matter display dual characteristics at appropriate conditions of interaction. This concept has been further confirmed by diffraction experiments using heavier particles such as the slow neutrons from a nuclear reactor.

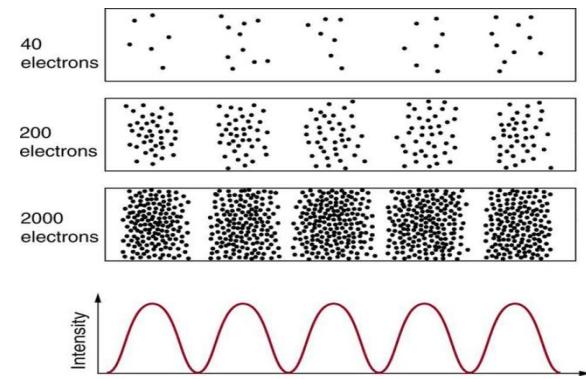
Hitachi in the 1980s showed the diffraction of electrons when scattered by a thin wire. It was observed that the electrons scattering patterns are very close to a diffraction pattern produced by a double slit experiment.

### Young's double slit experiment with particles

A double slit experiment with particles incident on the slits one at a time reveal some interesting outcomes. Experiments show that electrons (or photons) as particles are expected to arrive at some definite location on a screen, unlike a wave. But if a second electron (or photons) is incident at the slit, the second electron reaches a different location, often far outside any experimental uncertainty. If many electrons (or photons) are incident on the slit but one at a time then the measurements will display a statistical distribution of locations that appears like an interference pattern.



The building up of the diffraction pattern of electrons scattered from a crystal surface. Each electron arrives at a definite location, which cannot be precisely predicted. The overall distribution shown at the bottom can be predicted as the diffraction of waves having the de Broglie wavelength of the electrons.

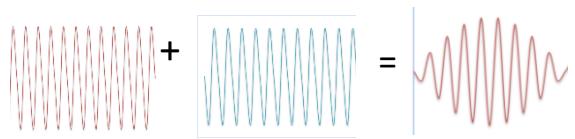


This experiment leads to concept of probabilities that are inherent in quantum mechanical systems. A quantum particle exhibits probabilistic behavior when there is no effort to detect the particle.

### Wave packets

The concept of matter waves requires a wave like (mathematical) representation of the moving particle where position and momentum of the particle can be estimated with reasonable accuracy. Sinusoidal representations result in a gross uncertainty in the position while providing a highly accurate estimation of the momentum.

The superposition of two waves of very close frequency and propagation constant results in a wave packet, frequency  $\omega + \Delta\omega$  and propagation constant  $k + \Delta k$ . Let  $y_1$  be a sinusoidal wave with angular frequency  $\omega$  and propagation constant  $k$  and  $y_2$  be a wave with frequency  $\omega + \Delta\omega$  and propagation constant  $k + \Delta k$ .



$$y_1 = A \sin(\omega t + kx) \text{ and}$$

$$y_2 = A \sin\{(\omega + \Delta\omega)t + (k + \Delta k)x\}$$

The superposition of the two waves gives a resultant

$$y = y_1 + y_2 = 2A \sin(\omega t + kx) \cdot \cos\left(\frac{\Delta\omega t + \Delta k x}{2}\right)$$

The first part is the original high frequency component and the second term is a low frequency component. This is the case of an amplitude modulated wave where the amplitude of the high frequency component is modulated according to the amplitude of the low frequency component. Since this is the resultant of a group of super imposed waves, it is referred to as a wave packet.

The momentum of the particle could be evaluated with the estimation of the wavelength of the waves in the wave packet. The position of the particle could be inferred from the region in which the amplitude (and hence the intensity) of the wave is a maximum.

This gives a reasonably accurate value of both momentum and position. The momentum is derived from the wavelength of the high frequency component and the position from the region of maximum amplitude of the wave packet.

We can define both a phase and group velocity for the wave packet.

The phase velocity of the waves is defined as the velocity of an arbitrary point marked on the wave (the high frequency component) as the wave propagates and is given by  $v_p = \frac{\omega}{k}$

The velocity of the wave packet (wave group) is defined as the group velocity and given by

$$v_g = \frac{d\omega}{dk}.$$

### **Relation between group velocity and particle velocity**

Group velocity of waves =  $v_g = \frac{d\omega}{dk}$

The angular frequency  $\omega = \frac{E}{\hbar}$  where E is the energy of the wave and hence  $d\omega = \frac{dE}{\hbar}$

The wave vector  $k = \frac{p}{\hbar}$  where p is the momentum and hence  $dk = \frac{dp}{\hbar}$

Therefore, the group velocity  $v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$

Since  $E = \frac{p^2}{2m}$  the group velocity  $v_g = \frac{dE}{dp} = \frac{p}{m} = v$  where v is the particle velocity.

### **Relation between group velocity and phase velocity**

The group velocity of the particle is given by  $v_g = \frac{d\omega}{dk} = \frac{d}{dk}(v_{ph} \cdot k) = v_{ph} + k \frac{dv_{ph}}{dk}$

However,  $\frac{dv_{ph}}{dk} = \frac{dv_{ph}}{d\lambda} \cdot \frac{d\lambda}{dk}$ .

And  $\frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$  hence  $v_g = v_{ph} - \frac{2\pi}{k} \frac{dv_{ph}}{d\lambda} = v_{ph} - \lambda \frac{dv_{ph}}{d\lambda}$

In a dispersive medium (where the velocity of the waves depends on the wavelength) the group velocity is given by the above equation.

When the group velocity of the wave packet is equal to the phase velocity the medium in which the wave propagate is a non-dispersive medium. In this case  $\frac{dv_{ph}}{d\lambda} = 0$  or the phase velocity is a constant with respect to wavelength.

### ***Evaluate the condition under which the group velocity of a wave packet is***

- i) Half the phase velocity and ii) twice the phase velocity**

The group velocity of a wave packet is given by  $v_g = v_{ph} - \lambda \frac{dv_p}{d\lambda}$

Case 1.  $v_g = v_{ph}/2$

$\frac{dv_p}{v_{ph}} = \frac{1}{2} \frac{d\lambda}{\lambda}$  This on integration yields  $\ln(v_{ph}) \propto \ln \sqrt{\lambda}$  or  $v_{ph} \propto \sqrt{\lambda}$

This implies that the phase velocity is proportional to the square root of the wavelength

Case 2.  $v_g = 2v_{ph}$

$\frac{dv_p}{v_{ph}} = -\frac{d\lambda}{\lambda}$  This on integration yields  $\ln(v_{ph}) \propto \ln \left(\frac{1}{\lambda}\right)$  or  $v_{ph} \propto \lambda^{-1}$

This implies that the phase velocity is inversely proportional to the wavelength.

### Uncertainty principle

Heisenberg's analysis of the wave packet revealed the spread in the estimation of the position and the spread in the propagation constant of the wave is intrinsically related.

A Fourier transform of the wave functions gives the distribution of the propagation constant. In summary the product of the standard deviations in the estimates of the position and the propagation constant was shown to be greater than or at the most equal to  $\frac{1}{2}$ . i.e.,  $\Delta x \cdot \Delta k \geq 1/2$

This then translates to the standard form of the uncertainty principle when the propagation constant is transformed to the momentum through the relation

$$p = \hbar k$$

The position and momentum of a particle cannot be determined simultaneously with unlimited precision. If one of the parameters is determined with high precision then the other must necessarily be imprecise, such that the product of the uncertainties is greater than or equal to  $\hbar/2$  i.e.,

$$\Delta x \cdot \Delta p \geq \hbar/2$$

where  $\Delta x$  is the uncertainty in the position and  $\Delta p$  is the uncertainty in the momentum determined simultaneously.

The uncertainty relation for energy E and time t for a physical system can be written as

$$\Delta E \cdot \Delta t \geq \hbar/2$$

Where  $\Delta E$  is the uncertainty in the energy E of a system and  $\Delta t$  is the uncertainty in the time in which this energy is estimated.

In the case of rotational motion, the uncertainty relation between the angular position  $\theta$  and the angular momentum L can be written as

$$\Delta \theta \cdot \Delta L \geq \hbar/2$$

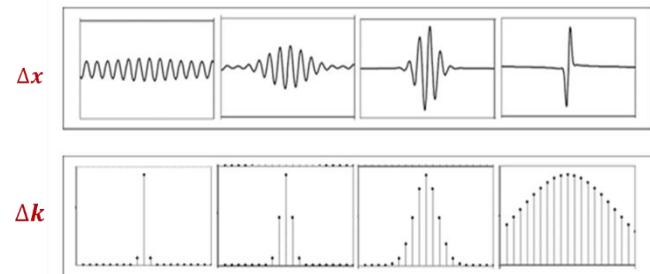
where  $\Delta \theta$  is the uncertainty in the angular position and  $\Delta L$  is the uncertainty in the angular momentum determined simultaneously.

### Heisenberg's Gamma ray microscope:

Heisenberg proposed the gamma ray microscope (as a thought experiment to illustrate the uncertainty principle) to locate the position of an electron. To be able to "observe" the electron, it should be "illuminated" by a radiation whose wavelength is comparable to the size of the scattering object. Hence it is evident that one should use  $\gamma$  rays to observe electrons, which in turn scatter the radiation onto the objective lens of the microscope. In order that we "see" the electron, the limit of resolution of the microscope should be comparable to the position uncertainty  $\Delta x$ .

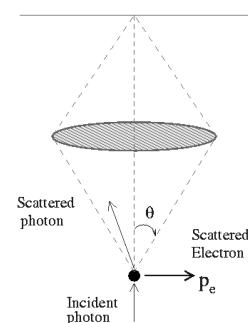
Thus, we get  $\Delta x \approx \frac{\lambda}{\sin \theta}$ .

However, when the high energy  $\gamma$  rays can impart momentum to the electrons (following the principles of Compton Effect).



***The more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa.***

***Heisenberg, uncertainty paper, 1927***



The maximum momentum imparted to the electron can be estimated from the maximum shift in the scattered photon momentum. If the momentum of the photons entering the microscope at a half cone angle  $\theta$  is  $\frac{h}{\lambda}$  then the maximum momentum gained by the electron in the x direction would be

$$p_x \approx \pm \frac{h}{\lambda} \sin \theta.$$

Thus, the minimum momentum of the electron would be uncertain by a factor  $\Delta p_x \approx 2 \frac{h}{\lambda} \sin \theta$

Thus the product of the uncertainties  $\Delta x \cdot \Delta p_x \approx \frac{\lambda}{\sin \theta} * 2 \frac{h}{\lambda} \sin \theta \approx 2h > \frac{h}{4\pi}$  conforms to the uncertainty principle.

This illustrates that in the simultaneous determination of the position and momentum of an electron results in an inherent uncertainty.

### **Electron's existence inside the nucleus**

The uncertainty principle can be used to illustrate the impossibilities in physical systems or the correctness of assumptions. Beta particle emission from radioactive nuclei is one such example. Experiments show that the beta emission is the emission of an electron with a high energy of about 4MeV by radioactive nuclei. If we assume the electron to be an integral part of the nucleus then we may be able to estimate the minimum energy of the electron using the uncertainty principle.

If the electron is part of the nuclei, then the position of the electron is uncertain to the extent of the nuclear diameter. The uncertainty in the position of the electron

$$\Delta x \approx 10^{-14} m$$

The minimum uncertainty in the momentum of the electron then can be estimated as

$$\Delta p = \frac{\hbar}{2 \cdot \Delta x} = 5.28 \times 10^{-21} kgms^{-1}$$

Hence the minimum momentum of the electron  $p$  has to be at least the uncertainty  $\Delta p$  and hence

$$\text{The kinetic energy of the electron } E = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{1}{2m} \left( \frac{\hbar}{2 \cdot \Delta x} \right)^2 \approx 96 \text{ MeV}$$

This implies that the energy of the electron emitted by the radioactive nuclei should be quite high if electron had to be integral member of the nuclei. Since the energies of the electron emitted by radioactive nuclei are very less compared to the estimate, we conclude that the electron cannot be a permanent part of the nuclei, thus illustrating the power of the uncertainty principle.

### **Wave functions**

A moving particle can be represented by a wave packet. The wave packet can be described by a function  $\Psi(x, y, z, t)$  which is referred to as the wave function or the state function.. The function  $\Psi$  though contains information about the physical state of the system, has no other physical interpretation. However, since the amplitude of the wave gives information on the probable position of the particle,  $\Psi$  can be termed as the **probability amplitude**.



The functions should have the following characteristics if it has to be representing a moving particle.

(1)  $\psi$  must be finite, continuous and single valued in the regions of interest.

Since  $\Psi(x, y, z, t)$  is a probability amplitude (as discussed in the definition of a wave packet) it is necessary that the function is **finite** and highly localized. The value of the function could change with the position of the particle but has to remain finite and **continuous** (as is obvious from the fact it is representing a wave packet). Since the physical parameters of the system are single valued the wave function has also to be **single valued**.

- (2) The derivatives of the wave function must be finite, continuous and single valued in the regions of interest.

Since the wave function is a continuous function, the derivatives of the function with respect to the variables must exist. For example if the function is a plane wave given by  $\psi = Ae^{i(kx-wt)}$  then the derivative of the function is  $\frac{\partial \psi}{\partial x} = Ae^{ikx}.ik = ik.\psi$ . It is obvious that the derivative of the function would inherit the properties of the wave function, and hence it has to be finite continuous and single valued.

- (3) The wave function  $\psi$  must be normalizable. i.e.,  $\int_{-\infty}^{+\infty} \psi^* \psi dV = 1$

The wave function  $\Psi(x, y, z, t)$  is a probability amplitude and the intensity of the wave (the point at which the energy of the wave is likely to be concentrated) is the square of the probability amplitude. Since the wave function can be a real or imaginary function it is evident that the square of the wave function  $|\Psi|^2 = \Psi^* \cdot \Psi$ .  $\Psi^*$  is the complex conjugate of the wave function. Thus, the product is representative of the intensity of the wave or the probability of finding the particle at any point in the wave packet and is called the **probability density**. Thus, the summation of all the  $\Psi^* \cdot \Psi$  for the extent of the wave packet should give the total probability of finding the particle. Thus  $\sum \Psi^* \cdot \Psi = 1$ . Since the wave function is a continuous function it can be written as

$$\int \Psi^* \cdot \Psi dx = 1$$

Since the wave function is highly localized this implies that the wave function  $\Psi$  should vanish at large values of  $x$ , i.e.  $\Psi \rightarrow 0$  as  $x \rightarrow \infty$ .

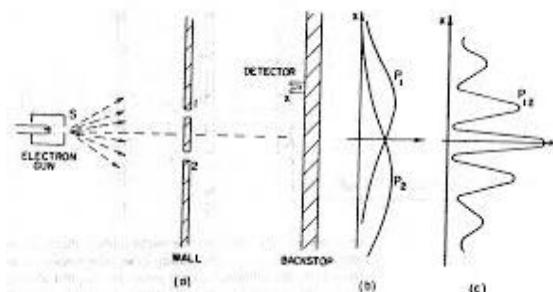
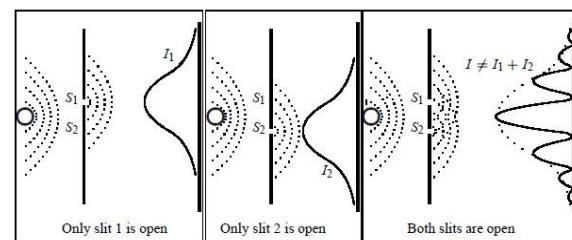
Hence the integral evaluated over all of space  $\int_{-\infty}^{+\infty} \Psi^* \cdot \Psi dx = 1$ . This is called as the normalization of the wave function. In effect the amplitude of the wave is normalized to ensure that the total probability of finding the particle is always equal to one.

The wave function  $\Psi$  satisfying the above conditions are called as well-behaved functions and can be used to represent the physical state of a system in quantum mechanics.

### Linear superposition of wave functions

The classical Young's double slit experiment with light waves demonstrates the diffraction of light. The experiment conceived photons passing through two closely spaced slits diffract and forms an interference pattern at the screen.

The experiment can be repeated with single photon emitted one at a time allowed to be incident on the slit with no particular alignment. The photon decides to enter either slit 1 or slit 2. The state of the photon entering slit 1 is described by the wave function  $\psi_1$  and  $\psi_2$  represents the wavefunction of the photons passing through slit 2. When slit 2 is closed and slit 1 is opened all photons preferentially go thru slit 1 and the intensity pattern of the photons on the screen will be given by  $P_1$ . Similarly when slit 1 is closed and slit 2 is opened all photons preferentially go thru slit 2 and the intensity pattern of the photons on the screen will be given by  $P_2$ . However, when both the slits are opened the intensity patterns do not add up. The resultant is an interference pattern which can be described as the superposition of the two photon states given by  $\psi_3 = \psi_1 + \psi_2$ .



If the photon beam is replaced by an electron beam then it is interesting to note that the electrons going through the slit behaves as waves and form an interference pattern on the screen.

This clearly demonstrates the wave behavior of electrons. If  $\psi_1$  represents the electrons passing through slit 1 and  $\psi_2$  represents the electrons passing through slit 2, then the probability densities  $P_1 = |\psi_1|^2$  and  $P_2 = |\psi_2|^2$ .

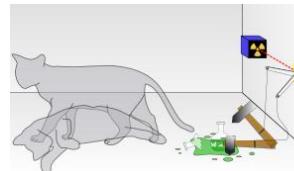
It is obvious that  $\psi_3 = \psi_1 + \psi_2$  represents the super imposition of the two states or super position of the two wave functions. Thus, the probability density of the new states should be given by

$$P_3 = |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi_1^* \psi_2 + \psi_2^* \psi_1 \text{ and is not equal to } |\psi_1|^2 + |\psi_2|^2.$$

Thus, we observe that the superposition of the two states yield a new state.

In general if  $\psi_1$  and  $\psi_2$  are two wave functions of a system then the linear superposition of the two states is also a possible quantum state  $\psi_3 = a * \psi_1 + b * \psi_2$

Another interesting observation is that any attempt to observe the events of which or how many electrons pass through each slit with a detector, the interference pattern is not observed and the intensity is a algebraic addition of the two intensities from the two slits. Thus, the superposed wave function  $\psi_3$  is non-existent and the wave function is said to have collapsed.



**Schrödinger's cat:** a cat, a flask of poison, and a radioactive source are placed in a sealed box. If an internal monitor (e.g. [Geiger counter](#)) detects radioactivity (i.e. a single atom decaying), the flask is shattered, releasing the poison, which kills the cat. The Copenhagen interpretation of quantum mechanics implies that after a while, the cat is simultaneously alive and dead. Yet, when one looks in the box, one sees the cat either alive or dead not both alive and dead. This poses the question of when exactly quantum superposition ends and reality collapses into one possibility or the other.

Thus, quantum systems are not subjected to observations, since the observations interfere with the quantum behavior of the particles being studied. This is the classic Schrodinger's cat paradox.

### Observables.

The physical parameters associated with the particle such as energy, momentum, kinetic energy, spin, etc. are observables of the state of a system. Experimental results can give us values of observables, and multiple measurements on the system at the same state should result in the same value or average values for the observables, if the state of the system is not modified by the measurement. Observables have real values and their accurate measurements would be limited by the principles of uncertainty.

The wave function carries information about the state of the system, or the observables can be extracted from the wave functions with the help of appropriate operators.

### Operators

The wave function describing a system in one dimension can be written as  $\psi(x, t) = e^{\frac{i}{\hbar}(px - Et)}$ . This function contains information about the observables of the system. The values of the observables can be inferred using a mathematical operator operating on the wave function.

Differentiating  $\psi$  with respect to position yields  $\frac{d\psi}{dx} = (\frac{ip}{\hbar})\psi$

Or the operation  $\left\{-i\hbar \frac{d}{dx}\right\}$  on  $\psi$  yields the momentum of the system.

$\hat{p} = \left\{-i\hbar \frac{d}{dx}\right\}$  is the momentum operator.

Differentiating the above yields  $\frac{d^2\psi}{dx^2} = \left(\frac{ip}{\hbar}\right)^2\psi$

Rearranging the terms and dividing by  $2m$  we get  $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \frac{p^2}{2m}\psi = KE\psi$

Thus, the operation  $\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\}$  on  $\psi$  yields the kinetic energy.

$\widehat{KE} = \{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\}$  is the kinetic energy operator

Differentiating  $\psi$  with respect to time yields  $\frac{d\psi}{dt} = (-\frac{iE}{\hbar})\psi$

Or the operation  $\{i\hbar\frac{d}{dt}\}$  on  $\psi$  yields the total energy of the system

$\widehat{E} = \{i\hbar\frac{d}{dt}\}$  is the total energy operator.

The position operator  $\widehat{x}$  is equivalent to multiplying the wave function by  $x$  itself  $\widehat{x} = x$ .

The potential energy operator is not explicitly defined as the potential can be inferred if the total energy and the kinetic energy of the system is known.

### **Expectation values:**

Quantum mechanics deals with probabilities and hence predicts only the most probable values of the observables of a physical system which are called the expectation values. These expectation values could be the average of repeated measurements on the system. The method of evaluating the expectation values is outlined as below.

Let  $\widehat{p}$  be an operator that gives the value of the momentum  $p$  when it operates on the wave function  $\psi$ .

The operation  $\psi^*\widehat{p}\psi = \psi^*p\psi = p\psi^*\psi$  where  $p$  is the value of the observable extracted from  $\psi$ . The many values of  $p$  extracted from the wave function can be averaged over the extend of the wave packet.

The same can be obtained by integrating the expression  $\psi^*\widehat{p}\psi$  over the range and dividing it by the total probability

$\int \psi^*\widehat{p}\psi dV = \int \psi^*p\psi dV = \langle p \rangle \int \psi^*\psi dV$  where  $\langle p \rangle$  is the most probable value of the momentum.

Thus the expectation value of the momentum is written as  $\langle p \rangle = \frac{\int \psi^*\widehat{p}\psi dV}{\int \psi^*\psi dV}$ .

If the integral is over all of space then the integrals could be evaluated between limits of  $\pm\infty$ . In this case it is observed that the denominator would be the total probability and can be written as 1. However, it is customary to write the expectation values in the standard form.

In the general case for an operator  $\widehat{A}$  when and hence the expectation value of the parameter  $A$  can be written as  $\langle A \rangle = \frac{\int \psi^*\widehat{A}\psi dV}{\int \psi^*\psi dV}$ .

### **Schrodinger's Wave equation**

The moving particle is described by a wave function and there is a need to have a wave equation which can describe this moving particle. Schrodinger's approach to describe the motion in terms of a differential equation is one of the most popular methods. (Dirac's operator mechanics with vector spaces is another method of describing the moving particle and is a computational friendly method.)

### The one dimensional time dependent Schrodinger's wave equation

The most general method of describing a system involves evaluating the system in terms of the state variables of position and time.

The total energy of a system is equal to the sum of kinetic energy and potential energy (which are observables of the system)

The energy expression can be written as  $E = KE + V$

Multiplying throughout with the wave function  $\psi$  we get

$$E\psi(x, t) = KE\psi(x, t) + V\psi(x, t) \quad \dots \dots \dots (1)$$

This equation can be written in terms of the corresponding operators as

$$\hat{E}\psi(x, t) = \hat{K}\psi(x, t) + V\psi(x, t)$$

which is an eigen value equation for the total energy of the system.

The total energy operator is  $\left\{ i\hbar \frac{\partial}{\partial t} \right\}$ , the kinetic energy operator is  $\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right\}$ .

Replacing the total energy and the kinetic energy terms with the respective operators we can rewrite the expression (1) as

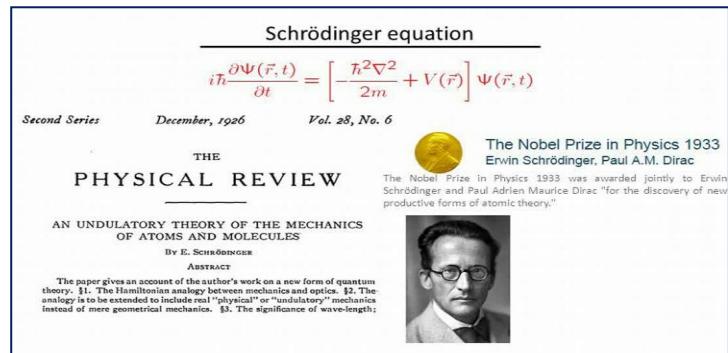
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

or

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + i\hbar \frac{\partial \Psi}{\partial t} - V\Psi = 0 \quad \dots \dots (2)$$

which is the Schrödinger's time dependent wave function since  $\Psi(x, t)$  is a function of both position and time.

The solution of the differential equation yields the wave function  $\Psi$  which is the state function of the system.



### The one dimensional time independent Schrodinger's wave equation

Generally any system in the steady state is time invariant and hence the wave function could be independent of time. In such a case we can write the wave function can be written as the product of two functions one that is position dependent and the other time dependent.

$$\text{Ie., } \Psi(x, t) = A e^{\frac{i}{\hbar}(px)} \cdot e^{-\frac{i}{\hbar}(Et)}$$

where  $\psi(x) = A e^{\frac{i}{\hbar}(px)}$  is the position dependent part and  $\phi(t) = e^{-\frac{i}{\hbar}(Et)}$  is the time dependent part.

Substituting  $\Psi(x, t) = \psi(x) \cdot \phi(t)$  in equation (2) we get

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x) \cdot \phi(t)}{\partial x^2} + i\hbar \frac{\partial \psi(x) \cdot \phi(t)}{\partial t} - V\psi(x) \cdot \phi(t) = 0$$

The total energy  $E$  of the steady state system being a constant, the total energy operator can be replaced by the value  $E$  with no loss of sense.

$$\frac{\hbar^2}{2m} \frac{d^2 \psi(x) \cdot \phi(t)}{dx^2} + E\psi(x) \cdot \phi(t) - V\psi(x) \cdot \phi(t) = 0$$

The above equation can be written as  $\left\{ \frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + E\psi(x) - V\psi(x) \right\} * \phi(t) = 0$

We recognize that the product of two functions is zero and since  $\phi(t) \neq 0$

$$\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + E\psi(x) - V\psi(x) = 0 \quad \dots \dots \dots (3)$$

This is the Schrödinger's time independent one dimensional wave equation. The solutions of the Schrodinger's wave equation yield the wave function  $\psi(x)$  which describes the physical state of the system.

The solution so obtained has to be checked for continuities at any boundaries and normalized to get the exact wave function of the system.

In general the Hamiltonian form of this equation is written as

$$\mathbf{H}\Psi = \mathbf{E}\Psi$$

Where the Hamiltonian operator  $\hat{H} = \hat{KE} + \hat{PE} = \left\{ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} - V \right\}$

### [Three dimensional Schrodinger's wave equation.]

The Schrodinger's wave equation for a 3D can be evolved by looking at the problem as three one dimensional problem in the independent variables **x, y and z**. The wave function of such a system can be written as

$\Psi(x, y, z) = \psi(x)\psi(y)\psi(z)$  where  $\psi(x)$ ,  $\psi(y)$  and  $\psi(z)$  are the three mutually independent wave functions of the particles in the orthogonal co-ordinate system.

The derivatives of the wave function can be written as partial derivatives of the wave function.

The SWE then can be written as

$$\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(x, y, z) + (E - V) \Psi(x, y, z) = 0$$

which can be simplified as

$$\frac{\hbar^2}{2m} \nabla^2 \Psi(x, y, z) + (E - V) \Psi(x, y, z) = 0$$

Where  $\nabla^2 = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$  is the Laplacian operator defined as

$$\nabla^2 = \nabla \cdot \nabla \text{ and the operator } \nabla = [\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}]$$

### [Linear superposition of wave functions from SWE.]

The wave function  $\psi(x)$  which is the solution of the differential equation  $\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) - V\psi(x) = 0$  is a state function. Since a system could have multiple states the solution of the wave equation can give us multiple wave functions  $\psi(x)$ . If  $\psi_1(x)$  represents a state 1 and  $\psi_2(x)$  represents a state 2 of the system then it can be seen that a linear combination of  $\psi_1(x)$  and  $\psi_2(x)$  is also a solution of the SWE. Thus  $\psi_{12}(x) = n.\psi_1(x) + m.\psi_2(x)$  will also be a solution of the SWE. It is obvious that the superposition of two waves is a wave packet and can represent the state of a system.

It is also evident that the probability densities however do not add to give the probability density of the new state and has to be estimated from the new wave function ]

### Template for solving problems in quantum mechanics using the Schrödinger's wave equation

*The Schrodinger's wave equation can be applied to any physical system and the solution of the wave equation yields the wave function of the system. The wave function is probability amplitude and contains information about the physical state (observables of the system). The wave function has to be a well behaved wave function to represent a moving particle.*

*The template for solving the Schrodinger's wave equation is:*

1. Define / set up the physical system (define particle nature, boundaries of potential, total energy of the particle etc)
2. Write the Schrodinger's wave equation and apply the known conditions
3. Obtain the general form of the wave function
4. Check / verify the wave function for it's characteristics
  - finiteness, discreteness and continuity of  $\psi$  and its derivatives,
  - normalization of the wave functions
5. Interpret the solution and get the implications on the quantum system.

### **Problem no 1. Free Particle solution**

A particle is said to be a free particle when it experiences no external forces.

Thus the force given by  $\mathbf{F} = -\frac{dV}{dx} = \mathbf{0}$ . This implies that either V is zero or V is a constant.

The simplest case then could be when the particle is moving in a region of zero potential i.e.,  $V=0$ .

The Schrödinger's time independent one dimensional wave equation for the system simplifies to

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) = 0 \quad \text{or} \quad \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$$

$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$  where  $k = \sqrt{\frac{2mE}{\hbar^2}}$  is the propagation constant.

The solution of this differential equation is  $\psi = Ae^{ikx} + Be^{-ikx}$  where A and B are constants which can be real or imaginary.

As a general concept the first part describes a forward moving wave packet (in increasing x direction) and the second part describes a backward moving wave packet (decreasing x direction)

The energy of the particle is given by  $E = \frac{\hbar^2 k^2}{2m}$ .

Since the free particle is moving in a zero potential region and there is no restriction on wave number or the energy of the particle, we conclude that the total energy of the particle is kinetic in nature with no implications of quantization.

This could be the quantum description of a classical free particle.

### Some typical solved Numericals

- 1.** Estimate the Compton shift for X rays scattered at  $95^\circ$  with respect to the incident direction. If the momentum of the scattered X rays is  $4.5 \times 10^{-24} \text{ kg m s}^{-1}$  estimate the wavelength of the incident X Rays.

The Compton shift is given by  $\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c} (1 - \cos \theta)$ .

$$\text{At } 95^\circ \text{ the shift is } \Delta\lambda = 2.427 \times 10^{-12} * (1 - \cos(95)) = 2.64 \times 10^{-12} \text{ m}$$

$$\text{Wavelength of the scattered X ray is } \lambda_f = \frac{h}{p} = 1.472 \times 10^{-10} \text{ m}$$

$$\text{Wavelength of the incident X ray is } \lambda_i - \Delta\lambda = 1.44 \times 10^{-10} \text{ m}$$

- 2.** In a Compton scattering of electrons with X rays discuss the condition under which the energy gained by the electron is maximum. If the wavelength of the incident X ray is 0.1nm calculate the maximum energy gained by the electron.

In Compton effect the maximum shift in the wavelength of the scattered X ray is when the angle of scattering is  $180^\circ$ . At this angle there is a head on collision with the electron and the electron moves along the incident direction. The momentum and hence the energy transfer are maximum under this condition.

The maximum momentum transfer is the maximum momentum loss of the X ray

$$= \frac{h}{\lambda} - \frac{h}{\lambda'} = \frac{h}{\lambda} - \frac{h}{\lambda + \Delta\lambda} = 3.07 \times 10^{-25} \text{ Kg m s}^{-1}.$$

The maximum energy transfer is the maximum energy loss of the X ray

$$= \frac{hc}{\lambda} - \frac{hc}{\lambda'} = \frac{hc}{\lambda} - \frac{hc}{\lambda + \Delta\lambda} = 575.16 \text{ eV}$$

- 3.** Estimate the energy of a non-relativistic electron if it to confined in a region of width  $10^{-14} \text{ m}$  and calculate the de Broglie wavelength of the electron with this energy. Comment on the results obtained.

The position of the electron is uncertain to the extent of  $10^{-14} \text{ m}$ .  $\Delta x \approx 10^{-14} \text{ m}$

$$\text{The minimum uncertainty in the momentum } \Delta p = \frac{\hbar}{2\Delta x} = 5.27 \times 10^{-21} \text{ kgms}^{-1} = p$$

$$\text{The kinetic energy of the electron } E = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{1}{2m} \left( \frac{\hbar}{2\Delta x} \right)^2 \approx 96 \text{ MeV} \quad \lambda = \frac{\hbar}{p} = 1.257 \times 10^{-13} \text{ m}.$$

The de Broglie wavelength > the width of the region, which implies the electron cannot be confined in this interval.

- 4.** Find the spread in the wavelength of a photon whose lifetime in the excited state is uncertain to  $10^{-10} \text{ s}$  if the wavelength of emission is 541nm.

The uncertainty relation for energy E and time t for a physical system can be written as

$\Delta E \cdot \Delta t \geq \hbar/2$  where  $\Delta E$  is the uncertainty in the energy E of a system and  $\Delta t$  is the uncertainty in the time in which this energy is estimated.

$$\Delta E = \frac{\hbar}{2\Delta t} = \Delta h\nu = h\Delta \left( \frac{c}{\lambda} \right) = \left| hc \cdot \frac{\Delta\lambda}{\lambda^2} \right|$$

$$\Delta\lambda = \frac{\lambda^2}{4\pi c \Delta t} = 7.76 \times 10^{-14} \text{ m}$$

Numericals

1. The energy lost by an incident X ray photon in a Compton Effect is  $1.064 \times 10^{-17}$  J. If the wavelength of the incident wavelength is  $1.5 \times 10^{-10} m$ , find the angle of the scattered X ray photon.
2. The shift in the wavelength of a X ray scattered by an electron is 2.42pm. Find the direction and magnitude of the momentum of the scattered electron.
3. Find the de Broglie wavelength of electrons moving with a speed of  $10^7$  m/s (**Ans**  $7.28 \times 10^{-11}$  m)
4. Compare the momenta and energy of an electron and photon whose de Broglie wavelength is 650nm (**Ans Ratio of momenta =1; ratio of energy of electron to energy of photon =**  $\frac{h}{2m\lambda c} = 1.867 \times 10^{-6}$ )
5. Calculate the de Broglie wavelength of electrons and protons if their kinetic energies are
  - i) 1% and ii) 5% of their rest mass energies. (**Ans Rest mass energy of electron =**  $8.19 \times 10^{-14}$  J; **rest mass energy of protons =**  $1.503 \times 10^{-10}$  J. The de Broglie wavelength  $\lambda = \frac{h}{\sqrt{2mkT}}$  Electron 1%  $\lambda = 1.72 \times 10^{-11} m$  Electron 5%  $\lambda = 7.68 \times 10^{-12} m$  Proton 1%  $\lambda = 9.33 \times 10^{-15} m$  Proton 5%  $\lambda = 4.17 \times 10^{-15} m$ )
6. An electron and a photon have a wavelength of 2.0 Å. Calculate their momenta and total energies.
7. What is the wavelength of an hydrogen atom moving with a mean velocity corresponding to the average kinetic energy of hydrogen atoms under thermal equilibrium at 293K? ( $\lambda = \frac{h}{\sqrt{3mkT}} = 1.47 \times 10^{-10} m$ )
8. The frequency of Surface tension waves in shallow water is given by  $v = (2\pi T/\rho\lambda)^{1/2}$ , where T is the surface tension,  $\rho$  is the density of the medium and  $\lambda$  the wavelength of the waves. Find the group velocity of the waves.
9. The relation between the wavelength  $\lambda$  and frequency  $v$  of electromagnetic waves in a wave guide is given by  $\lambda = c/\sqrt{v^2 - v_0^2}$ . Find the group velocity of the waves.
10. The speed of an electron is measured to be 1 km/s with an accuracy of 0.005%. Estimate the uncertainty in the position of the particle.
11. The spectral line of Hg green is 546.1 nm has a width of  $10^{-5}$  nm. Evaluate the minimum time spent by the electrons in the upper state before de excitation to the lower state. (**Ans:**  $\Delta t = \frac{\hbar}{2\Delta E} = \left| \frac{\lambda^2}{4\pi c \Delta \lambda} \right| = 7.91 \times 10^{-9} s$ )
12. The uncertainty in the location of a particle is equal to its de Broglie wavelength. Show that the corresponding uncertainty in its velocity is approx. one tenth of its velocity. (**Ans:**  $\Delta p = \frac{\hbar}{2\Delta x} = \left| \frac{\hbar}{4\pi \lambda} \right| = \frac{p}{4\pi}$  Hence  $\Delta v = \frac{v}{4\pi} = \frac{v}{12.56} \approx \frac{v}{10}$ )
13. Determine the maximum wavelength shift in the Compton scattering of photons from protons.  
(Ans =  $2.64 \times 10^{-5}$  Å)
14. Show that for a free particle the uncertainty relation can also be written as  $\Delta x \cdot \Delta \lambda = \left| \frac{\lambda^2}{4\pi} \right|$  where  $\Delta x$  is the uncertainty in location of the wave and  $\Delta \lambda$  the simultaneous uncertainty in wavelength.
15. Discuss the following functions to be taken as acceptable wave functions:  
 i:  $N e^{ax}$  ii:  $N e^{ax^2}$  iii:  $N e^{-ax^2}$  iv:  $\frac{N e^{-ax^2}}{5-x}$

16. A wave function is given by  $\psi(x) = Ne^{ikx}$  in the region  $0 < x < a$ . Find the normalization constant N.

17. Find the expectation values of position and momentum for the wave function defined by  $\psi(x) = Ne^{ikx}$  in the region  $-a < x < a$

18. Find the normalisation constant B for the wave function  $\Psi = B[\sin(\pi x/L) + \sin(2\pi x/L)]$  (

**Ans**  $B = \sqrt{\frac{1}{L}}$ )

**Unit II – Quantum Mechanics of simple systems**

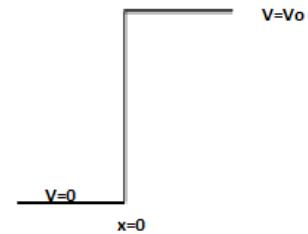
Topics covered under this unit

1. **Solutions of the wave equation to interpret a moving particle encountering a potential step**
  - a. Energy of the particle greater than the potential step
  - b. Energy of the particle less than the potential step
2. **Solutions of the wave equation to interpret a moving particle encounter a potential barrier**
  - a. Barrier tunneling
  - b. Radioactive alpha decay as a case of barrier tunneling
3. **Solutions of the wave equation to interpret a moving particle confined to a region with infinite potentials at the boundaries**
  - a. One dimensional potential well
  - b. Two dimensional potential well
  - c. Three dimensional potential well
4. **Qualitative discussions of the solutions of the wave equation to describe a moving particle confined to a region with finite potentials at the boundaries**
5. **Solutions of the wave equation to interpret a system if two particles connected with a bond as a harmonic oscillator**
6. **Discussions of the wave functions of a hydrogen atom**
7. **Concept of Fermions, Fermi Dirac Statistics**
8. **Concept of Density of States**

### Problem no. 2 - Potential Steps

The behavior of a moving particle when it encounters a potential field along its path is the first step in solving problems in Quantum Mechanics. In reality the potential field varies inversely as the distance from the source of the potential (i.e.,  $V \propto \frac{1}{r}$ ). However, the solution of the Schrödinger's wave equation becomes difficult if the actual potential variations are considered. It is therefore necessary and sufficient if the potentials are approximated to simpler (solvable) systems.

This leads to the concept of potential steps where the potential energy vs. distance graphs show a discrete jump from a zero value to a constant value  $V_0$ . However the behavior of the wave function (representing the particle) can have different responses depending on the energy of the particle as compared to the energy of the potential step. The energy of the particle can be greater or less than the energy of the potential step.



The problem can be divided as a two region problem, region I in which the potential  $V=0$  and the region II in which the potential  $V=V_0$ .

The Schrödinger's wave equation  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$

for the region I with  $V=0$  this becomes  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$

The solution of the equation in region I is given by

$$\psi_1 = A e^{ik_1 x} + B e^{-ik_1 x}$$

where  $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$  and the deBroglie wavelength  $\lambda_1 = \frac{\hbar}{\sqrt{2mE}}$

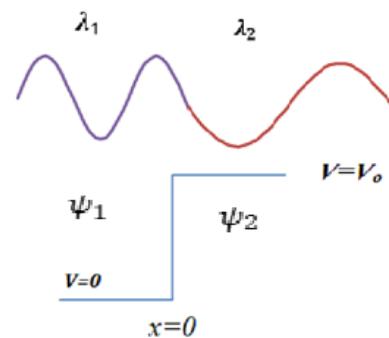
The component with the positive exponent represents the oncoming wave and the negative exponent represents the reflected wave at the boundary  $x=0$

In region II the nature of the wave function will depend on the energy  $E$  of the particle in comparison to the energy of the potential step.

**Case I.** If the energy  $E$  of the particle is greater than the energy of the potential ( $E > V_0$ ) then the Schrödinger's wave equation for the region II can be written as

$$\frac{\partial^2 \psi_{II}}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_{II} = 0$$

with the solution being  $\psi_{II} = C e^{-ik_{II}x} + D e^{ik_{II}x}$  where  $k_{II} = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ . The nature of the wave function remains cyclic and the particle propagates in region II with reduced kinetic energy ( $E - V_0$ ). The first term of the wave function is non-existing since there cannot be a reflection after  $x > 0$  as there is no disruption in the potential.



The momentum in the second region is given by

$\hbar k_{II} = \sqrt{2m(E - V_0)}$  and the corresponding deBroglie wavelength  $\lambda_{II} = \frac{\hbar}{\sqrt{2m(E - V_0)}}$  which is longer than the deBroglie wavelength in region I.

In this case the constants B and D can be found in terms of A by applying the boundary condition that the wave function and its derivatives are finite and continuous at  $x = 0$ .

**at  $x = 0$**   $\psi_{I(x=0)} = \psi_{II(x=0)}$  gives  $A + B = D$

**at  $x = 0$**   $d\psi_{I(x=0)} = d\psi_{II(x=0)}$  gives  $(A - B)k_I = Dk_{II}$

Solving the simultaneous equations we get  $D = 2A * \left(\frac{k_I}{k_I \text{ and } k_{II}}\right)$

$D = 2A * \left(\frac{k_I}{k_I + k_{II}}\right)$  and  $B = A * \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)$

It is seen that the coefficient B of the reflected component is non zero implying that there is a small probability of reflection at  $x=0$  even if the energy of the particle is greater than the potential step  $V_0$ .

The flux of incident particles is given by  $\psi_1^* \psi_1 \times v_1 = A^* A v_1$

The reflection coefficient can be written as  $R = \frac{\text{reflected flux}}{\text{incident flux}} = \frac{B^* B v_1}{A^* A v_1} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2$

and the transmission coefficient  $T = \frac{\text{transmitted flux}}{\text{incident flux}} = \frac{D^* D v_{II}}{A^* A v_I}$  where  $v_I$  and  $v_{II}$  are the velocities of the particles in the two regions.

Thus, the transmission co-efficient  $T = \left(\frac{4k_I k_{II}}{k_I + k_{II}}\right) = \frac{4\sqrt{E(E-V_0)}}{(\sqrt{E} + \sqrt{E-V_0})^2}$

It is observed that  $R+T = 1$ , i.e. the flux incident has to be partially reflected and partially transmitted.

R and T are the relative probabilities of reflection and transmission at the potential step.

### Case II Energy of the particle < $V_0$ .

In region I the behavior of the particle is the same at the previous case (since  $V=0$ ) and the wave function will be

$$\psi_1 = A e^{ik_1 x} + B e^{-ik_1 x}$$

If the energy E of the particle is lesser than the energy of the potential step ( $E < V_0$ ), then the Schrödinger's wave equation for the region II can be written as

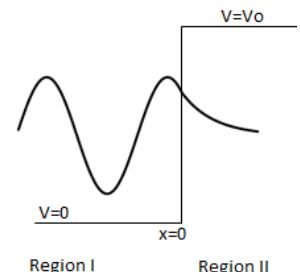
$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0$$

with the solution being  $\psi_2 = F e^{-\alpha x} + G e^{\alpha x}$  where  $\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

The second part of the wave function  $G e^{\alpha x}$ , makes  $\psi_2$  infinite for large values of  $x$  and hence cannot be part of the wave function. Setting the coefficient  $G$  to be zero the wave function reduces to

$$\psi_2 = F e^{-\alpha x}$$

The wave function has a finite value and decays exponentially in region II. Thus there exists a finite probability for the particle to be found in region II



(since  $\psi_2^* \psi_2$  is non zero) which is unlike the classical solution.

(In an exponential decay the wave function is significant till it decays to  $\frac{1}{e}$  of the value at  $x=0$ . At  $x=0$  the value of the function  $\psi_2 = F$ . The changes in this function  $\psi_2 = Fe^{-\alpha x}$  become insignificant at some  $\Delta x$ .

The function evaluated at  $\Delta x$  gives  $\psi_2(\Delta x) = Fe^{-\alpha \Delta x} = F * \frac{1}{e} = F * e^{-1}$ .

This implies  $\alpha * \Delta x = 1$  or  $\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_o-E)}}$ .

The wave function becomes insignificant at a distance  $\Delta x = \frac{\hbar}{\sqrt{2m(V_o-E)}}$  which is the penetration depth in region II. The penetration depth increases as the energy of the particle increases.

In the second region the kinetic energy of the particle is negative which implies that the particle cannot physically exist in the second region.

We conclude that when a particle (or beam of particles with identical E) is incident on a potential step, there is a quantum mechanical effect which -

- the particle can be reflected back even if the energy of the particle  $E > V_o$ .
- the particle can have a small but finite probability of being in the second region even if  $E < V_o$ .

### **Problem no. 3 - Potential Barrier**

The potential barrier is a region in space where the potential is a constant  $V_o$  for all  $0 < x < L$  and  $V=0$  for the all  $x < 0$  and  $x > L$

A particle of mass m and energy  $E < V_o$ , incident on the potential barrier is represented by a forward moving wave. Since  $E < V_o$  classically we expect the particle to be reflected back at the potential barrier and there is no probability of finding the particle in the region beyond the barrier.

In **region I** with  $V=0$  the Schrödinger's wave equation becomes  $\frac{\partial^2 \psi_I}{\partial x^2} + \frac{2m}{\hbar^2} E \psi_I = 0$  (1)

The solution of the equation in region I is given by

$$\psi_I = Ae^{ik_1 x} + Be^{-ik_1 x} \quad (2)$$

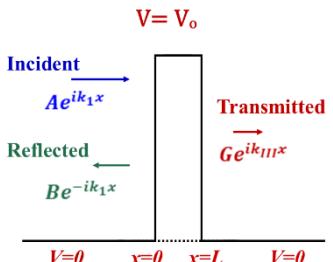
where  $k_I = \sqrt{\frac{2mE}{\hbar^2}}$  and the deBroglie wavelength  $\lambda_I = \frac{\hbar}{\sqrt{2mE}}$

The first term in equation 2 represents the incident wave and the second term represents the reflected component.

In **region II** since  $E < V_o$ , the Schrödinger's wave equation for the region II can be written as

$$\frac{\partial^2 \psi_{II}}{\partial x^2} - \frac{2m}{\hbar^2} (V_o - E) \psi_{II} = 0 \quad (3)$$

with the solution being  $\psi_{II} = De^{-\alpha x}$  where  $\alpha = \sqrt{\frac{2m(V_o-E)}{\hbar^2}}$  (4)



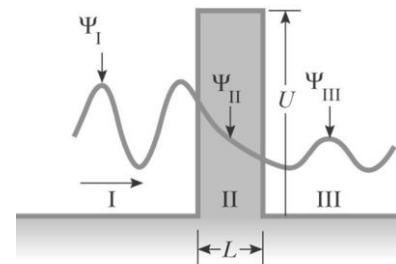
In region II the nature of the wave function changes to an exponentially decaying function. The penetration depth is given by  $\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$  (5)

And in **region III**, the potential being 0, the wave equation is  

$$\frac{\partial^2 \psi_{III}}{\partial x^2} + \frac{2m}{\hbar^2} E \psi_{III} = 0$$

and the wave function is given by  $\psi_{III} = G e^{ik_{III}x}$  (6)

where  $k_{III} = \sqrt{\frac{2mE}{\hbar^2}}$  and the deBroglie wavelength  $\lambda_{III} = \frac{\hbar}{\sqrt{2mE}}$



The amplitude of the reflected and transmitted waves can be evaluated in terms of the incident amplitude by applying the boundary conditions

$$\psi_I = \psi_{II} \text{ at } x = 0 \quad \text{and} \quad \psi_{II} = \psi_{III} \text{ at } x = L$$

$$\text{and} \quad \frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx} \text{ at } x = 0 \quad \text{and} \quad \frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \text{ at } x = L$$

The transmission coefficient which gives the probability of the particles being transferred to the third region can be estimated as  $T = \frac{\text{transmitted flux}}{\text{incident flux}} = \frac{G^* G v_3}{A^* A v_1}$

where  $v_1$  and  $v_3$  are the velocities of the particle in region I and III. Since the energy of the particle is the same in the two regions the velocities are also same and

the transmission coefficient can be evaluated approximately as

$$T = \frac{G^* G}{A^* A} \approx 16 \frac{E}{V_o} \left[ 1 - \frac{E}{V_o} \right] e^{-2\alpha L} \cong e^{-2\alpha L}$$

Thus the probability of transmission is more if either  $\alpha$  or  $A$  is small. Smaller  $\alpha$  implies smaller  $(V_o - E)$ . Thus particles with higher energy have higher transmission probability through the barrier.

If the width of the barrier **L is less than the penetration depth  $\Delta x$**  then there is a finite probability that the particle is transmitted across the barrier.

This process of transmission through a potential barrier even when the energy of the particle is lesser than the barrier potential is known as barrier tunneling or the quantum mechanical tunneling.

It is also noted that for all values of E, there is always a reflected component which is given by  $R = 1 - T$  which is higher than the transmitted coefficient.

*[The particle in the second region has a negative Kinetic energy and this is not a physical reality. However, the particle can exchange energies with the field (potential) without violating the uncertainty principle  $\Delta E \cdot \Delta t = \frac{\hbar}{4\pi}$ . Thus the energy exchange has to happen in a time interval of  $\Delta t = \frac{\hbar}{4\pi\Delta E}$ . This gives a time interval which is extremely small of the order of femto seconds. Thus, the particle has to cross the barrier almost instantaneously]*

### Radioactive alpha decay as a case of barrier tunneling

Emission of alpha particles (Helium nuclei) in the decay of radioactive elements can be example of tunneling.

The positive charge on the nucleus creates a nonlinear potential barrier around the nucleus. This potential barrier is estimated to be as high as 20MeV at the surface.

In the radioactive  $\alpha$  decay of the nucleus, two protons and two neutrons are emitted as a single entity (a doubly charged He nucleus). The process of radioactive decay of  $\alpha$  particles with low energies compared to the barrier potential could be explained as a case of barrier tunneling.

The potential which varies inversely as the distance from the surface of the nucleus can be approximated to a triangular potential. This can then be modeled as a series of rectangular potentials of thin slices of thickness  $\Delta r$ . The potential barrier for each of these slices decrease by a small  $\Delta V$ , which gives  $\alpha_n =$

$$\sqrt{\frac{2m(V_n - E)}{\hbar^2}}$$

The transmission coefficients for each of the slice of potential barrier can be evaluated with  $T_n = e^{-2\alpha_n \Delta r}$  and the total transmission probability is the product of all these individual transmission probabilities. This gives a reasonable

estimate of the tunneling probabilities of alpha particles.

Tunneling rate is very sensitive to small changes in energy and size of the nucleus and account for the wide range of decay times to different radioactive nuclei.

Taking the alpha particles to be in a state of constant motion with a very high kinetic energy, the frequency of approach to the nuclear surface can be estimated to be the diameter of the nucleus divided by the velocity of the particles. This frequency when multiplied by the transmission co-efficient gives us the probability that an alpha particle is emitted out of the nucleus. The inverse of this probability is then the mean lifetime for alpha decay of the radioactive nucleus.

#### Problem no. 4 - Particle in a Box with infinite potentials at the walls

A particle with mass  $m$  and energy  $E$  is confined in a one dimensional box with infinite potential at the boundaries. Defining the boundaries to be  $x = -\frac{a}{2}$  and  $x = +\frac{a}{2}$  where the potential tends to infinity.

The particle is confined to the region  $-\frac{a}{2} < x < +\frac{a}{2}$  and cannot be found in regions outside the boundaries  $x < -\frac{a}{2}$  and  $x > +\frac{a}{2}$ . The potential inside the region  $-\frac{a}{2} < x < +\frac{a}{2}$  is  $V=0$ .

The Schrödinger's wave equation  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$

in the region within the well  $V=0$  this becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

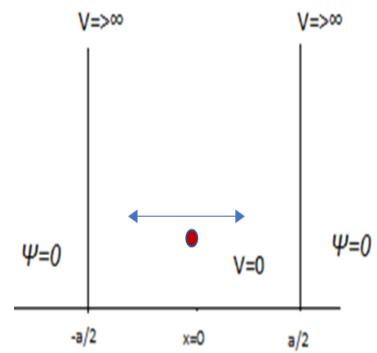
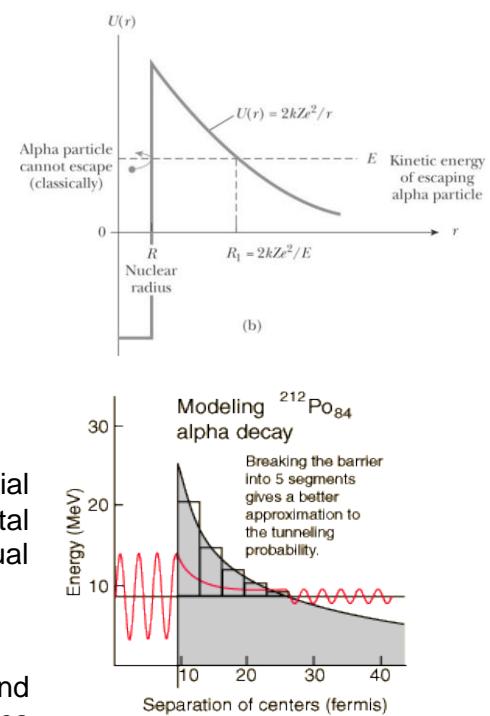
The solution of the equation in region  $-\frac{a}{2} < x < +\frac{a}{2}$  is given by

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

Applying the boundary condition that  $\psi = 0$  at  $x = -\frac{a}{2}$  and  $x = +\frac{a}{2}$

At  $x = -\frac{a}{2}$   $\psi(x = -\frac{a}{2}) = A \sin(-k \frac{a}{2}) + B \cos(k \frac{a}{2}) = 0$  gives

$$-A \sin(k \frac{a}{2}) + B \cos(k \frac{a}{2}) = 0$$



At  $x = \frac{a}{2}$   $\psi\left(x = \frac{a}{2}\right) = A\sin\left(k \frac{a}{2}\right) + B\cos\left(k \frac{a}{2}\right) = 0$  gives

$$A\sin\left(k \frac{a}{2}\right) + B\cos\left(k \frac{a}{2}\right) = 0 \quad [2]$$

The two conditions imply that (since sine and cosine functions cannot be zero at the same time) if **A = 0 then B ≠ 0** and **if A ≠ 0 then B = 0** since when  $\sin\left(k \frac{a}{2}\right) = 0$ ,  $\cos\left(k \frac{a}{2}\right) ≠ 0$  and vice versa.

Taking the first condition that  $A = 0$  and  $B ≠ 0$  implies that when

$$\cos\left(k \frac{a}{2}\right) = 0, \quad k \frac{a}{2} = (2N - 1)\frac{\pi}{2} \text{ or } k = (2N - 1)\frac{\pi}{a} n \text{ odd multiple of } \frac{\pi}{a}$$

The second condition  $B = 0$  then  $A ≠ 0$  which implies that

$$\sin\left(k \frac{a}{2}\right) = 0 \text{ or } k \frac{a}{2} = N\pi \text{ or } k = 2N\frac{\pi}{a} \text{ (an even multiple of } \frac{\pi}{a} \text{ )}$$

The above two conditions can be combined and generalized to give the allowed values of the propagation constant (wave number)

$$k = \frac{n\pi}{a} \text{ with } n = 1, 2, 3, \dots$$

The wave function then reduces to

$$\psi(x) = A \cos(kx) \text{ for } n \text{ odd and}$$

$$\psi(x) = A \sin(kx) \text{ for } n \text{ even}$$

The allowed values of k give the allowed states with energy  $E_n = \frac{h^2 n^2}{8ma^2}$

The wave functions can be normalized for the individual states to give the constants A and B.

The constant A can be evaluated by normalizing the wave function ie., integrating the function between limits of  $-\frac{a}{2}$  and  $\frac{a}{2}$   $\int \psi^* \psi dx = 1$

$$\int_{-a/2}^{a/2} \left[ A \sin\left(\frac{n\pi}{a} x\right) \right]^2 dx = \frac{A^2}{2} \int_{-a/2}^{a/2} \left[ 1 - \cos\left(\frac{2n\pi}{a} x\right) \right] dx$$

$$\text{This on integration gives } \frac{A^2}{2} \left[ x - \frac{L}{2n\pi} \sin\left(\frac{2n\pi}{a} x\right) \right]_{-a/2}^{a/2} = \frac{A^2}{2} [a - 0] = 1$$

$$\text{This gives a value of } A = \sqrt{\frac{2}{a}}$$

The exact form of the wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a} x\right) \text{ for } n \text{ odd} \quad (\text{even parity})$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \text{ for } n \text{ even} \quad (\text{odd parity})$$

[Parity of a function is determined by changing the sign of the variable. If the function remains unchanged then it is defined as an even parity functions and if the function changes sign then it is an odd parity function.

If  $\psi(-x) = \psi(x)$  then the function has an even parity and

if  $\psi(-x) = -\psi(x)$  then the function has an odd parity.]

### Eigen functions and Eigen values

Eigen functions are exact wave functions which represent the state of the system completely. Eigen functions are exact solutions of the Schrodinger's wave equation.

The even parity Eigen function of a particle in a infinite potential well  $\psi_n = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right)$  and odd parity Eigen function of a particle in a infinite potential well  $\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$

The first three states correspond to n=1,2 and 3

The Eigen functions are

$$\psi_1 = \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right)$$

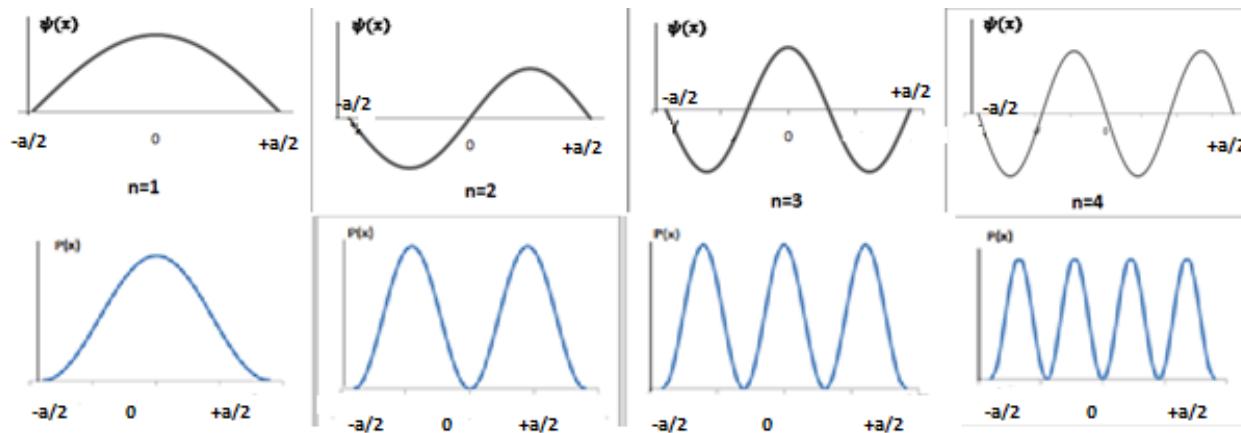
$$\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$$

$$\psi_3 = \sqrt{\frac{2}{a}} \cos\left(\frac{3\pi x}{a}\right)$$

Eigen values of the system are the exact values of the physical parameters of the system obtained from an Eigen function using operators.

The Eigen energy values is given function  $E_n = \frac{\hbar^2 n^2}{8mL^2}$  where n = 1,2 3...

And the Eigen values are  $E_1 = \frac{\hbar^2}{8ma^2}$      $E_2 = \frac{\hbar^2 2^2}{8ma^2}$      $E_3 = \frac{\hbar^2 3^2}{8ma^2}$



Probability density  $\psi^* \psi$  for the first three states is obtained by squaring the corresponding wave functions  $\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$  or  $\psi_n = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right)$ . The square of the function is close to a gaussian shape.

In the first state n=1, the probability of finding the particle is maximum at  $x = 0$  and the area under the curve represents the total probability of finding the particle in the ground state which is 1.00

In the second state n=2, the probability of finding the particle is maximum at  $x = -a/4$  and  $x = +a/4$ . The area under one segment of the curve represents the probability of finding the particle in the first excited state and is  $1/2 = 0.5$ .

In the third state  $n=3$ , the probability of finding the particle is maximum at  $x = -\frac{a}{3}$ ,  $x = 0$  and  $x = +\frac{a}{3}$ . The area under one segment of the curve represents the probability of finding the particle in the first excited state and is  $\frac{1}{3} = 0.333$ .

In general, the probability of finding the particle in the  $n^{\text{th}}$  state, in a segment of length  $a/n$  is  $\frac{1}{n}$ .

The probability of finding the particle between two limits in the well is given by the expression

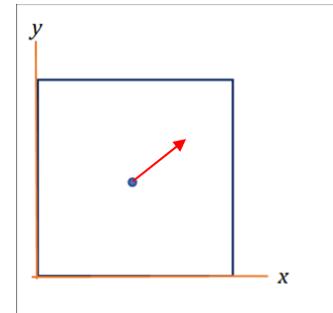
$P = \int_{x_1}^{x_2} \left[ A \cos \left( \frac{n\pi}{a} x \right) \right]^2 dx \text{ or } \int_{x_1}^{x_2} \left[ A \sin \left( \frac{n\pi}{a} x \right) \right]^2 dx$ , depending on whether the state  $n$  is odd or even. Note that this probability will be less than 1 if the limits are not the boundaries of the well.

The Eigen values of the momentum and the  $p_n = \hbar k = n \frac{\hbar}{2a}$

### Particle in a 2D well of infinite potential at the boundaries

A particle in a two dimensional well has two degrees of freedom and can move in XY plane. This can be treated as a case of particle confined in a well with infinite potentials at the boundaries of the x and y directions. The momentum  $\mathbf{P}$  of a particle moving in the x y plane can be resolved into two independent momentum components  $\mathbf{P}_x$  and  $\mathbf{P}_y$  along the x and y directions.

The problem can be analyzed as two independent problems for the x and y directions and the solutions would be similar to the one dimensional infinite potential well problem.



The Schrodinger's equation can be written as  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$

$\frac{\partial^2 \psi}{\partial x^2} + k_x^2 \psi = 0$  where  $k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$  and the solutions to this are

The eigen functions for the x direction

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}} \cos \left( \frac{n_x \pi}{a} x \right) \text{ for } n_x \text{ odd} \quad (\text{even parity})$$

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{n_x \pi}{a} x \right) \text{ for } n_x \text{ even} \quad (\text{odd parity})$$

with the eigen values for energy as  $E_x = \frac{\hbar^2 n_x^2}{8mL^2}$  where  $n_x$  can take values 1,2,3,4,5,....

The particle's movement in the y direction can be analysed similarly.

The Schrodinger's equation can be written as  $\frac{\partial^2 \psi}{\partial y^2} + \frac{2m}{\hbar^2} E \psi = 0$

$\frac{\partial^2 \psi}{\partial y^2} + k_y^2 \psi = 0$  where  $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$  and the solutions to this are

The eigen functions for the y direction

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}} \cos \left( \frac{n_y \pi}{a} y \right) \text{ for } n_y \text{ odd} \quad (\text{even parity})$$

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}} \sin \left( \frac{n_y \pi}{a} y \right) \text{ for } n_y \text{ even} \quad (\text{odd parity})$$

with the eigen values for energy as  $E_y = \frac{\hbar^2 n_y^2}{8mL^2}$  where  $n_y$  can take values 1,2,3,4,5....

The total energy of the system is then  $E_n = E_x + E_y = \frac{\hbar^2 n_x^2}{8mL^2} + \frac{\hbar^2 n_y^2}{8mL^2} = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2)$

The allowed energy states of the particle are then decided by the allowed values of  $n_x$  and  $n_y$ .

The first allowed state is the ground state of the system and given by  $E_{11} = 2 \frac{\hbar^2}{8mL^2} = 2E_0$  where  $E_0 = \frac{\hbar^2}{8mL^2}$ .

The second allowed state of the system is given by  $E_{21} = 5E_0$  which is also the energy of the state  $E_{12}$ . There are two allowed states for the same energy value of  $5E_0$ . This state is then doubly degenerate.

In general, for a 2D system in when  $n_x = n_y$  the energy state is a single state and when  $n_x \neq n_y$  the energy state has a degeneracy factor of 2.

The separation between energy states does not increase monotonically as in the 1D system.

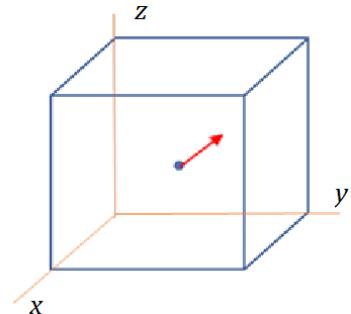
The wave functions of the corresponding states can be written as

$$\psi_{11} = \frac{2}{a} \cos\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \text{ for the first allowed state with } n_x = n_y = 1$$

$$\psi_{21} = \frac{2}{a} \sin\left(\frac{2\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \text{ for the second allowed state with } n_x = 2 \text{ and } n_y = 1$$

$$\psi_{12} = \frac{2}{a} \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}y\right) \text{ for the allowed state with } n_x = 1 \text{ and } n_y = 2$$

From the wave functions we realize that the two states are different but has the energy eigen value of  $5E_0$ . Such states are referred to as degenerate states.



### **Particle in a 3D Box of infinite potential at the boundaries**

A particle in a three dimensional well has three degrees of freedom and can move in 3D space. This can be treated as a case of particle confined in a box of sides L with infinite potentials at the boundaries of the x, y and z directions. The momentum **P** of a particle moving in space can be resolved into three independent momentum components **P<sub>x</sub>**, **P<sub>y</sub>** and **P<sub>z</sub>** along the coordinate axes.

This problem can be analysed as three independent problems for the x, y and z directions and the individual solutions will be similar to the one dimensional infinite potential well problem.

The Schrodinger's equation can be written as  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$

$\frac{\partial^2 \psi}{\partial x^2} + k_x^2 \psi = 0$  where  $k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$  and the solutions to this are

The eigen function for the x directions

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_x \pi}{a} x\right) \text{ for } n_x \text{ odd} \quad (\text{even parity})$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a} x\right) \text{ for } n_x \text{ even} \quad (\text{odd parity})$$

with the eigen values for energy as  $E_x = \frac{\hbar^2 n_x^2}{8mL^2}$  where  $n_x$  can take values 1,2,3,4,5....

The particle's movement in the y direction can be analysed.

The Schrodinger's equation can be written as  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$

$\frac{\partial^2 \psi}{\partial y^2} + k_y^2 \psi = 0$  where  $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$  and the solutions to this are

The eigen function for the y directions

$$\psi_n(y) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_y \pi}{a} y\right) \text{ for } n_y \text{ odd} \quad (\text{even parity})$$

$$\psi_n(y) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_y \pi}{a} y\right) \text{ for } n_y \text{ even} \quad (\text{odd parity})$$

with the eigen values for energy as  $E_y = \frac{\hbar^2 n_y^2}{8mL^2}$  where  $n_y$  can take values 1,2,3,4,5....

The particle's movement in the z direction can be analysed.

The Schrodinger's equation can be written as  $\frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} E \psi = 0$

$\frac{\partial^2 \psi}{\partial z^2} + k_z^2 \psi = 0$  where  $k_z = \sqrt{\frac{2mE_z}{\hbar^2}}$  and the solutions to this are

The eigen functions for the z direction

$$\psi_n(z) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_z \pi}{a} z\right) \text{ for } n_z \text{ odd} \quad (\text{even parity})$$

$$\psi_n(z) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_z \pi}{a} z\right) \text{ for } n_z \text{ even} \quad (\text{odd parity})$$

with the eigen values for energy as  $E_z = \frac{\hbar^2 n_z^2}{8ma^2}$  where  $n_z$  can take values 1,2,3,4,5....

The total energy of the system is then

$$E_n = E_x + E_y + E_z = \frac{\hbar^2 n_x^2}{8ma^2} + \frac{\hbar^2 n_y^2}{8ma^2} + \frac{\hbar^2 n_z^2}{8ma^2} = \frac{\hbar^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

The allowed energy states of the particle are then decided by the allowed values of  $n_x$ ,  $n_y$  and  $n_z$ .

The first allowed state is the ground state of the system and has an energy

$$E_{111} = 3 \frac{\hbar^2}{8ma^2} = 3E_o \text{ where } E_o = \frac{\hbar^2}{8ma^2}.$$

The second allowed state of the system is given by  $E_{211} = 6E_o$  which is also the energy of the state  $E_{121}$  and  $E_{123}$ . There are three allowed states for the same energy value of  $6E_o$ . This state is then triply degenerate.

The analysis of the first few states reveal that the states are non degenerate when  $n_x = n_y = n_z$ . The states have a degeneracy factor of 3 whenever two of the numbers  $n_x$ ,  $n_y$  and  $n_z$  are equal and not equal to the third.

When all the three numbers  $n_x, n_y$  and  $n_z$  are unequal then the energy state would have a degeneracy of 6.

Further the separation between energy states does not increase monotonically as in the 1D system.

The wave functions of the corresponding states can be written as

for the first allowed state with  $n_x = 1, n_y = 1$  and  $n_z = 1$

$$\psi_{111} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

the second allowed state with  $n_x = 2, n_y = 1$  and  $n_z = 1$

$$\psi_{211} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \sin\left(\frac{2\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

the allowed state with  $n_x = 1, n_y = 2$  and  $n_z = 1$

$$\psi_{121} = \frac{2}{a} \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

for the allowed state with  $n_x = 1, n_y = 1$  and  $n_z = 2$

$$\psi_{112} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}y\right) \sin\left(\frac{n_z\pi}{a}z\right)$$

From the wave functions we realize that the three states are different but has the energy Eigen value of  $6E_0$ .

### Problem no. 5 - Finite potential well

The finite potential well is a closer approximation to real potentials in solids. The particle can be confined to a region with constant potential  $V_0$  at the walls  $|x| > \frac{L}{2}$ . Inside the potential well region of  $-L/2$  to  $+L/2$  the potential is zero. In this case the SWE for the three regions can be solved to get the nature of the wave functions.

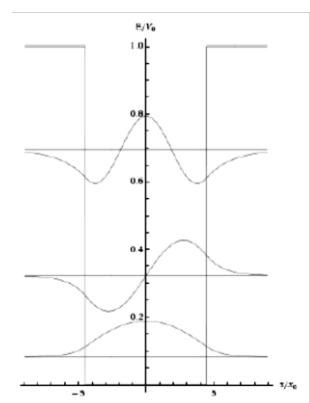
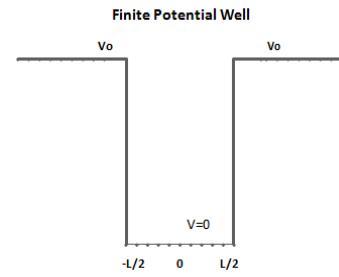
However, these do not result in an exact solution and approximation methods are used. The nature of the wave functions in the three regions can be written as

$$\psi_1 = De^{\alpha x} \text{ where } \alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \text{ for the region } x < -L/2$$

$$\psi_2 \cong A \cos(k_2 x) \text{ for odd values of } n \quad \text{or}$$

$$\psi_2 = A \sin(k_2 x) \text{ for even values of } n \quad \text{where } k_2 = \sqrt{\frac{2mE}{\hbar^2}} \text{ for the region } -L/2 < x < L/2$$

The cosine solutions show even parity (symmetric when sign of the function becomes negative) and the sine solutions exhibit odd parity (anti symmetric when sign of the function becomes negative). However, it is to be noted that the wave function  $\psi_2$  would not be zero at the boundaries of  $-\frac{L}{2}$  and  $+\frac{L}{2}$ .



$$\psi_3 = Ge^{-\alpha x} \text{ where } \alpha = \sqrt{\frac{2m(V_o - E)}{\hbar^2}} \text{ for the region } x > L/2$$

The continuity of the wave functions and their derivatives at the boundaries  $-\frac{L}{2}$  and  $+\frac{L}{2}$  gives the conditions

$$\alpha = k \tan(k \frac{L}{2}) \text{ or } \sqrt{(V_o - E)} = \sqrt{E} \tan\left(\sqrt{\frac{2mE}{\hbar^2}} * \frac{L}{2}\right) \text{ for}$$

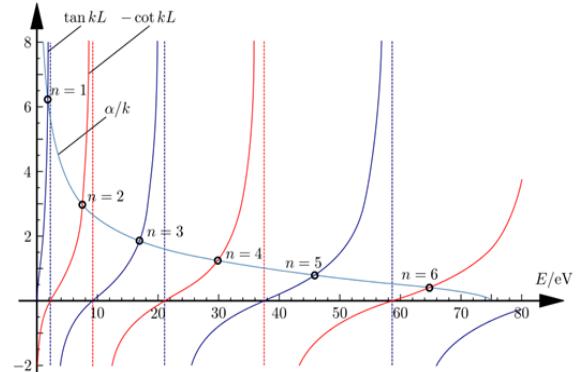
$n=1$

and

$$\alpha = -k \cot(k \frac{L}{2}) \text{ or } \sqrt{(V_o - E)} = -\sqrt{E} \cot\left(\sqrt{\frac{2mE}{\hbar^2}} * \frac{L}{2}\right)$$

for  $n=2$

It can be seen that the right-hand side and left-hand side of the equations contain the same variable  $E$  and the nature of variations of the functions on either sides are quite different and hence an exact solution do not exist. (Equations of this type are called transcendental equations.)



The energy values of the particle inside the well region can be found from graphical or approximate methods. The variation of the left-hand side and the right-hand side could be plotted on the same graph as a function. The points of intersection of the LHS and RHS plots are the solutions as the values of  $E$  satisfy both the equations.

Thus, the different energy states could be evaluated.

Since the particle is in the finite potential well, at least one solution to the problem exists. Or one energy state exists for the particle in the finite potential well. The number of solutions would obviously depend on the height of the finite potential  $V_o$ .

From the expression for the energy of an infinite potential well we can write the energy of the particle in a finite potential well as

$$E_{infinite} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} = \frac{\hbar^2 n^2}{2m(\text{width of the well where } \psi \rightarrow 0)^2}$$

In the case of the finite potential well we can define the effective width of the well as the points where the wave function becomes insignificant. Thus, the effective width of the well is the width of the well plus twice the penetration depth of the particle in that energy state. The penetration depths in the regions of the potential  $V_o$  is given by  $\Delta x = \frac{h}{\sqrt{2m(V_o - E_x)}}$  which is a function of  $E_x$ .

The effective width of the box (defined approx as the points at the wave function becomes insignificant of zero) is then larger and can be approximated as  $L + 2\Delta x$

In the case of the finite potential well the energy of the particle can be written as

$$E_{finite} = \frac{\hbar^2 \pi^2 n^2}{2m(\text{width of the well where } \psi \rightarrow 0)^2} = \frac{\hbar^2 \pi^2 n^2}{2m(L + 2\Delta x)^2}$$

Hence the energy values are less than the energy values for the corresponding states of an infinite potential well of the width  $L$ .

### Problem no. 6 - Harmonic Oscillator

Harmonic oscillator is one of the most fundamental systems in quantum mechanics which gives insight to a variety of problems such as the vibrational molecular spectroscopy.

The classical harmonic oscillator is a bound particle subjected to oscillations about a mean position. However, a restoring force that is proportional to the displacement of the particle from a mean position keeps the amplitude of the oscillations within limits. The force equation of such a system in classical physics is  $\mathbf{F} = \mathbf{ma} = m \frac{d^2\mathbf{x}}{dt^2} = -k\mathbf{x}$  where  $k$  is the force constant given by

$m\omega^2$  where  $\omega = \sqrt{\frac{k}{m}}$  is the frequency of vibration and  $m$  is the mass of the system.

The potential energy of the system is evaluated as

$$V = - \int \mathbf{F} dx = \int kx dx = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2.$$

Consider a diatomic molecule with the masses of the atoms as  $m_1$  and  $m_2$  bound by a bond that is springy in nature. This can be studied as a spring mass system with spring constant (which basically depend on the bond strength). In this case the effective mass  $\mu$  of the system will decide the frequency of oscillations  $\omega = \sqrt{\frac{k}{\mu}}$  and the potential energy of the system can be written as  $V(x) = \frac{1}{2} \mu\omega^2 x^2$ .

Using this form of the potential in the Hamiltonian  $H\Psi$  we get

$$-\frac{\hbar^2}{2\mu} \frac{d^2\Psi(x)}{dx^2} + V\Psi(x) = -\frac{\hbar^2}{2\mu} \frac{d^2\Psi(x)}{dx^2} + \frac{1}{2} \mu\omega^2 x^2 = E\Psi(x)$$

The Schrodinger wave equation can be written as

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2\mu}{\hbar^2} \left( E - \frac{1}{2} \mu\omega^2 x^2 \right) \Psi(x) = 0$$

Notice the term  $E - \frac{1}{2} \mu\omega^2 x^2$  is positive since  $V(x)$  cannot increase infinitely.

A solution to this can be attempted by substituting  $\xi = \gamma x$  ( $\xi$  is pronounced as zai) and  $\gamma = \sqrt{\frac{\mu\omega}{\hbar^2}}$

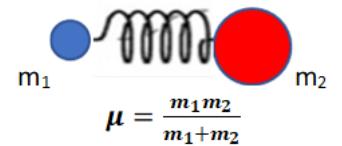
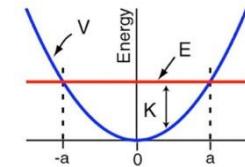
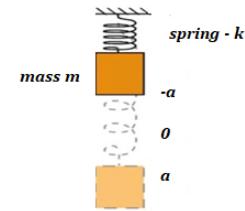
The eigen function is of the form  $\Psi_n(x) = N_n H_n(\gamma x) e^{-\frac{1}{2}(\gamma x)^2}$

where  $n=0,1,2,3,4\dots$   $N_n = \sqrt{\left[ \frac{\gamma}{2^n n! \sqrt{\pi}} \right]}$  and

$H_n(\xi)$  are the Hermite polynomials described by

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi) \text{ for } n \geq 1$$

The first two terms of the Hermite polynomial are  $H_0(\xi) = 1$  and  $H_1(\xi) = 2\xi$  which can be used to find the successive terms.



$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\psi_0(x) = N_0 H_0(\xi) e^{-\frac{1}{2}\xi^2} = \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2}$$

$$\psi_1(x) = N_1 H_1(\xi) e^{-\frac{1}{2}\xi^2} = \sqrt{\frac{2}{\sqrt{\pi}}} \cdot \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{3}{4}} \cdot x \cdot e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2}$$

The solutions yield the Eigen energy values of the system as

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

This gives the allowed energy states as  $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \dots \dots$

Thus, the minimum energy state of the system is a non-zero  $= \frac{1}{2}\hbar\omega$  where  $\omega$  is the fundamental frequency of vibration. The higher energy states are then equally spaced at  $\hbar\omega$  which is unlike the energy of states in the particle in a box solution.

[To verify that the wave functions are solutions of the SWE, we can substitute  $\psi_0(x)$  and the corresponding energy  $E_0 = \left(\frac{1}{2}\right)\hbar\omega$  in the Schrodinger's wave equation.

$$\frac{d}{dx}\{\psi_0(x)\} = \frac{d}{dx} \left\{ \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2} \right\} = \left\{ -\left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} \cdot \frac{\mu\omega}{\hbar} x e^{-\frac{1}{2}\frac{\mu\omega}{\hbar}x^2} \right\} = -\frac{\mu\omega}{\hbar} x \psi_0(x)$$

Differentiating once again  $\frac{d}{dx} \left[ -\frac{\mu\omega}{\hbar} x \psi_0(x) \right] = -\left(\frac{\mu\omega}{\pi\hbar}\right) \left\{ \psi_0(x) - \frac{\mu\omega}{\hbar} x^2 \psi_0(x) \right\}$

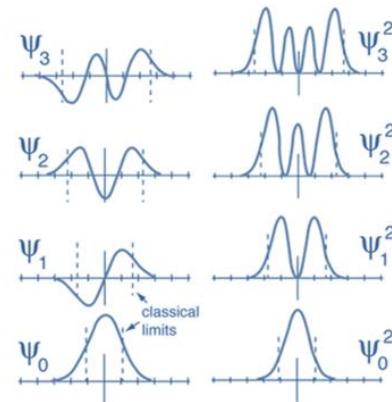
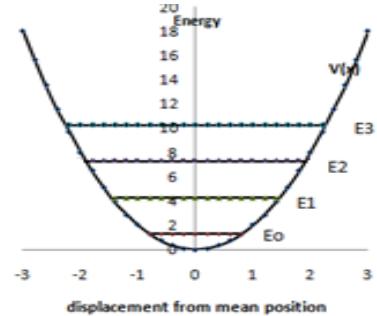
Substituting this in the SWE gives

$$\begin{aligned} & -\left(\frac{\mu\omega}{\hbar}\right) \left\{ \psi_0(x) - \frac{\mu\omega}{\hbar} x^2 \psi_0(x) \right\} + \frac{2\mu}{\hbar^2} \left( \left(\frac{1}{2}\right)\hbar\omega - \frac{1}{2}\mu\omega^2 x^2 \right) \psi_0(x) = \\ & -\left(\frac{\mu\omega}{\hbar}\right) \psi_0(x) + \left(\frac{\mu\omega}{\hbar}\right)^2 x^2 \psi_0(x) + \frac{2\mu}{\hbar^2} \left(\frac{1}{2}\right)\hbar\omega - \frac{2\mu}{\hbar^2} \frac{1}{2} \mu\omega^2 x^2 \psi_0(x) = 0 \end{aligned}$$

Thus, we note that  $\psi_0(x)$  satisfies the SWE and hence is an eigen function of the system

Similarly, verify that  $\psi_1(x)$  also satisfies the SWE with the corresponding energy  $E_1 = \left(\frac{3}{2}\right)\hbar\omega.$

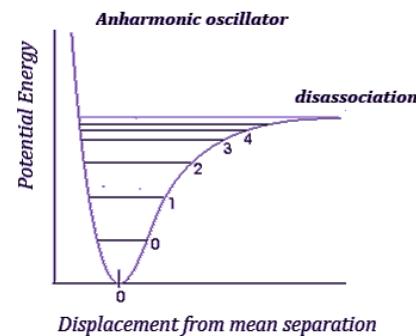
The wave functions of the system can be graphically inferred by considering each of the states to be equivalent to a one-dimensional finite potential well. The width of the well corresponds to the maximum displacement in that state. Therefore, the wave functions of the finite potential well that we inferred are useful even in this case. However, each state has an increasing width and the tails of the decaying wave functions also increase as the energy of the state increases. The probability distribution functions for the first few states are also shown in the figure.



The real potential energy variations deviate from the ideal parabolic potential energy curve. The bonding results in exchange of electrons / sharing of electrons resulting in a deviation of the electrostatic interactions. The deviation is treated as a perturbation of the harmonic oscillator potential with an addition term for the potential.

The result of this variation results in energy levels which are not uniformly distributed and the separation between the energy levels decrease for larger values of  $n$ .

This analysis helps us understand the vibration energy states of a diatomic molecule and forms the fundamental analysis of the Infra Red absorption by the molecular. This analysis can be extended to understand the vibrational states of lattices in a crystal which leads to the concept of phonons in crystals.



### Problem 7: Discussion of the solutions to the Hydrogen atom problem.

The hydrogen atom is the simplest possible stable atom with one proton in the nucleus and one electron in the orbital. In the ground state, the system exhibits perfect spherical symmetry. Hence the possibility of looking for a solution to the Schrodinger's wave equation for the states of the electron could be attempted. Though the problem looks very simple as a case of only two particles, the mathematical analysis of the solutions is very exhaustive.

The methodology and the solutions are discussed to present a picture of how the quantum numbers of a system evolves out naturally from the solution of the differential equation in three dimensions.

The 3D SWE in cartesian co-ordinate system can be written as

$$\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(x, y, z) + (E - V) \Psi(x, y, z) = 0$$

Since the hydrogen atom exhibits a spherical symmetry it is prudent to write the Schrodinger's wave equation in the spherical co-ordinate system ( $r, \theta, \varphi$ ).

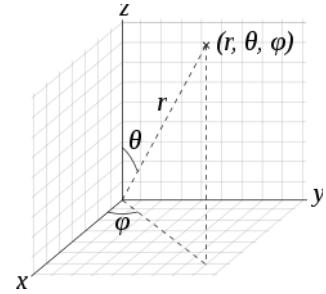
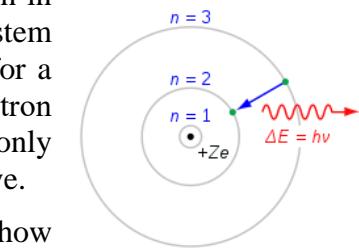
[ the transition to the spherical coordinate system from the cartesian coordinate system is possible with the transition relations

$$x = r \sin \theta \cos \varphi, y = r \sin \theta \sin \varphi \text{ and } z = r \cos \theta$$

where  $r = \sqrt{x^2 + y^2 + z^2}$  is the radius vector

$\theta = \tan^{-1} \left( \frac{\sqrt{x^2+y^2}}{z} \right)$  is the polar angle (varying between 0 to  $2\pi$  and

$\varphi = \tan^{-1} \left( \frac{y}{x} \right)$ ] is the azimuthal angle (varying between 0 to  $2\pi$  ]



In spherical polar co-ordinate system, the SWE can be written as

$$\frac{\hbar^2}{2\mu r^2 \sin \theta} \left[ \sin \theta \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Psi}{\partial \varphi^2} \right] + (E - V(r)) \Psi(r, \theta, \varphi) = 0$$

where the wave function in spherical polar co-ordinates is  $\Psi(r, \theta, \varphi)$ .

$$\text{The potential energy term can be written as } V(r) = \frac{e^2}{4\pi\epsilon_0 r}$$

The wave function can be resolved into three independent components in the three independent variables  $r, \theta$  and  $\varphi$ .

$$\Psi(r, \theta, \varphi) = R(r) \cdot \Theta(\theta) \cdot \Phi(\varphi)$$

The Schrodinger's wave equation can be resolved into three mutually independent equations using the method of separation of variables as

$\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \varphi^2} = -m_l^2$  with the solution  $\Phi(\varphi) = A e^{im_l \varphi}$  where  $m_l = 0, \pm 1, \pm 2, \dots$  is the magnetic quantum number (which gives the possible orientations of the quantized angular momentum of the system).

Substituting for the expression  $\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \varphi^2}$  we can separate the expressions in  $R$  and  $\Theta$  as

$$\frac{m_l^2}{\sin^2 \theta} - \frac{1}{\theta \sin \theta} \left[ \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) \right] = l(l+1)$$

where  $l$  is an arbitrary constant which an integer greater than or equal to  $m_l$ . This puts a restriction on  $m_l = 0, \pm 1, \pm 2, \dots, \pm l$

In general,  $l = 0, 1, 2, 3, \dots, n-1$  is the angular momentum quantum number which describes the quantized angular momentum of the orbital electron as  $\mathbf{L} = \sqrt{l(l+1)} \cdot \hbar$

The radial part of the wave equation

$$\frac{1}{R} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \right] + \frac{2\mu r^2}{\hbar^2} [E - V(r)] = l(l+1)$$

We observe that the energy of the system is dependent only on the solution of this equation which gives the radial component of the wave function as

$$R_{nl(r)} = \frac{1}{r} \rho^{l+1} e^{-\rho} \cdot v(\rho)$$

The variable  $\rho = \frac{r}{an}$  where  $n$  is an integer  $n = 1, 2, 3, \dots$  and  $a \equiv \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} = 0.529 \times 10^{-10} m$  is the Bohr radius.

$v(\rho)$  is a polynomial of degree  $j_{max} = n - l - 1$  given by  $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$

whose co-efficient are given by the recursion formula  $c_{j+1} = \left\{ \frac{2(j+l+1)-\rho_o}{(j+1)(j+2l+2)} \right\} c_j$  and  $\rho_o = 2n$

The normalized radial wave function  $R_{nl(r)} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^l$

where  $n$  is the principal quantum number defined by  $n = 1, 2, 3, \dots$

The first few radial wave functions can be written as

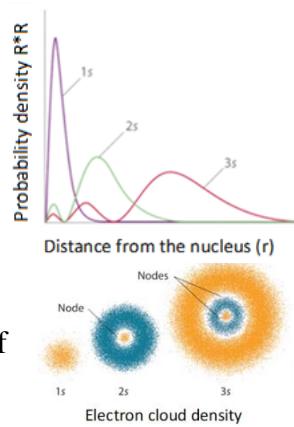
$$R_{10}(r) = 2a^{-3/2} e^{-r/a} \text{ for } n=1 \text{ and } l=0$$

$$R_{20}(r) = \frac{1}{\sqrt{2}} a^{-3/2} \left( 1 - \frac{1}{2} \frac{r}{a} \right) e^{-r/2a} \text{ for } n=2 \text{ and } l=0$$

$$R_{21}(r) = \frac{1}{\sqrt{24}} a^{-3/2} \left( \frac{r}{a} \right) e^{-r/2a} \text{ for } n=2 \text{ and } l=1$$

These wave functions can be shown to be solutions of the radial wave equation. Then by induction we conclude that the radial wave function is a solution of the radial part of the SWE.

The probability of finding the electron at a distance  $r$  from the nucleus can be estimated using the probability density. The plot shows the probability of locating the electron in the three states 1s, 2s and 3s.



The eigen energy simplifies to  $E_n = -\frac{\hbar^2 k^2}{2\mu} = -\frac{\mu e^4}{8\pi^2 \epsilon_0^2 \hbar^2 \rho_o^2} = -\frac{\mu e^4}{8\pi^2 \epsilon_0^2 \hbar^2 \cdot 4n^2}$

$$E_n = - \left[ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2} = - \left[ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2} \quad \text{where } n=1,2,3, \dots$$

The energy is written as negative to indicate that the system is in a bound state. This implies that when the energy of the system goes to zero the binding between the particles is broken and the particles are free particles. This happens for a large value of  $n \rightarrow \infty$

The ground state energy of the system can be evaluated as  $E_1 = - \left[ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] = -13.6 \text{ eV}$

The different allowed energy states correspond to the different values of  $n$ . This enables to estimate the energy of transition between different states, which gives us the absorption or emission spectra of the atom.

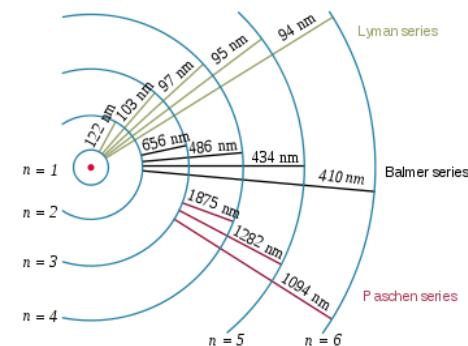
The energy difference between two states can be evaluated as

$$\Delta E = E_{n1} - E_{n2} = - \left[ \left\{ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right\} \frac{1}{n_1^2} - \left\{ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right\} \frac{1}{n_2^2} \right]$$

The transitions from states with  $n > 1$  to  $n = 1$  result in spectral lines in the ultraviolet region which is the Lyman series.

The transitions from states with  $n > 2$  to  $n = 2$  result in spectral lines in the visible region which is the Balmer series.

The transitions from states with  $n > 3$  to  $n = 3$  result in spectral lines in the infra red region which is the Paschen series.



The predicted values of the wavelengths of the spectral lines of the Hydrogen atom ( $\Delta E = \frac{hc}{\lambda}$ ) agree with the observed wavelengths in the emission spectra of the Hydrogen atom.

The same analysis can be used to study hydrogen like atoms with a single electron in the outer most orbital such as Deuterium, doubly ionized Lithium, etc. The effective mass  $\mu$  can be estimated and gives reasonably correct values of the energy of the states and hence their spectral characteristics.

### [ Verification of the eigen functions of the radial equation:

The radial part of the wave equation

$$\left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \right] + \frac{2\mu r^2}{\hbar^2} [E - V(r)] R = l(l+1) R$$

For the state  $n=2, l=0$  the radial equation  $R_{20}(r) = \frac{1}{\sqrt{2}} a^{-3/2} \left( 1 - \frac{1}{2} \frac{r}{a} \right) e^{-r/2a}$

The radial wave equation  $\left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial R_{20}}{\partial r} \right) + \right] + \frac{2\mu r^2}{\hbar^2} [E - V(r)] R_{20} = 0$

The energy  $E_2 = - \left[ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{2^2}$  and the potential  $V(r) = \frac{e^2}{4\pi\epsilon_0 r}$

The first term of the Radial wave equation:

Differentiating  $\mathbf{R}_{20}$  with respect to  $r$  once

$$\frac{\partial \mathbf{R}_{20}}{\partial r} = \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{1}{2a} e^{-r/2a} - \frac{1}{2a} e^{-r/2a} + \frac{r}{(2a)^2} e^{-r/2a} \right) = \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{1}{a} e^{-r/2a} + \frac{r}{(2a)^2} e^{-r/2a} \right)$$

Multiplying the result with  $r^2$        $r^2 \frac{\partial \mathbf{R}_{20}}{\partial r} = \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{r^2}{a} e^{-r/2a} + \frac{r^3}{(2a)^2} e^{-r/2a} \right)$

Differentiating the result once again with respect to  $r$

$$\begin{aligned} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \mathbf{R}_{20}}{\partial r} \right) &= \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{2r}{a} e^{-r/2a} - \frac{r^2}{a} e^{-r/2a} \times \left( -\frac{1}{2a} \right) + \frac{3r^2}{(2a)^2} e^{-r/2a} + \frac{r^3}{(2a)^2} e^{-r/2a} \times \left( -\frac{1}{2a} \right) \right) \\ &= \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{2r}{a} e^{-r/2a} + \frac{2r^2}{(2a)^2} e^{-r/2a} + \frac{3r^2}{(2a)^2} e^{-r/2a} - \frac{r^3}{(2a)^3} e^{-r/2a} \right) \\ \frac{\partial}{\partial r} \left( r^2 \frac{\partial \mathbf{R}_{20}}{\partial r} \right) &= \frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{2r}{a} e^{-r/2a} + \frac{5r^2}{(2a)^2} e^{-r/2a} - \frac{r^3}{(2a)^3} e^{-r/2a} \right) \end{aligned}$$

Evaluating the second term, substituting for  $E_2$  &  $V(r)$  and simplifying

$$\begin{aligned} \frac{2\mu r^2}{\hbar^2} [E_2 - V(r)] &= \left[ -\frac{2\mu r^2}{\hbar^2} \left[ \frac{\mu}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{2^2} - \frac{2\mu r^2}{\hbar^2} \frac{e^2}{4\pi\epsilon_0 r} \right] = \left[ -\frac{r^2}{(2a)^2} + \frac{2r}{a} \right] \\ \frac{2\mu r^2}{\hbar^2} [E_2 - V(r)] \mathbf{R}_{20} &= \left[ -\frac{2r^2}{(2a)^2} + \frac{2r}{a} \right] \times \frac{1}{\sqrt{2}} a^{-3/2} \left( 1 - \frac{1}{2} \frac{r}{a} \right) e^{-r/2a} \\ &= \frac{1}{\sqrt{2}} a^{-3/2} \left( 1 - \frac{1}{2} \frac{r}{a} \right) \left[ -\frac{2r^2}{(2a)^2} + \frac{2r}{a} \right] e^{-r/2a} \\ &= \frac{1}{\sqrt{2}} a^{-3/2} \left[ -\frac{r^2}{(2a)^2} + \frac{2r}{a} + \frac{r^3}{(2a)^3} - \frac{2r^2}{2a^2} \right] e^{-r/2a} \\ &= \frac{1}{\sqrt{2}} a^{-3/2} \left[ \frac{r^3}{(2a)^3} - \frac{5r^2}{(2a)^2} + \frac{2r}{a} + \right] e^{-r/2a} \end{aligned}$$

The sum of the two terms

$$\frac{1}{\sqrt{2}} a^{-3/2} \left( -\frac{2r}{a} e^{-r/2a} + \frac{5r^2}{(2a)^2} e^{-r/2a} - \frac{r^3}{(2a)^3} e^{-r/2a} \right) + \frac{1}{\sqrt{2}} a^{-3/2} \left[ \frac{r^3}{(2a)^3} - \frac{5r^2}{(2a)^2} + \frac{2r}{a} + \right] e^{-r/2a} = 0$$

Thus,  $\mathbf{R}_{20}$  is a solution of the radial wave equation. It can be verified similarly for wave functions of any state. ]

***Additional inputs for conceptual understanding.***

**[ Particle in a Box with infinite potentials at the walls (boundaries at  $x=0$  to  $x=L$ )**

A particle in an one dimensional box is confined to be within the boundaries ( $x=0$  and  $x=L$ ) where the potential tends to infinity. The particle cannot be found outside the boundary  $x < 0$  and  $x > L$ . The potential inside the well  $V=0$ .

The Schrödinger's wave equation  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$

in the region within the well  $V=0$  this becomes  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

The solution of the equation in region  $0 < x < L$  is given by

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

Applying the boundary condition that  $\psi = 0$  at  $x = 0$  and  $x = L$

At  $x=0$   $\psi(x = 0) = A \sin(k0) + B \cos(k0) = 0$  gives  $B = 0$

The wave function then reduces to  $\psi(x) = A \sin(kx)$

At  $x=L$   $\psi(L) = A \sin(kL) = 0$ .

If  $A=0$  the wave function does not exist and hence  $kL = n\pi$

Or  $k = n \cdot \frac{\pi}{L}$ , thus propagation constant can be only multiples of  $\frac{\pi}{L}$

This also gives us the energy  $E_n = \frac{\hbar^2 n^2}{8mL^2}$

The wave function then reduces to  $\psi(x) = A \sin\left(\frac{n\pi}{L} x\right)$

The constant  $A$  can be evaluated by normalizing the wave function ie.,  $\int_0^L \psi^* \psi dx = 1$

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

$$\text{Which on integration gives } \frac{A^2}{2} \left[ 1 - \frac{L}{2n\pi} \sin\left(\frac{2n\pi}{L} x\right) \right]_0^L = \frac{A^2}{2} [L - 0] = 1 .$$

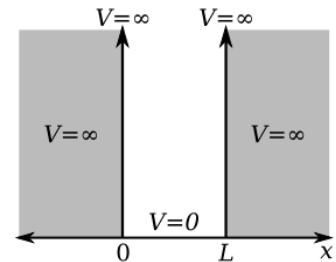
$$\text{This gives a value of } A = \sqrt{\frac{2}{L}}$$

$$\text{The exact form of the wave function becomes } \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$$

**Eigen functions and Eigen values**

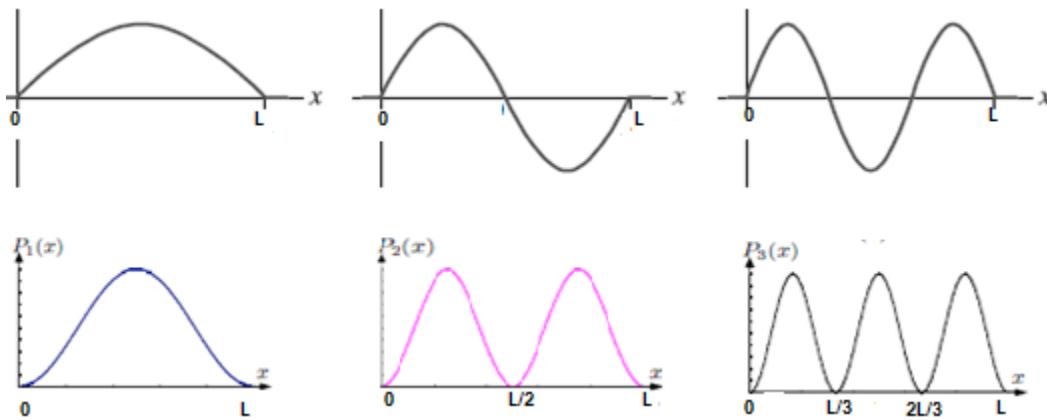
The Eigen function of a particle in a infinite potential well  $\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$  and the Eigen energy values is given function  $E_n = \frac{\hbar^2 n^2}{8mL^2}$  where  $n = 1, 2, 3, \dots$

The first three states correspond to  $n=1, 2$  and  $3$



The Eigen functions are  $\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$     $\psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$     $\psi_3 = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$

And the Eigen values are  $E_1 = \frac{\hbar^2}{8mL^2}$     $E_2 = \frac{\hbar^2 2^2}{8mL^2}$     $E_3 = \frac{\hbar^2 3^2}{8mL^2}$



Probability density  $\psi^* \psi$  for the first three states is obtained by squaring the wave function

$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ . The square of the function is close to a Gaussian shape.

In the first state  $n=1$  the probability of finding the particle is maximum at  $L/2$  and the area under the curve represents the total probability of finding the particle in the ground state which is 1.00

In the second state  $n=2$  the probability of finding the particle is maximum at  $L/4$  and  $3L/4$ . The area under one segment of the curve represents the probability of finding the particle in the first excited state and is  $1/n = 0.5$ .

In the third state  $n=3$  the probability of finding the particle is maximum at  $L/6$ ,  $L/3$  and  $+5L/6$ . The area under one segment of the curve represents the probability of finding the particle in the first excited state and is  $1/n = 0.333$ .

In general, the probability of finding the particle in the  $n^{\text{th}}$  state, in a segment of length  $L/n$  is  $1/n$ . ]

### Concept of Fermions, Fermi Dirac Statics

One of the factors which is used in classification of fundamental particles is the concept of the spin of the particle. The spin is a measure of the intrinsic angular momentum possessed by a particle. According to quantum mechanics all particles with a **spin  $\pm\frac{1}{2}$**  or **odd integral multiples of  $\pm\frac{1}{2}$**  are classified as Fermions and all particles with integral or zero spin are classified as Bosons.

Fermions include electrons, protons, neutrons. Electrons which are Fermions form the fundamental idea of the development of the periodic table. The fermionic nature of electrons in a metal is responsible for the behavior of electrons in a metal.

In any given system with a collection of electrons (which are identical and indistinguishable particles) there is a distribution of the electrons in available energy states following Pauli's Exclusion Principle. At very low temperatures all the available electrons are arranged in discrete energy states and the highest occupied electron state is referred to as the **Fermi Energy** of the system.

### Fermi Dirac statistics, Fermi factor

The occupation probabilities of the different energy states with fermions at different temperatures are estimated using the Fermi Dirac statistics.

The Fermi factor gives the probability of an energy state  $E$  either above or below the Fermi energy  $E_f$  of the system to be occupied at a temperature  $T$  and is expressed as

$$F_d = \frac{1}{\left( e^{\left( \frac{E-E_f}{k_B T} \right)} + 1 \right)}$$

Estimation of the Fermi factor at  $T=0K$  gives distinct results for  $E < E_f$  and  $E > E_f$ .

- If  $E < E_f$  then for  $E - E_f$  is negative, then the Fermi factor  $F_d = \frac{1}{\left( e^{-\left( \frac{\Delta E}{k_B T} \right)} + 1 \right)}$ .

At 0K this becomes  $F_d = \frac{1}{\left( e^{-\infty} + 1 \right)} = 1$ . This implies that at 0K all electron states below the Fermi level are filled states.

- If  $E > E_f$  then for  $E - E_f$  is positive, then the Fermi factor  $F_d = \frac{1}{\left( e^{\left( \frac{\Delta E}{k_B T} \right)} + 1 \right)}$ .

At 0K this becomes  $F_d = \frac{1}{\left( e^{\infty} + 1 \right)} = 0$ . This implies that at 0K all electron states above the Fermi level are empty states.

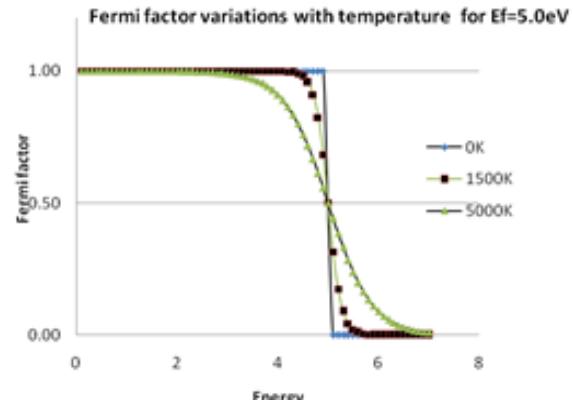
- For  $T > 0$  and  $E = E_f$  the Fermi factor  $F_d = \frac{1}{\left( e^{\left( \frac{E-E_f}{k_B T} \right)} + 1 \right)} = \frac{1}{e^0 + 1} = \frac{1}{2} = 0.5$ . This gives a

probability of occupation of 50% for the Fermi energy.

The variation of the fermi factor with energy for different temperatures can be graphically represented as shown:

At 0 K, the fermi factor has the maximum value of one up to the fermi energy and beyond that  $F_d$  is consistently zero.

At higher temperatures, the fermi factor is a constant one up to approximately  $E_f - kT$  and decreases from 1 to 0.5 at  $E_f$ . Beyond  $E_f$ ,  $F_d$  decreases to zero approx. at  $E_f + kT$ .



The Fermi energy has a weak temperature dependence and is given by

$$E_f = E_{f0} \left[ 1 - \frac{\pi^2}{12} \left( \frac{k_B T}{E_{f0}} \right)^2 \right]$$

where  $E_{f0}$  is the Fermi energy at zero Kelvin. At normal temperature ranges the ratio of  $\frac{k_B T}{E_{f0}}$  is very low and hence can be approximated to be a constant equal to the value at zero Kelvin.

### Fermi temperature

The arrangement of electrons in discrete energy states leads to the concept that only electrons near the Fermi energy are excited into the states above  $E_f$  (referred to as the conduction states for free electrons in a metal and it may be really difficult to excite all the valence electrons into the conduction states). If the temperature of the metal is  $T$  then  $k_B T$  is the thermal energy available to the electrons in the metal. The thermal energy required to excite the last electron at the bottom of the energy band if termed as  $k_B T_f$ , then at temperature  $T_f$  the electron would have an energy  $E_f = k_B T_f$ . This temperature is termed as the Fermi temperature of electrons in the metal.

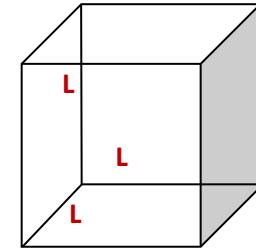
### Fermi velocity

From the above analysis only a small fraction of electrons close to the Fermi energy can be taking part in the conduction processes. The electrons excited into the conduction states have energies very close to the Fermi energy. These conduction electrons then possess a kinetic energy which may be equal to Fermi energy.

The kinetic energy of the electrons near the Fermi energy is  $E_f = \frac{1}{2}mv_f^2$  where  $v_f$  the Fermi velocity of conduction electrons is  $v_f = \sqrt{\frac{2E_f}{m}}$ .

### Density of states derivation

The electrons in a metal can be approximated to the particle in a box in three dimensions, since under normal conditions the electrons cannot escape the boundaries of the metal. Consider a mono-valent metal in the form of a cube of side  $L$ . Inside the metal the electrons can be assumed to be moving in a zero potential field.



The three-dimensional Schrödinger's wave equation can be written as three one dimensional Schrödinger's wave equation and their corresponding solutions analyzed.

The  $x$  component of the particle motion can be described by the wave function which is the solution of the SWE

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) = 0$$

This gives the Eigen energy value for the  $x$  component as  $E_{n_x} = \frac{\hbar^2 n_x^2}{8mL^2}$

Similarly, the energy in the other two dimensions can be evaluated as  $E_{n_y} = \frac{\hbar^2 n_y^2}{8mL^2}$  and  $E_{n_z} = \frac{\hbar^2 n_z^2}{8mL^2}$

The total energy of the electron can be written as

$$E_n = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\hbar^2}{8mL^2} R^2 \quad \text{----- (1) where } R^2 = n_x^2 + n_y^2 + n_z^2$$

The number of states with energy  $E$  can be evaluated by studying the variation of the combinations of  $n_x$ ,  $n_y$  and  $n_z$ . It can be deduced that every combination of  $n_x$ ,  $n_y$  and  $n_z$  result in an energy state as per equation (1).

(The  $n$  space corresponds to the momentum space since  $k = n \frac{\pi}{L}$ . Thus the combinations can give the picture of particles moving in different directions.) When  $n_x$ ,  $n_y$  and  $n_z$  are equal the energy state is unique and is nondegenerate. It is also noted that the energy states can be degenerate with degeneracy of 3 when two of the three  $n_x$ ,  $n_y$  and  $n_z$  are equal and degeneracy of 6 when all the three are not equal.

The distribution of energy states depending of the combinations of  $n_x$ ,  $n_y$  and  $n_z$  can be evaluated analyzing the  $n$  space formed by  $n_x$ ,  $n_y$  and  $n_z$ .

It is observed that every combination of  $n_x$ ,  $n_y$  and  $n_z$  gives additional unit volume in ***n space*** from which we conclude that evaluating the number of states is equivalent to evaluating the volume of the ***n space***.

It is also noticed that the degenerate energy states with the same energy values lie on the surface of an octant of a sphere with the center at the origin. Hence it is sufficient to find the volume of the octant of a sphere of radius  $R$  to evaluate the number of energy states up to  $R$  i.e., the combination of  $n_x$ ,  $n_y$  and  $n_z$ .

The sensitivity of the increase in the states with increasing  $n_x$ ,  $n_y$  and  $n_z$  can be found from the change in the volume of the octant if the radius changes from  $R$  to  $R+dR$  realizing that  $R \gg dR$ .

The volume of the shell of thickness  $dR$  is then given by  $\frac{\pi R^2 dR}{2}$ . This is also then the number of energy states available between  $R$  and  $R+dR$ .

The energy expression  $E_n = E_0 R^2$  gives us  $R^2 = \frac{E_n}{E_0}$  and  $dR = \frac{dE}{2\{E_n E_0\}^{1/2}}$

Therefore the number of energy states between  $E$  and  $E+dE$  is given by

$$\frac{\pi R^2 dR}{2} = \frac{\pi}{4} \frac{E_n}{E_0} \frac{dE}{\{E_n E_0\}^{1/2}} = \frac{\pi}{4} \cdot \frac{E_n^{1/2}}{E_0^{3/2}} dE$$

Substituting for  $E_0 = \frac{\hbar^2}{8mL^2}$  we get the number of energy states between  $E$  and  $E+dE$  as

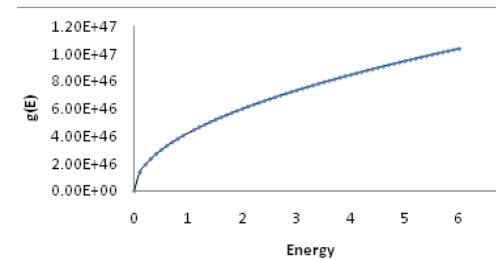
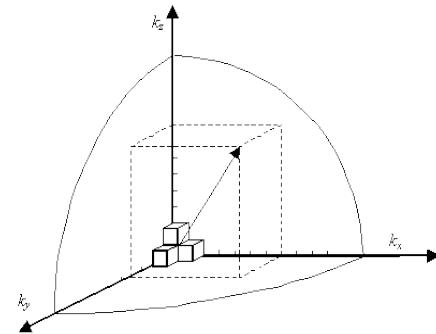
$$\frac{\pi}{4} \cdot \left( \frac{8mL^2}{\hbar^2} \right)^{3/2} E^{1/2} dE$$

The number of electrons states per unit volume can be estimated taking into consideration the Pauli's exclusion principle and allowing two electrons with opposite spins in each energy state.

The density of states for electrons in a metal gives the number of electron states per unit volume with energy  $E$

$$g(E) dE = \frac{\pi}{2} \left( \frac{8m}{\hbar^2} \right)^{3/2} E^{1/2} dE$$

This shows that the distribution of electrons in energy states vary non-linearly with increasing energy  $E$ .



**Numericals**

1. Electrons with energies of 4.00 eV are incident on a potential step 3.0 eV high. Find the probability of reflection at  $x=0$  and transmission for  $x>0$ . (**Ans R= 19.20% ;T =19.20%**)
2. A proton with energy E is incident on a potential step of height 3.5eV. If the de Broglie wavelength of the particle after transmission is 1.228 nm, find the energy of the proton.
3. A beam of identical electrons is incident on a barrier 6.0 eV high and 2 nm wide. Find the energy of the electrons if 1% of the electrons are to get through the barrier. (**Ans =5.963eV**)
4. An electron and a proton with the same energy E approach a potential barrier whose height U is greater than E. Comment on their tunneling probability.
5. A current beam 10 pico amperes (of identical electrons) is incident on a barrier 5.0 eV high and 1 nm wide. Find the transmitted current strength if the energy of the electrons is 4.9ev. (**Ans = T=3.93%** Transmitted current =  $10\text{pA} \times 0.0393 = 0.393\text{pA}$ )
6. Show that the probability of finding a particle trapped in an infinite potential well between  $x$  and  $x+\Delta x$  is approx  $\Delta x/L$  and is independent of  $x$ .
7. Find the probability that a particle in a box of width L can be found between 0 and  $L/n$  when the particle is in the nth state
8. A particle in an infinite potential well of width a. Find the probability of finding the particle between  $a/3$  and  $2a/3$  in the ground and third excited states. (**Ans:**)
9. What is the minimum energy of an electron trapped in a one dimensional region the size of an atomic nucleus ( $1 \times 10^{-14}$  m)? (**Ans 3.77 Gev**)
10. Find the energy required to excite a particle in a box of width 'a' from the second excited state to the fifth state. ()
11. Show that the probability of occupancy of an energy level  $\Delta E$  above the Fermi level is the same as that of the probability of non-occupancy of an energy level  $\Delta E$  below the Fermi level.
12. Estimate the probability of occupancy of an energy level 0.1 eV above the Fermi level for Copper with  $E_f = 7.0\text{eV}$  for i) 100K ii) 300K iii) 1000K
13. Find the temperatures at which the occupancy of an energy state 0.3 eV above the Fermi level has an occupancy probability of i) 0.01 and ii) 0.05

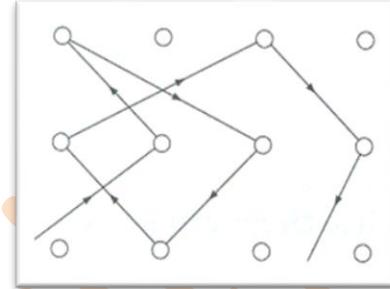
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## 1 Basics of CFET, expressions for electrical parameters

Drude and Lorentz proposed the classical free electron theory of electrical conductivity of metals (as early as 1904). The model of conductivity of free electrons is based on the following assumptions:

- (1) The valence electrons of the atoms of the metal contribute to the conduction process either electrical or thermal. The electrons move in an array of ion cores (which are nuclei surrounded by inner electrons excluding the valence electrons). All the valence electrons are free electrons and are treated as conduction electrons which are in a state of random motion (like the molecules in an ideal gas).
- (2) The effect of positive ion cores on the electrons is considered to be constant and hence neglected.
- (3) The electrostatic repulsion between the electrons is neglected.
- (4) The electrons in the metal are considered equivalent to molecules in a gas and the gas laws are made applicable to the electrons in a metal. Accordingly, the distribution of energy and velocity is assumed to follow Maxwell-Boltzmann statistics.



The average velocity of electrons in the metal is dependent on the temperature of the metal and is termed as the thermal velocity of electrons  $v_{th} = \sqrt{\frac{3kT}{m}}$ . At 300K the thermal velocity of the electrons is  $v_{th} \approx 10^5 \text{ ms}^{-1}$ .

However this random motion of the electrons do not contribute to a net drift of electrons across the metal and hence no current flows through the material

The conduction electrons in the lattice are scattered by collisions with the ionic cores and other electrons. The mean time between collisions is the relaxation time of the electrons in the metal and the distance between successive collisions is the mean free path. Taking the mean lattice parameter of 10nm as the mean free path  $\lambda$ , the relaxation time can be estimated as  $\tau = \frac{\lambda}{v_{th}} \approx 10^{-15} \text{ s}$ .

**Drift Velocity :** In the presence of an Electric field E the electrons show a net drift across the metal in a direction opposite to that of the electric field. The velocity of the electrons across the metal in the presence is known as the drift velocity  $v_d$ .

The force equation for the electron's motion can be described by  $m \frac{dv}{dt} = eE - kmv$  where the last term accounts for the loss of energy due to the scattering which is proportional to the momentum of the electrons and k is the coefficient of scattering loss.

In the equilibrium condition this leads to an average velocity for the electrons which is the drift velocity  $v_d = \frac{eE}{km}$

Dimensionally  $k$  should be  $(\text{time})^{-1}$ .

The decay of the drift velocity to zero in the absence of the electric field yields that  $k = \frac{1}{\tau}$  where  $\tau$  is the relaxation time – the time between successive collisions or the time for the drift velocity to fall to  $1/e$  times its steady value in the presence of an electric field.

The drift velocity  $v_d = \frac{e\tau E}{m} = \mu E$  where  $\mu = \frac{e\tau}{m}$  is the **electron mobility or the charge carrier mobility**. The mobility  $\mu = \frac{e\tau}{m} = \frac{v_d}{E}$  is the drift velocity per unit electric field.

The drift velocity of electrons is extremely low compared to the thermal velocity. To illustrate, the drift velocity of electrons experiencing an electric field of  $1\text{V/m}$  is of the order of  $10^{-4}\text{ ms}^{-1}$ .

#### **Expression for Electrical conductivity:**

The current through a conductor with an electron concentration  $n$  of cross section  $A$  and length  $L$  at an applied electric field  $E$  can be evaluated as

$$I = nev_d A \text{ where } v_d \text{ is the drift velocity given by } v_d = \frac{e\tau E}{m}$$

$\therefore I = neA \frac{e\tau E}{m}$  or  $J = \frac{I}{A} = \frac{ne^2\tau}{m} E = \sigma E$  where  $\sigma$  is a constant for a given metal and is the conductivity of the metal

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

The resistivity of the metal is  $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}$ .

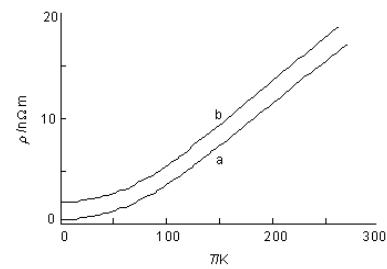
Thus the resistivity of a metal is inversely proportional to the concentration of free electrons and the relaxation time of electrons in the metal.

## **2 Experimental temperature dependence of the resistivity**

Experiments show that resistivity of metals in general vary linearly with temperature in the normal operating temperatures.

At these temperatures the resistivity  $\rho_{sc}$  results from the scattering of the electrons moving with high thermal velocities in random directions.

However at very low temperatures the resistivity  $\rho_{res}$  is found to saturate to a non zero finite value, which is dependent on the impurity concentration in the metal.



Hence two independent types of resistivities determine the total resistivity of the metal. Since the phenomena are independent of each other the net resistivity would be the sum of the two resistivity components which is known as the Mattheissen's rule.

$$\rho = \rho_{res} + \rho_{sc}$$

Hence  $\frac{m}{ne^2\tau} = \frac{m}{ne^2\tau_{res}} + \frac{m}{ne^2\tau_{sc}}$ . This gives us the effective relaxation time as  $\frac{1}{\tau} = \frac{1}{\tau_{res}} + \frac{1}{\tau_{sc}}$

## Unit III: Application of Quantum Mechanics to Electrical Transport in Solids

### 3 Draw backs of CFET and quantum corrections.

The classical free electron theory failed to correlate the experimental results of many phenomena such as the temperature dependence of resistivity, specific heat of electrons etc.

- a. According to the classical free electron theory the resistivity of a metal is given by  $\rho = \frac{m}{ne^2\tau}$ . For a given material the temperature dependence of resistivity arises from the temperature dependence of the relaxation time  $\tau = \frac{\lambda}{v_{th}}$ . Since the mean free path of the electrons is assumed to be a constant for a wide range of metals, the temperature dependence of the thermal velocity should affect the relaxation time. For a given temperature  $v_{th} = \sqrt{\frac{3k_B T}{m}}$  and hence  $v_{th} \propto \sqrt{T}$  or  $\tau \propto T^{-\frac{1}{2}}$ . Since the resistivity  $\rho \propto \tau^{-1}$ , the temperature dependence of resistivity can be inferred to be  $\rho \propto \sqrt{T}$ . But experimental observations show that  $\rho \propto T$  and hence the classical free electron conduction model fails to explain the correct temperature dependence of resistivity of metals.
- b. The contribution of electrons to the specific heat of the metal can be estimated using the principle that the specific heat  $C_{el} = \frac{dU}{dT}$ . Considering one mole of a mono valent metal, the energy of the valence electrons is given by  $U = \frac{3}{2} k_B T \cdot N_{avg}$ . Hence the specific heat of the electrons should be equal to  $C_{el} = \frac{dU}{dT} = \frac{3}{2} k_B \cdot N_{avg} = \frac{3}{2} R$  which is a constant. However experimental estimation of the specific heat of electrons is only approximately 1% of the theoretical value and is also found to be temperature dependent. Thus, the theory fails to explain the actual specific heat dependence of electrons in metals.
- c. The electrical conductivity of metals, given by  $\sigma = \frac{ne^2\tau}{m}$ , should be dependent on the free electron concentration for a given temperature, assuming that the relaxation time is more or less constant. However, it is found that mono valent Copper with lesser electronic concentration has a higher electrical conductivity as compared to trivalent Aluminum. Similarly Zinc with higher electronic concentration has lesser conductivity than Aluminum. Experimental results show that there is no linear dependence of the electronic concentration on the conductivity of metals.

Thus, the classical free electron theory fails to explain the experimental observations. It is obvious that some of the assumptions of the CFET are over estimations or under estimations of the physical parameters and hence need to be corrected.

#### 4 Quantum model of valence electrons in a metal - Fermi energy

Metals have a very high concentration of valence electrons  $\approx 10^{28} m^{-3}$ . According to the quantum mechanical principles these valence electrons in a metal have to be in discrete energy states following Pauli's exclusion principle. This requires the energy states of the atomic levels to split into discrete closely spaced energy states to accommodate all the valence electrons. At 0K such an arrangement leads to a sea of energy levels which have a separation as small as  $\approx 10^{-20} eV$ . The upper most occupied energy state at 0K is then termed as the Fermi energy of the metal. Thus at 0K all the states below the Fermi energy are filled and all the states about the Fermi energy are empty.

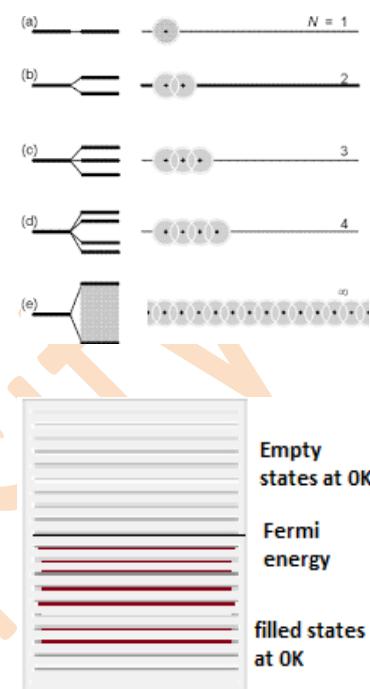
By convention electrons above the Fermi level should contribute to the conduction process and the valence electrons are below the Fermi level. (The electrons in states below the Fermi level do not contribute to the conduction process). Thus according to this model not all the valence electrons in a metal are conduction electrons.

The effective number of electrons above the Fermi level could be approximated as  $n_{eff} = n \frac{kT}{E_f}$ .

The effective number of electrons above the Fermi level for copper ( $E_f=7eV$ ) at 300K can be calculated to be  $n_{eff} = n \frac{kT}{E_f} = n * 0.0036 = n * 0.36\%$ . Thus a small fraction of the available valence electrons are excited into states above the Fermi level, which contribute to the conductivity of the material.

This quantum model of the free electrons gives rise to the following modifications to the classical free electron theory:

- The valence electrons in the metal are arranged in discrete energy states following Pauli's exclusion principle. Only electrons close to the Fermi level participate in the conduction process.
- The occupation probability of the electron states are described by the Fermi Dirac distribution function applicable to fermions.
- The conduction electrons in a metal move in array of positive ions, colliding with the ionic centers and other electrons resulting in the resistance of the material.



- The electrostatic interactions namely, the electron – electron interaction and the electron – ion interactions are negligible.
- The electrons undergo random scattering due to the vibrating ionic centers giving rise to resistance to flow of electrons.

## 5 Fermi Dirac statistics, Fermi factor

The occupation probabilities of electrons in the different energy state at different temperatures are estimated using the Fermi Dirac statistics for Fermions. (All particles with spin  $\pm \frac{1}{2}$  are classified as Fermions. Fermions follow the Fermi Dirac statistics for particles which are indistinguishable.)

The Fermi factor  $F_d = \frac{1}{\left(e^{\left(\frac{(E-E_f)}{k_B T}\right)}+1\right)}$  gives the probability of an energy state E to be occupied at a temperature T

Estimation of the Fermi factor at T=0K gives distinct results for  $E < E_f$  and  $E > E_f$ .

- If  $E < E_f$  then for  $E - E_f$  is negative, then the Fermi factor  $F_d = \frac{1}{\left(e^{-\left(\frac{(E-E_f)}{k_B T}\right)}+1\right)}$ .

At 0K this becomes  $F_d = \frac{1}{\left(e^{(-\infty)}+1\right)} = 1$ . This implies that at 0K all electron states below the Fermi level are filled states.

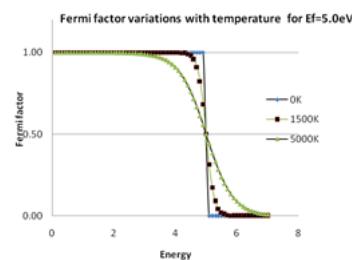
- If  $E > E_f$  then for  $E - E_f$  is positive, then the Fermi factor

$$F_d = \frac{1}{\left(e^{\left(\frac{(E-E_f)}{k_B T}\right)}+1\right)}.$$

At 0K this becomes  $F_d = \frac{1}{\left(e^{(+\infty)}+1\right)} = 0$ . This implies that at 0K all electron states above the Fermi level are empty states.

- For  $T > 0$  and  $E = E_f$  the Fermi factor  $F_d = \frac{1}{\left(e^{\left(\frac{(E-E_f)}{k_B T}\right)}+1\right)} = \frac{1}{e^0+1} = \frac{1}{2} = 0.5$ . This gives a

probability of occupation of 50% for the Fermi energy.



The Fermi energy has a weak temperature dependence and is given by

$$E_f = E_{f0} \left[ 1 - \frac{\pi^2}{12} \left( \frac{k_B T}{E_{f0}} \right)^2 \right]$$

where  $E_{f0}$  is the Fermi energy at zero Kelvin. At normal temperature ranges the ratio of  $\frac{k_B T}{E_{f0}}$  is very low and hence can be approximated to be a constant equal to the value at zero Kelvin.

## 6 Fermi temperature

The arrangement of electrons in discrete energy states leads to the concept that only electrons near the Fermi energy are excited into the conduction band and it may be really difficult to excite all the valence electrons into the conduction band. If the temperature of the metal is T then  $k_B T$

is the thermal energy available to the electrons in the metal. The thermal energy required to excite the last electron at the bottom of the energy band if termed as  $k_B T_f$ , then at temperature  $T_f$  the electron would have an energy  $E_f = k_B T_f$ . This temperature is termed as the Fermi temperature of electrons in the metal.

Evaluating the temperature for Copper with Fermi energy as 7 eV gives the value of the Fermi temperature as approximately 81000K. It is obvious that at such high temperatures the metal cannot be in the solid state and hence this is only a representative temperature which highlights the point that all valence electrons cannot be conduction electrons.

## 7 Fermi velocity

From the above analysis it is clear that only a small fraction of electrons close to the conduction band can be taking part in the conduction processes. The electrons excited into the conduction band have energies very close to the Fermi energy. These conduction electrons then possess a kinetic energy which may be equal to the Fermi energy.

The kinetic energy of the electrons near the Fermi energy is  $E_f = \frac{1}{2}mv_f^2$  where  $v_f$  the Fermi velocity of conduction electrons is  $v_f = \sqrt{\frac{2E_f}{m}}$ . Fermi velocity for conduction electrons in Copper gives  $v_f = 1.06 \times 10^6 \text{ ms}^{-1}$ .

This velocity is greater than the thermal velocity of electrons (as per the CFET). The electrons in the conduction band are in a state of random motion and the scattering of the electrons by the lattice is the origin of the electrical resistance of the metal.

## 8 Density of states derivation

The electrons in a metal can be approximated to the particle in a box in three dimensions, since under normal conditions the electrons cannot escape the boundaries of the metal. Consider a mono-valent metal in the form of a cube of side  $L$ . Inside the metal the electrons can be assumed to be moving in a zero potential field.

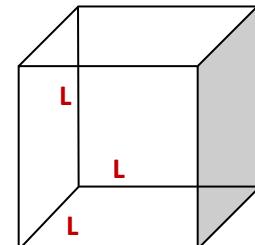
The three dimensional Schrödinger's wave equation can be written as three one dimensional Schrödinger's wave equation and their corresponding solutions analysed.

The x component of the particle motion can be described by the wave function which is the solution of the SWE

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) = 0$$

This gives the Eigen energy value for the x component as  $E_{n_x} = \frac{\hbar^2 n_x^2}{8mL^2}$

Similarly the energy in the other two dimensions can be evaluated as  $E_{n_y} = \frac{\hbar^2 n_y^2}{8mL^2}$  and  $E_{n_z} = \frac{\hbar^2 n_z^2}{8mL^2}$



## Unit III: Application of Quantum Mechanics to Electrical Transport in Solids

The total energy of the electron can be written as

$$E_n = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\hbar^2}{8mL^2} R^2 \quad \text{----- (1) where } R^2 = n_x^2 + n_y^2 + n_z^2$$

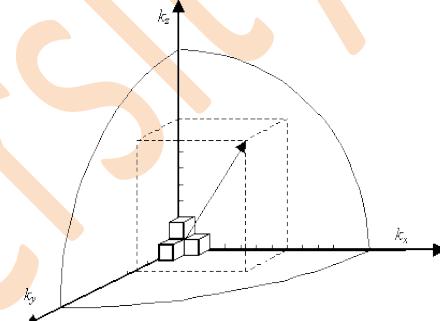
The number of states with energy E can be evaluated by studying the variation of the combinations of  $n_x$ ,  $n_y$  and  $n_z$ . It can be deduced that every combination of  $n_x$ ,  $n_y$  and  $n_z$  result in an energy state as per equation (1).

(The  $n$  space corresponds to the momentum space since  $k = n \frac{\pi}{L}$ . Thus the combinations can give the picture of particles moving in different directions.) When  $n_x$ ,  $n_y$  and  $n_z$  are equal the energy state is unique and is non degenerate. It is also noted that the energy states can be degenerate with degeneracy of 3 when two of the three  $n_x$ ,  $n_y$  and  $n_z$  are equal and degeneracy of 6 when all the three are not equal.

The distribution of energy states depending of the combinations of  $n_x$ ,  $n_y$  and  $n_z$  can be evaluated analyzing the  $n$  space formed by  $n_x$ ,  $n_y$  and  $n_z$ .

It is observed that every combination of  $n_x$ ,  $n_y$  and  $n_z$  gives additional unit volume in ***n space*** from which we conclude that evaluating the number of states is equivalent to evaluating the volume of the ***n space***.

It is also noticed that the degenerate energy states with the same energy values lie on the surface of an octant of a sphere with the center at the origin. Hence it is sufficient to find the volume of the octant of a sphere of radius  $R$  to evaluate the number of energy states up to  $R$  i.e., the combination of  $n_x$ ,  $n_y$  and  $n_z$ .



The sensitivity of the increase in the states with increasing  $n_x$ ,  $n_y$  and  $n_z$  can be found from the change in the volume of the octant if the radius changes from  $R$  to  $R+dR$  realizing that  $R \gg dR$ .

The volume of the shell of thickness  $dR$  is then given by  $\frac{\pi R^2 dR}{2}$ . This is also then the number of energy states available between  $R$  and  $R+dR$ .

The energy expression  $E_n = E_0 R^2$  gives us  $R^2 = \frac{E_n}{E_0}$  and  $dR = \frac{dE}{2\{E_n E_0\}^{1/2}}$

Therefore the number of energy states between  $E$  and  $E+dE$  is given by

$$\frac{\pi R^2 dR}{2} = \frac{\pi}{4} \frac{E_n}{E_0} \frac{dE}{\{E_n E_0\}^{1/2}} = \frac{\pi}{4} \cdot \frac{E_n^{1/2}}{E_0^{3/2}} dE$$

Substituting for  $E_0 = \frac{\hbar^2}{8mL^2}$  we get the number of energy states between  $E$  and  $E+dE$  as

$$\frac{\pi}{4} \cdot \left( \frac{8mL^2}{\hbar^2} \right)^{3/2} E^{1/2} dE$$

The number of electrons states per unit volume can be estimated taking into consideration the Pauli's exclusion principle and allowing two electrons with opposite spins in each energy state.

The density of states for electrons in a metal gives the number of electron states per unit volume with energy E

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

This shows that the distribution of electrons in energy states vary non-linearly with increasing energy E.

The probability that an energy state is occupied is given by the fermi factor

$$F_d = \frac{1}{1 + e^{\frac{(E-E_f)}{k_B T}}}$$

And hence the occupancy of the states described by N(E) is determined by the factor

$$N(E) = g(E) * F_d$$

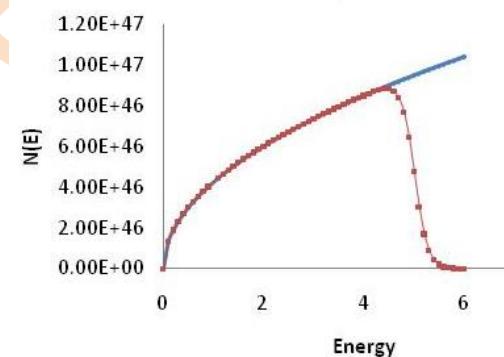
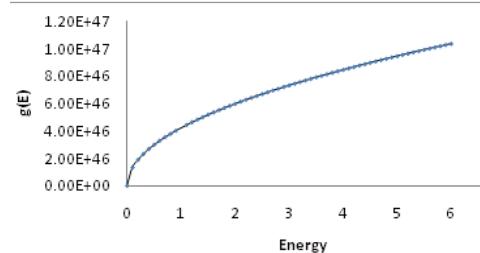
This in effect is multiplying g(E) by a number between 0 and 1 depending on the position of the energy relative to the Fermi energy and the temperature.

The states below  $E_f - k_B T$  are completely occupied as  $F_d$  is 1.

The states in the range of  $k_B T$  below the Fermi level are emptied and the probability of occupancy  $F_d$  is between 1 and 0.5.

The states above  $E_f$  in a range  $k_B T$  are now occupied and the probability of occupancy lies between 0.50 and 0.00.

The variation of N(E) with E can be graphically represented as shown for a representative material with Fermi energy of 5eV.



## 9 Expression for Fermi energy, average electron energy

The Fermi energy of metals can be evaluated from the fact that all available electrons occupy energy levels below the Fermi level  $E_f$  at 0K. This means that the density of occupied states  $N(E) = g(E) * F_d$  when evaluated for all levels from 0 to  $E_f$ , should result in the total count of electrons in the metal, ie.,

$$\text{The total free electronic concentration } n = \int_0^{E_f} N(E) dE = \int_0^{E_f} g(E) * F_d dE .$$

We know that  $F_d$  has to be 1 for all energy levels below  $E_f$  at 0K and hence

$$n = \int_0^{E_f} N(E) dE = \int_0^{E_f} g(E) dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE = \frac{\pi}{3} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

This gives us a method of estimating the Fermi energy of the system if the number of valence electrons per unit volume is known.

The Fermi energy can be estimated if the concentration of free electrons is known and can be evaluated as

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

Average energy of electrons in a metal at 0K

Since the distribution of electrons in the different energy states shows a non linear variation, the average energy of the electron is not the simple average of the electron's max and min energy. From the graph of  $N(E)$  vs  $E$  we observe that  $N(E)$  states have energy  $E$  which implies that the total energy of all electrons in filled states upto  $E_f$  should be the summation of all  $N(E)*E$

The average energy of the electron =  $\frac{\text{total energy of all electrons in different energy states}}{\text{total number of electrons}}$

$$\frac{\int_0^{E_f} g(E) * E * F_d dE}{\int_0^{E_f} g(E) * F_d dE} = \frac{\frac{\pi}{2} \left(\frac{8m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE * E}{\frac{\pi}{2} \left(\frac{8m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE}$$

This on integration gives the average energy  $E = \frac{3}{5} E_f = 0.6 * E_f$

#### Merits of Quantum free electron theory:

#### Heat capacity due to free electrons

The electronic specific heat (contribution to the specific heat from the conduction electrons) can be evaluated in the light of the fact that only electrons close to the Fermi level participate in the conduction. Hence the heat absorption happens due to that fraction of electrons. This number can be estimated as the effective number of electrons (in one mole of the metal for a mono valent metal) in the conduction process as  $n_{\text{eff}} = \frac{N_a}{E_f} \cdot k_B T$ .

Hence if the average thermal energy of the electrons is taken to be  $\frac{3}{2}k_B T$  then the total energy of electrons in one mole of the material  $U = n_{\text{eff}} \cdot \frac{3}{2}k_B T = \frac{3}{2}k_B T \cdot \frac{N_a}{E_f} \cdot k_B T = \frac{3}{2} \cdot \frac{N_a}{E_f} \cdot k_B^2 T^2$

Hence the specific heat  $C_{\text{el}} = \frac{dU}{dT} = 3 \cdot \frac{N_a}{E_f} \cdot k_B^2 T = 3R \cdot \frac{kT}{E_f}$

Thus, the electronic specific heat is a fraction of the value predicted by the CFET (since  $\frac{kT}{E_f}$  is a fraction less than 1% for most metals) and is temperature dependent. This analysis gives the correct correlation with the experimental results.

A more accurate evaluation of the electronic specific heat of mono valent metals (using the ideas of the number of electrons in the levels above  $E_f$  and their average energy values) results in the relation

$$C_{el} = \frac{\pi^2}{2} N * \frac{k_B^2 T}{E_f}$$

### **Temperature dependence of the resistivity**

According to the classical free electron theory resistivity of the electrons originates from the scattering mechanism in which the ionic centers are stationary.

The quantum free electron theory takes into account the thermal vibrations of the ionic array which accounts for the scattering of electrons. The amplitude of the random vibrations of the lattice ions is proportional to temperature. When the ions vibrate the lattice presents an effective cross sectional area for scattering of  $\pi r^2$  where  $r$  is the amplitude of vibration. But the increasing amplitude also result in an increase in the probability of electron scattering.

Thus the mean free path  $\lambda$  of the electrons reduces with increasing temperature. The electron mean free path  $\lambda$  is inversely proportional to the scattering cross section and hence  $\lambda \propto 1/T$

The expression for conductivity  $\sigma = \frac{ne^2\tau}{m} = \frac{ne^2\lambda}{mv_f}$  shows that the conductivity is proportional to the mean free path. Hence the conductivity will be inversely proportional to temperature or resistivity  $\rho \propto T$  as is found experimentally.

### **Relation between electrical conductivity and thermal conductivity (Wiedemann-Franz law and Lorenz number)**

From the discussions of the electronic arrangement it is obvious that the electrons close to the Fermi energy are responsible for the electrical or thermal conduction and hence it should be possible to find a relation between the two seeming different physical phenomena.

It is known that the thermal conductivity of the metal  $K = \frac{1}{3} \cdot \frac{C}{V} \cdot v \cdot L$

Where  $C$  is the electronic specific heat given by  $C_{el} = \frac{\pi^2}{2} N \cdot \frac{k_B^2 T}{E_f}$ ,

$V$  the volume,  $v$  is the velocity of electrons and  $L$  the mean free path. The mean free path of electrons is given by  $L = v \cdot \tau$ . Taking velocity to be the Fermi velocity  $v_F$  (since most of the conduction electrons are located about the Fermi energy) the expression for the thermal conductivity can be written as

$$K = \frac{1}{3} \cdot \frac{1}{V} \cdot \frac{\pi^2}{2} N \cdot \frac{k_B^2 T}{E_f} \cdot v_F \cdot v_F \tau = \frac{\pi^2}{6} \cdot n \cdot \frac{k_B^2 T}{E_f} \cdot v_F^2 \cdot \tau.$$

where  $n = \frac{N}{V}$  is the concentration of free electrons.

$$K = \frac{\pi^2}{3} \cdot n \cdot \frac{k_B^2 T}{E_f} \cdot \frac{mv_F^2}{2m} \cdot \tau = \frac{\pi^2}{3} \cdot n \cdot \frac{k_B^2 T}{m} \cdot \tau$$

The electrical conductivity of the metal is then given by  $\sigma = \frac{ne^2\tau}{m}$

The ratio of the thermal conductivity to electrical conductivity can be calculated as

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

This is the Wiedemann-Franz law. It was noticed by Lorenz that the ratio  $\frac{K}{\sigma T} = \frac{\pi^2}{3e^2} k_B^2$  is a constant irrespective of the metal and is called the Lorenz number.

The Lorenz number has a value  $= 2.4 \times 10^{-8} \text{ W}\Omega\text{K}^{-2}$ .

### **Short comings of quantum free electron theory**

The quantum free electron theory though successful in giving correct dependencies of some of the electrical parameters and the specific heat of electrons, was not able to explain

Differences in conduction in metal, semiconductor and insulator, and the origin of the band gap in semiconductors and insulators are not explained.

Experimentally observed positive Hall co-efficient observed in some metals like Zinc, Magnesium, lead etc.

These demerits could be reflective of the real potentials of the ionic centers in the lattice which was ignored in the development of the model. The presence of the potentials can significantly affect the wave function of the electrons.

### **11. Motion of electron in periodic potential (one dimensional treatment)**

The free electrons in a metal are not free from electrostatic potentials and move in a periodic potential due to the regular arrangement of the ionic centers.

The potential is lower close to the positive ions in the lattice (and in some cases basis) positions. The electrons experience a potential with the same periodicity as the lattice. The columbic potential in the real crystal can be approximated by rectangular potentials.

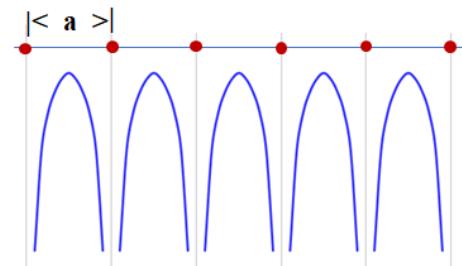
If  $V(x)$  is the potential at  $x$  then, it can be seen from the figure that

$V(x + a) = V(x)$  which means that the potential is periodic and invariant under the translation through the lattice parameter.

However, the wave function of the free electrons

$\Psi(x) = e^{ikx}$  is modulated by the periodic potential and can be written as

$\Psi(x) = e^{ikx} \cdot V_k(x)$  where  $k$  is the wave number of the electron waves. This is known as the Bloch function.



### Kronig-Penney model, allowed energy zones/energy bands

In the Kronig-Penney model the periodic potential is approximated as a long chain of coupled finite square wells, of barrier height  $V_0$ , with a period 'a', and barrier thickness c.

The wave function of the electron is a modulated wave of the form  $\psi(x) = e^{ikx} \cdot V_k(x)$ .

A solution to the Schrödinger's equation exists if the dispersive wave number of the electron k is related to the energy through the equation:

$$\cos(ka) = \frac{ma}{\hbar^2} V_0 \cdot c \cdot \frac{\sin(Ka)}{Ka} + \cos(Ka)$$

where  $K = \sqrt{\frac{2m(E)}{\hbar^2}}$ . We notice that the above is a transcendental equation and has approximate solutions.

The left hand side of the equation is bound with upper and lower limits of +1 to -1.

The right side of the equation has oscillations of decreasing amplitude with increasing  $ka$ . However, the solutions exist only for those allowed range of  $k = n\frac{\pi}{a}$ . Thus, there exists a range of allowed energy states and forbidden energy states.

In the limit  $\frac{ma}{\hbar^2} V_0 \cdot c$  tends to infinity  $\sin(Ka) = 0$  which implies  $K = \frac{n\pi}{a}$  and hence the energy  $E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$ .

In the limit  $\frac{ma}{\hbar^2} V_0 \cdot c$  tends to zero  $\cos(Ka) = 1$  which implies  $k = K$  and hence the energy  $E = \frac{\hbar^2 K^2}{2m}$  which is the solution for a free particle.

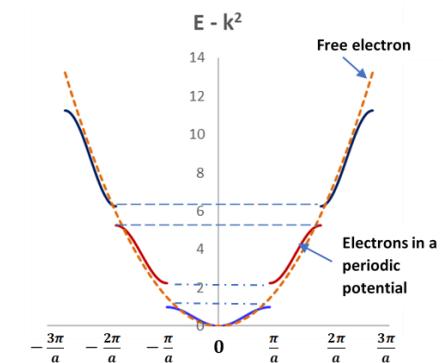
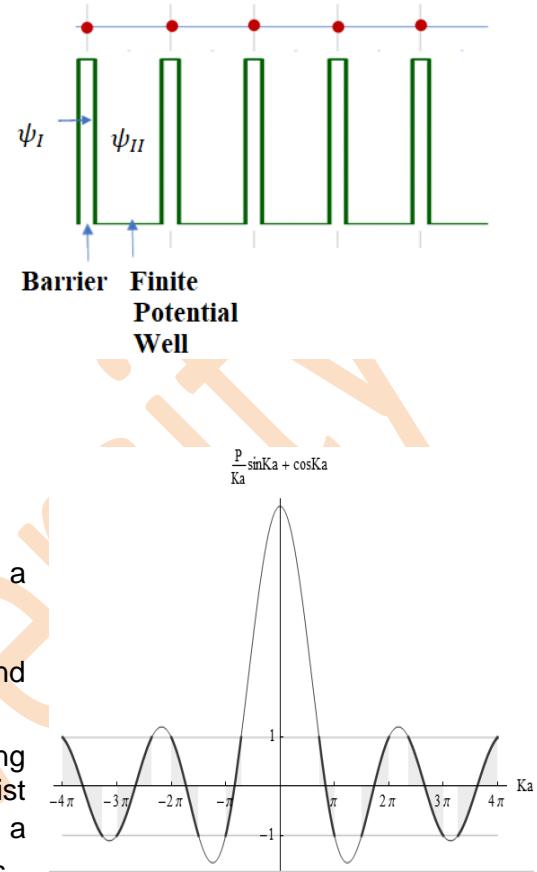
The  $E(k)$  – k diagram for the system show discontinuity in the energy at the zone boundary of  $k = \pm n\frac{\pi}{a}$ . (The parabolic variation of E for the free electrons is shown for comparison).

Since the functions are symmetric (and periodic with period of  $2\frac{\pi}{a}$ ), it is possible to represent the energy band diagram in a single zone of  $+\frac{\pi}{a}$  to  $-\frac{\pi}{a}$ .

The lowest allowed energy state is non-zero. The lowest band is the completely filled inner band followed by a band of forbidden energy states (shaded).

The next band of allowed states represents the valence band.

The upper most occupied states form the conduction band.



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Thus, we observe allowed and forbidden energy states for the electrons in the material.

Materials are then classified as metals, semiconductors or insulators on the basis of the Fermi energy of the material.

In the case of conductors, the Fermi level is in the uppermost band the conduction band. All states below the Fermi level are filled and all levels above the Fermi energy are empty. Thus, metal are characterized by a partially filled conduction band.

In the case of materials with a completely filled valence band and completely empty conduction band, the Fermi energy is theoretically the midpoint of the energy band gaps. Materials with energy gap of 3-5 eV are classified as semiconductors. At normal temperatures it is possible for the electrons in the valence band to move into the conduction in the case of metals and semiconductors.

Materials with energy band gap greater than 5eV are classified as Insulators in which the electron conduction is impossible and attempts to excite the electrons lead to a dielectric breakdown.

### Concept of Effective mass

The motion of electrons in the crystal is governed by the energy equation  $E = \frac{\hbar^2 k^2}{2m}$  which shows that the energy is nonlinearly dependent on the propagation constant  $k$ .

Differentiating the expression twice with respect to  $k$

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*}$$

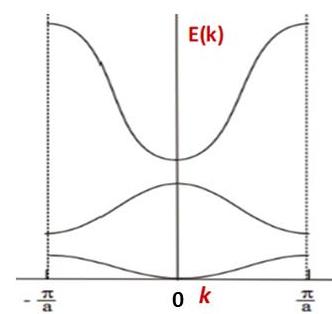
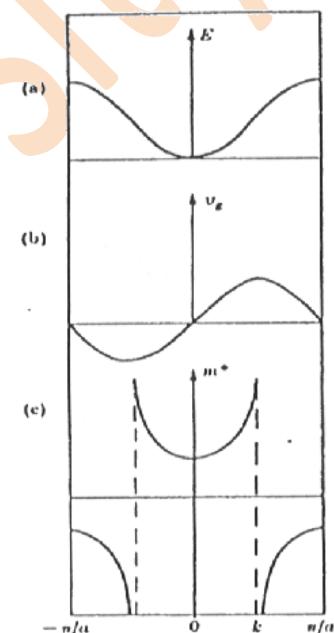
it is observed that  $m^* = \left(\frac{1}{\hbar^2} \frac{d^2E}{dk^2}\right)^{-1}$  is not a constant and depends on the non linearity of  $E$ . This means that the charge carriers have an effective mass which depends on the curvature of  $E-k$ .

Higher curvature (larger  $\frac{d^2E}{dk^2}$ ) means smaller effective mass and smaller curvature results in higher effective mass.

It can be seen that the slope of the E-K curve is minimum at the band edges and hence the effective mass of the charge carriers are highest at the band edges.

Since curvature of the  $E-k$  is positive in the conduction band the effective mass is +ve and the curvature in the valence band is negative indicating a negative mass. However, this can be construed to be the motion of a charge carrier with a charge of the opposite type as that of electrons. This leads to the concept of hole conduction in the valence band. The effective mass of electrons can be higher or lower than the rest mass of the electrons and depends on the position of the electron in the particular band.

The concept of the effective mass helps understand the mobility of charge carriers in a system particularly in semiconductors. In most compound semiconductors the effective mass of electrons and holes are much smaller than the rest mass of electrons. These materials exhibit a higher mobility of charge carriers.



### **Superconductivity**

Superconductivity was first discovered by H. Kammerlingh Onnes in 1911 while studying the resistivity of Mercury. He observed that if Mercury is cooled below 4.1K its electrical resistance falls by a factor of  $10^6$ . This drastic increase in the conductivity in certain metals has been termed superconductivity. The temperature at which the conductivity of the metal increases sharply is known as the transition temperature  $T_c$ . About 30 metals exhibit superconductivity, with superconducting transition temperatures between 0K and 9.3K.

Some of the key observations about superconductors are:

- Superconductivity is not observed in Mono valent metals
- The phenomena is exhibited by metals for which the valence electrons number are between 2 & 6.
- Metals which are highly resistive at normal temperatures show superconductivity at very low temperatures.
- The current in the super conductor persists for a long time of the order of  $10^5$  years.
- Superconductivity is destroyed by a high magnetic field or excessive currents through the superconductor.
- Ferromagnetic and anti ferromagnetic materials are not superconductors

### **Meissner effect.**

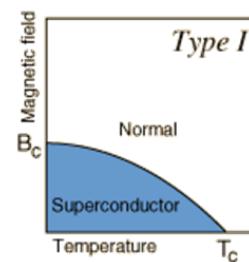
A superconducting material when subjected to a magnetic field and cooled to temperatures below the critical temperatures, it expels the magnetic lines of flux from its interior. The material then behaves as a perfect diamagnetic. This effect is called the Meissner effect.

When the material is in the normal conducting state, it allows the magnetic lines of force to pass through the material.

### **Critical Field**

A critical temperature  $T_c$  of superconducting material is dependent on the strength of the external magnetic fields. The presence of a strong external field drives the material into the normal conducting state. The strength of the magnetic field at which the material loses its superconducting state is known as the Critical Field  $H_c$ . The critical field strength is temperature dependent and is related to the Critical temperature by the relation

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

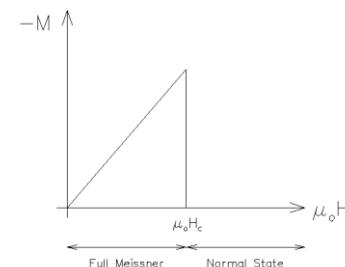


### **Type I and type II superconductors**

Superconductors are **classified** into two major categories as type I and type II superconductors based on the Meissner effect exhibited by the material.

**Type I superconductors** are generally pure metals which behave like a perfect diamagnetic material in the superconducting state (exhibiting a complete Meissner effect).

In the case of type I superconductors the critical temperature is dependent on the magnitude of an applied external magnetic field. Higher magnetic fields lower the critical field at which the material

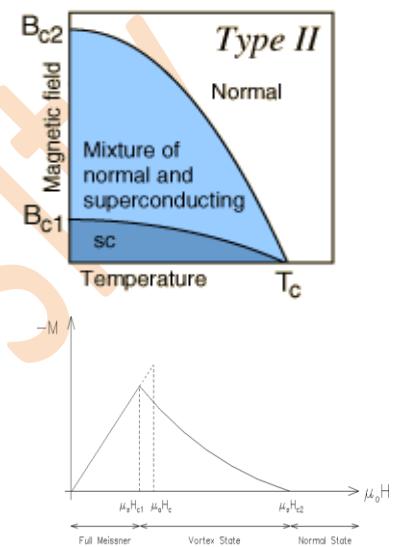


remains as a superconductor as shown.

External fields tend to induce magnetization in the material. The induced negative magnetic moment of the material increases with the applied external magnetic fields in the superconducting state. At the critical magnetic field, the material loses diamagnetic behavior, and the net magnetic moment falls to zero. The critical magnetic field strength for Type I superconductors is low.

Type I superconductors are also known as soft superconductors.

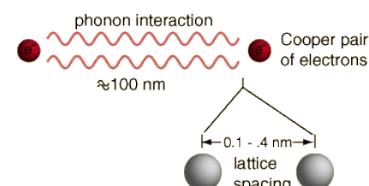
**Type II superconductors** are generally alloys of different metals. They were found to have much higher critical fields and therefore could carry much higher current densities while remaining in the superconducting state.



External magnetic fields induce magnetization of the material in the superconducting state and remain in the normal superconducting state up to a critical field  $H_{c1}$ . As the field is increased further, it is observed that the material partially allows the magnetic lines of force to penetrate the material, indicating the simultaneous presence of normal and superconducting states in the material up to a second critical field  $H_{c2}$  beyond which the material reverts back to its normal conducting states.

#### BCS theory

The properties of Type I superconductors were modeled successfully by the efforts of John Bardeen, Leon Cooper, and Robert Schrieffer in what is commonly called the BCS theory. A key conceptual element in this theory is the pairing of electrons close to the Fermi level into Cooper pairs through interaction with the crystal lattice. This pairing results from a slight attraction between the electrons related to lattice vibrations; the coupling of the electrons to the lattice is called a phonon interaction.



Electron pairs behave very differently from single electrons (which are fermions and must obey the Pauli exclusion principle), whereas electron pairs act more like bosons (which can condense into the same energy level).

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The electron pairs have a slightly lower energy and hence are delicately stable. The pairs require an energy of about 0.001eV to be separated which is referred to as the energy gap for the paired state to the unpaired state.

In the paired state the charge carriers do not show the kind of collision interactions which lead to ordinary resistivity. Below the critical temperature, the system is then in an extremely low resistive state.

Bardeen, Cooper, and Schrieffer received the Nobel Prize in 1972 for the development of the theory of superconductivity.

### Applications of Superconductivity:

Superconductors find extensive applications in a variety of fields. Some of the significant applications are :

SQUIDs which are superconducting quantum interference devices are capable of sensing extremely weak magnetic fields. They form the sensors in the MRI scanning used in the medical fields.

Strong magnets made using superconducting materials are used for magnetic levitation. Such magnets also form the core of the magnetic confinement that is required to contain the plasma in fusion experiments.

Superconducting systems are potential candidates for creating QUBITs which are fundamental to creating quantum computers.

Research is on to create room temperature superconductors which can then reduce the loss of energy in power transmission.

## Solved Numericals:

1. Estimate the Fermi factor of an energy state 0.01eV below the Fermi level at 500K

The Fermi factor  $f_D = \frac{1}{e^{(E-E_f)/kT} + 1}$  gives the probability of occupancy of an energy state E above or below the Fermi energy at temperature T.

The Fermi factor for an energy state 0.01 eV below the Fermi level at 500 K

$$f_d = 1/(e^{((-0.01 * [1.6 \times 10] ^{-19}) / (1.38 \times 10^{-23} * 500))} + 1) = 0.558$$

2. If the Fermi energy of the metal is 3.75 eV calculate the molar specific heat at 500 K

The molar electronic specific heat is given by  $C_{el} = dU/dT = 3N_a/E_f \cdot k_B^2 T$

At 500K the electronic specific heat = 0.29 J/mol

3. Determine the free electron concentration, the Fermi velocity for electrons in a metal with Fermi energy of 5.10 eV.

The concentration of free electrons in a metal is related to the Fermi energy as

$$n = \pi/3 (8m/h^2)^{3/2} \times E_f^{3/2}$$

For E=5.10eV      n =  $5.211 \times 10^{28} \text{ m}^{-3}$ .

The Fermi velocity of electrons is given by  $E_f = 1/2 m [v_f]^2$  Hence  $v_f = \sqrt{(2E_f/m)} = 1.34 \times 10^6 \text{ ms}^{-1}$ .

4. A mono valent metal has  $5 \times 10^{28}$  valence electrons per m<sup>3</sup>. Estimate the number of electron energy states per unit volume in the metal between 2eV and 2.005eV from the concept of the density of states.

The density of states for electrons in a metal gives the number of electron states per unit volume with

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

$$E = 2.00 \text{ eV} \quad dE = 0.005 \text{ eV}$$

$$\text{Hence } g(E)dE = \frac{\pi}{2} (8m/h^2)^{3/2} E^{1/2} dE = 4.80 \times 10^{25} \text{ per m}^3.$$

## Problem set

1. A certain conductor has a free electron concentration of  $5.9 \times 10^{28} \text{ m}^{-3}$ . What current density in the conductor will correspond to a drift velocity of  $1/1.6 \text{ mm s}^{-1}$ ? Calculate the mobility of charge carriers given conductivity as  $6.22 \times 10^7 (\Omega\text{m})^{-1}$ . (Ans :)
2. Calculate the free electron concentration, mobility and drift velocity of electrons in an Al wire of diameter 0.5mm, length 5m, resistance of 60 milli ohms that carries a current of 15A . Al has 3 free electrons At wt of Al=26.98 and density  $2.7 \times 10^3 \text{ kg m}^{-3}$ .

## Unit III: Application of Quantum Mechanics to Electrical Transport in Solids

3. Find the relaxation time and mobility of conduction electrons in a metal having  $6.5 \times 10^{28}$  electrons  $\text{m}^{-3}$  if the resistivity of the metal is  $1.43 \times 10^{-8}$  ohm m
4. There are  $1020$  electrons per  $\text{m}^{-3}$  in a material having a resistivity of  $0.1$  ohm  $\text{-m}$ . Find the charge mobility and the electric field needed to produce a drift velocity of  $1\text{ms}^{-1}$ .
5. A copper wire of radius  $1\text{mm}$  and length  $10$  meter carries a direct current of  $5$  ampere. Calculate the drift velocity of electrons in copper if  $n = 5 \times 10^{28}/\text{m}^3$ .
6. Silver has a density of  $10.5 \times 10^3 \text{ Kgm}^{-3}$  and atomic weight of  $107.9$ . If conductivity of silver at  $27^\circ\text{C}$  is  $6.8 \times 10^7 (\text{ohm}\cdot\text{m})^{-1}$ , find the mean free path of electrons as per the classical free electron theory.
7. Calculate the relaxation time of conduction electrons in a metal of resistivity of  $1.55 \times 10^{-8} \Omega \text{ - m}$  and an electronic concentration of  $6 \times 10^{28}$  per  $\text{m}^3$ .
8. Show that the probability of occupancy of an energy level  $\Delta E$  above the Fermi level is the same as that of the probability of non-occupancy of an energy level  $\Delta E$  below the Fermi level.
9. Estimate the probability of occupancy of an energy level  $0.1 \text{ eV}$  above the Fermi level for Copper with  $E_f = 7.0 \text{ eV}$  for i)  $100\text{K}$  ii)  $300\text{K}$  iii)  $1000\text{K}$
10. Find the temperatures at which the occupancy of an energy state  $0.3 \text{ eV}$  above the Fermi level has an occupancy probability of i)  $0.01$  and ii)  $0.05$
11. Calculate the Fermi energy of electrons in a mono valent metal with atomic weight  $132.9 \times 10^{-3} \text{ kg/mol}$  and density of  $1.9 \times 10^3 \text{ kg/m}^3$  at  $0\text{K}$ .
12. Estimate the energy for which the probability of occupation at  $300\text{K}$  is  $0.1$  for copper with Fermi energy of  $7.0 \text{ eV}$ . Comment on the probability of this level to be  $0.5$ .
13. The Fermi temperature of two metals A and B are in the ratio  $1.103$ . If the electron concentration of metal A is  $5.86 \times 10^{28} \text{ m}^{-3}$ , find the Fermi velocity of electrons in metal B. (Ans:  $1.325 \times 10^6 \text{ ms}^{-1}$ .)
14. Calculate the density of states with energy between  $4\text{eV}$  and  $4.005\text{eV}$  in copper with Fermi energy of  $7.02\text{eV}$ . ( $E = 4\text{eV} = 4 * 1.6 \times 10^{-19} \text{ J}$  and  $dE = .005 * 1.6 \times 10^{-19} \text{ J}$  mass of electron =  $9.1 \times 10^{-31} \text{ kg}$ )

**Contents**

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## 1. Introduction to Magnetic Materials

Every material when placed in an external magnetic field  $\mathbf{H}$  responds in different magnitudes and different ways. Some materials get magnetized either temporarily or permanently, others do not get magnetized but repulse the external magnetic fields. Materials are classified according to the magnetization state of the material.

The intensity of magnetization ( $M$ ) of a material is defined as the dipole moment per unit volume of the material.

$$M = \frac{m * 2l}{2l * a} = \frac{m}{a} \text{ which is the dipole strength per unit area of cross section.}$$

*The first truly scientific study of magnetism was made by the Englishman William Gilbert (1540–1603), who published his classic book *On the Magnet* in 1600. He experimented with lodestones (magnetite) and iron magnets, formed a clear picture of the Earth's magnetic field, and cleared away many superstitions that had clouded the subject. From his experiments, he concluded that the Earth was itself magnetic and that this was the reason compasses pointed north (previously, some believed that it was the pole star (Polaris) or a large magnetic island on the north pole that attracted the compass).*

*The existence of isolated magnetic poles, or monopoles, is not forbidden by any known law of nature, and serious efforts to find monopoles have been made [P. A. M. Dirac, Proc. R. Soc. Lond., A133 (1931) p. 60; H. Jeon and M. J. Longo, Phys. Rev. Lett., 75 (1995) pp. 1443–1446]. The search has not so far been successful.*

$$\text{The magnetization of the material } M = \chi_m H$$

where the magnetic susceptibility  $\chi_m$  of the material is the ratio of the magnetization  $\mathbf{B}$  to the magnetic field  $\mathbf{H}$  ie.,  $\chi_m = \frac{M}{H}$

Consider a long solenoid of length  $l$  with air as the core and having  $n$  turns. The magnetic field strength when a current  $I$  flows through the solenoid  $H = \frac{nI}{l}$  A/m.

$$\text{The magnetic flux density } B_o = \mu_0 H \text{ Tesla (Wb /m}^2\text{)}$$

$$\text{Where } \mu_0 = 4\pi \times 10^{-7} \text{ H/m or } (4\pi \times 10^{-7} \text{ TmA}^{-1})$$

When a material of susceptibility  $\chi_m$  is introduced inside the solenoid the total magnetic flux of the system is the sum of the flux due to the coil and the flux due to the magnetization of the material.

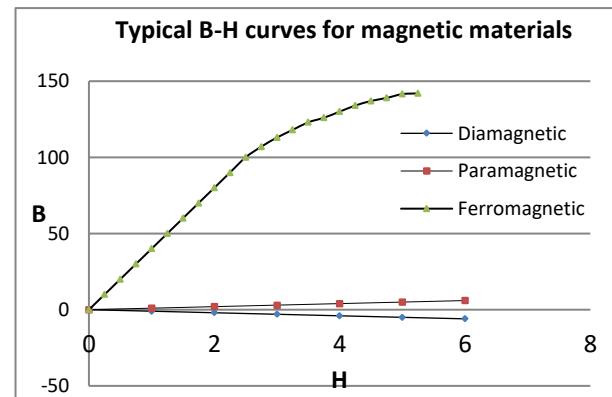
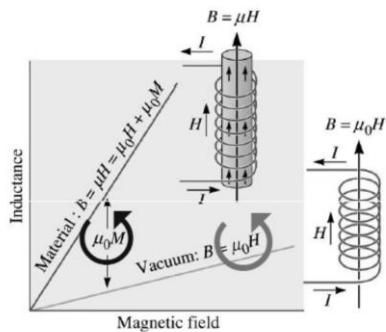
$$B = \mu_0 H + \mu_0 M = \mu_0 (H + M) = \mu_0 (H + \chi_m H) = \mu_0 (1 + \chi_m) H$$

Defining the relative permeability of the material  $\mu_r = (1 + \chi_m)$

The magnetic flux density  $B = \mu_0 \mu_r H = \mu H$ , where  $\mu = \mu_0 \mu_r$  is the permeability of the material.

Magnetic materials can be classified on their susceptibility to be magnetized by an external magnetic field and on their relative permeability.

Materials with susceptibilities less than 0 ( $\chi_m$  negative) are classified as diamagnetic materials. They tend to repel the lines of force of the external magnetic field. The diamagnetic susceptibilities are in the range of  $-10^{-3}$  to  $-10^{-6}$ . Diamagnetic materials possess a relative permeability less than 1.



Materials with a small positive susceptibility  $>0$  ( $\chi_m$  positive) are classified as paramagnetic materials. Paramagnetic materials tend to show feeble magnetization in the presence of an external field. The susceptibility of the material is of the order of  $10^{-4}$  to  $10^{-5}$  and relative permeability is slightly more than 1.

Materials with a large positive susceptibility  $>>0$  ( $\chi_m$  positive and large) are classified as ferromagnetic materials. Ferromagnetic materials are easily magnetized in the presence of an external magnetic field and exhibit a large relative permeability of the order of  $10^5$ - $10^6$ .

## 2. Origin of Magnetism in materials

Any current loop creates a magnetic field with the direction of the current deciding the direction of the field. It is imperative that the atomic level currents due to the electrons in the orbits could result in magnetic fields. The spin of the electrons can also be one of the major contributors to the magnetization in materials. In addition, there is also a feeble contribution from the nuclei as well which could be neglected for all practical evaluations. The net contribution from an atom to the magnetization would depend on the magnitudes of the individual components and the statistical behavior of the collection of atoms would decide the magnetic susceptibility of the material.

The basic atomic model of orbiting electrons around the nucleus constitutes tiny current loops at atomic levels. If the electrons are assumed to move in an orbit of radius  $r$  with a constant speed  $v$ , the period of rotation  $T$ , then the current  $I = \frac{e}{T} = \frac{e\omega}{2\pi} = \frac{ev}{2\pi r}$

The magnetic moment associated with the electron's moment in the orbit

$$\mu_e = I \cdot A = I * \pi r^2 = \frac{ev}{2\pi r} \pi r^2 = \frac{1}{2} evr = \frac{1}{2} e\omega r^2$$

The angular momentum of the orbiting electron  $L = m_e vr$  and the magnetic moment can be written as

$$\mu_{orb} = \left(\frac{e}{2m_e}\right) L$$

Thus the magnetic moment of the electron is proportional to its angular momentum. The ratio of the magnetic moment to the angular momentum  $\gamma = \frac{\mu_{orb}}{L} = \left(\frac{e}{2m_e}\right)$  is known as the gyro magnetic ratio. Due to the negative charge of the electron, the vectors  $\vec{\mu}$  and  $\vec{L}$  point in opposite directions and perpendicular to the plane of the orbit. The angular momentum of the electron is a multiple of  $\hbar$  (quantum mechanical concepts).

The magnetic effect of the orbital motion of the electron is either zero or very small because of the cancellation of the magnetic moments of electrons orbiting in opposite directions.

Apart from the orbital magnetic moments, electrons have the property of spin and a spin angular momentum  $\vec{S}$  associated with it.  $\vec{S}$  is of the same order as the angular momentum  $\vec{L}$ .

The magnetic moment due to the spin of the electrons is almost twice that of the orbital movement and the contribution from the spin to the magnetic moment can be written as  $\mu_{spin} = \sqrt{s(s+1)} \frac{e\hbar}{m}$ .

The total magnetic moment of an atom is the vector sum of orbital and spins magnetic moments.

The net magnetic moment due to electrons

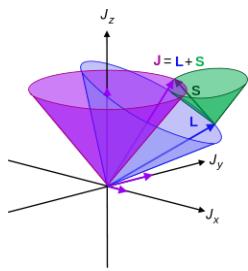
$$\mu_e = g_e \frac{e\hbar}{2m}$$

where  $g_e$  is the Lande g factor (spectroscopic splitting factor of the energy levels) given by  $g_e = 1 + \frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}$

From this the smallest non zero value of the spin magnetic moment due to electrons (when  $s=j$  and  $l=0$ ) is obtained as  $\mu_s = \frac{e\hbar}{m}$

This is twice the orbital magnetic moment and hence determines the susceptibility of materials. The magnetic moment being quantized; the smallest unit of magnetic moment  $\mu_B = \frac{e\hbar}{2m} = 9.27 \times 10^{-24} \text{ J/T}$  is called the Bohr magneton.

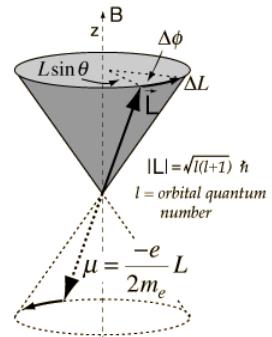
The magnetic moments of protons and neutrons are much smaller than the electron magnetic moment and are usually neglected.



### 3. Larmor precession

A magnetic moment directed at some finite angle with respect to the applied magnetic field direction, experiences a torque  $\mu \times B$ . This causes  $\mu$  to precess (rotate) about the magnetic field direction. (This is analogous to the precession of a spinning top around the gravity field.)

For static magnetic moments or classical current loops, the torque tends to line up the magnetic moments with the magnetic field  $B$ , so this represents its lowest energy configuration.



In the case of an electron in orbit around a nucleus, the magnetic moment is proportional to the angular momentum of the electron. The torque exerted by the external field produces a change in angular momentum which is perpendicular to that angular momentum, causing the magnetic moment to precess around the direction of the magnetic field rather than settle down in the direction of the magnetic field. This is called Larmor precession.

When a torque is exerted perpendicular to the angular momentum  $L$ , it produces a change in angular momentum  $\Delta L$  which is perpendicular to  $L$ , causing it to precess about the  $z$  axis. The effect of the torque as follows:

$$\tau = \mu \times B = |\mu B \sin \theta| = \frac{\Delta L}{\Delta t} = \frac{L \sin \theta \Delta \phi}{\Delta t} = L \sin \theta \omega_L$$

The precession angular velocity (Larmor frequency) is given by  $\frac{d\phi}{dt} = \omega_L = \frac{e}{2m_e} B$  since  $\frac{\mu}{L} = \left(\frac{e}{2m_e}\right)$ .

The Larmor frequency forms the basis for magnetic resonance.

The Larmor precession frequency for electrons is 14GHz/ T which forms the basis of the electron spin resonance.

The Larmor precession frequency for protons is 7.8 MHz/ T which forms the basis of the Nuclear magnetic resonance.

Thus, the magnetic moment due to a precessing charge can be evaluated as

$\mu_{\text{ind}} = \frac{1}{2} e \omega r^2 = \frac{B e^2 r^2}{4m}$  where  $r$  is the radius of the precessing orbit. The sign of this induced magnetic moment is negative by Lenz's law (it opposes the magnetic field that induced the precession).

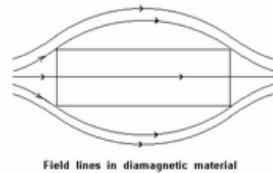
If there are  $N_a$  number of atoms per unit volume and each atom contains  $Z$  electrons we can estimate the total induced magnetisation as  $\mathbf{M} = N_a Z \mu_{ind} = -\frac{N_a Z e^2 r^2 B}{4m} = -\frac{N_a Z e^2 r^2 \mu_0 H}{4m}$

Hence the induced susceptibility  $\chi_m = \frac{M}{H} = -\frac{N_a Z e^2 r^2 \mu_0}{4m}$ .

This will yield an extremely small negative value of the order of  $10^{-5}$  for most materials and is recognized as the diamagnetic response of all materials.

#### 4. Diamagnetic materials

Diamagnetism is a property due to which certain materials are repelled by both poles of a magnet. When a short rod of diamagnetic material is placed in a magnetic field, it aligns itself at right angles to or across the direction of the magnetic lines of force. The meaning of term "diamagnetic" in Greek is "across magnetic".



The orbital motion of electrons is equivalent to tiny atomic current loops, producing magnetic fields. In most materials, the magnetic fields of the orbiting electrons balance each other and add up to zero in the absence of an external field. However, in the presence of an external magnetic field, the interaction of external field with the electrons induces an internal field which tends to align the current loops in a direction opposite to the applied field.

This effect on atomic scale is similar to that due to Lenz's law induced magnetic fields tend to oppose the change which created them. If magnetic response is only due to these phenomena then the material is classified as diamagnetic. Diamagnetism is exhibited by a substance only in the presence of an externally applied magnetic field.

Atoms with closed electronic shells and sub shells are generally diamagnetic (-ve  $\chi_m$  and  $\mu_r < 1$ ). The classical diamagnetic susceptibility is given by

$$\chi_{dia} = -\frac{Ne^2 \mu_0}{6m} \langle r^2 \rangle$$

where  $N$  is the number of atoms per unit volume and  $\langle r^2 \rangle$  is the average value of the square of the radius of the current loops. From the above it is observed that diamagnetic susceptibility is temperature independent.

All materials have inherent diamagnetism. Diamagnetism is detectable and observable only with sensitive instruments and in the presence of powerful magnets. Examples of diamagnetic substances include water, wood, sodium chloride, most organic compounds such as petroleum, some plastics, and many metals including copper, particularly the heavy metals with many core electrons, such as mercury, gold, bismuth and antimony. Most substances usually considered as nonmagnetic may be strictly called as diamagnetic.

The volume magnetic susceptibility of water is  $= -9.05 \times 10^{-6}$

Bismuth the most strongly diamagnetic material has  $= -1.66 \times 10^{-4}$ .

However, superconductors show strong diamagnetic effect (and offer no resistance to the formation of the current loops and conduction of electricity). Lines of magnetic flux are deflected away from the material due to diamagnetism and are expelled completely. These materials can be used in creating strong repulsive magnetic fields and are used in levitation experiments / applications.

## 5. Para magnetism

Paramagnetic materials are weakly attracted by magnetic fields. When a small rod of paramagnetic material is placed in a magnetic field, it aligns with or alongside the lines of force. The term paramagnetic is derived from a Greek word meaning “alongside magnetic”.

Para magnetism is generally a characteristic of materials with partially filled 3d shells, where the Hund's rule restricts the anti-parallel alignment resulting in the net spin magnetic moment for the atoms.

Pierre Curie (1859–1906) was a French physicist who worked extensively on magnetic materials. He and his wife, Marie (Skłodowska) Curie (1867–1934), later became famous for their research on radioactivity.

Materials with unpaired electron spins in the atomic / molecular orbitals have permanent magnetic dipoles even in the absence of an applied field. These dipoles are randomly oriented and do not interact with one another. The thermal energy of the system being greater than the magnetic energy  $k_B T > \mu_B B$ , the thermal agitation result in random ordering and a net zero magnetic moment.

In the presence of an external magnetic field these dipoles tend to align to the applied direction leading to a net magnetic moment in the direction of the applied field. The induced magnetization is weak and linearly dependent on the applied magnetic field. When the magnetic field is removed, the dipoles relax back to their normal random orientation and the magnetization becomes zero. Aluminium, Oxygen titanium, FeO are some examples of materials which are attracted by a magnetic field.



## 6. Quantum theory of Paramagnetic materials (solids).

Some of the features of the quantum theory of Para magnetism are:

The magnetic dipoles of a molecule / atom /ion in a material can be written as

$$\mu = g\mu_B m_j$$

where  $g_e$  is the Lande g factor and  $\mu_B$  is the Bohr magneton. In an external magnetic field  $B$  the dipoles are allowed only certain fixed orientations of the total angular momentum  $J$  and described by  $M_j$ .

For a given  $J$  (the total angular momentum) the allowed orientations are  $2j+1$  ( $j, j-1, j-2, \dots, 0, \dots, -j$ )

and the energy of interaction with an external magnetic field  $B$  is given by

$$E_j = \mu \cdot B = g\mu_B m_j \cdot B = g\mu_o \mu_B H m_j$$

For a material with  $N$  dipoles per unit volume, the net magnetization is the statistical average of the allowed  $m_j$  orientations and is given by

$$M = N \left[ \frac{\sum_{j=0}^{m_j} m_j g \mu_B * \exp\left(\frac{m_j g \mu_o \mu_B H}{kT}\right)}{\sum \exp\left(\frac{m_j g \mu_o \mu_B H}{kT}\right)} \right] \quad \text{eqn. 1.0}$$

Clearly the magnetization will depend on the value of the exponent  $\left(\frac{m_j g \mu_o \mu_B H}{kT}\right)$ .

**Case 1:** If  $m_j g \mu_o \mu_B H \ll kT$  i.e. the thermal energy is significantly higher (high temperatures) than the magnetic interaction energy with field, the ratio will be much less than 1.

Expanding the exponential terms as a power series and simplifying the terms the net magnetization

$$\mathbf{M} = Ng\mu_B * \frac{g\mu_0\mu_B H}{KT} \frac{j(j+1)}{3} = \frac{Ng^2\mu_0\mu_B^2 H}{KT} \frac{j(j+1)}{3}$$

The magnetic susceptibility  $\chi = \frac{\mathbf{M}}{H} = \frac{Ng^2\mu_0\mu_B^2}{KT} \frac{j(j+1)}{3} = \frac{C}{T}$  which is the classical Curie's law of paramagnetic

$$\left\{ \begin{array}{l} \text{Simplification of the expression} \left[ \frac{\sum_{-j}^{+j} m_j g \mu_0 \mu_B H / kT}{\sum \exp(m_j g \mu_0 \mu_B H / kT)} \right] \\ \text{Let } \exp(m_j g \mu_0 \mu_B H / kT) = \exp^{m_j x}, \text{ then the expression simplifies to} \frac{\sum_{-j}^{+j} m_j * \exp(m_j x)}{\sum \exp(m_j x)} \end{array} \right.$$

Since the exponent is small we can expand the exponential term as a series (summation neglecting the higher order term

$$\text{in } x, \frac{\sum_{-j}^{+j} m_j (1 + m_j x)}{\sum (1 + m_j x)} = \frac{\sum_{-j}^{+j} m_j + \sum_{-j}^{+j} m_j^2 x}{\sum_{-j}^{+j} 1 + \sum_{-j}^{+j} m_j x}$$

$m_j$  can take values from  $-j$  to  $= j$  including 0 and  $x$  is independent of  $j$  and hence

$$\sum_{-j}^{+j} m_j = j + (j - 1) + \dots + 1 + 0 - 1 - 2 \dots - (j - 1) - j = 0$$

$$\sum_{-j}^{+j} m_j^2 = 2 \times [1^2 + 2^2 + \dots + (j - 1)^2 + (j)^2] = 2 \times \frac{j(j+1)(2j+1)}{6} = \frac{j(j+1)(2j+1)}{3}$$

$$\sum_{-j}^{+j} 1 = 2j + 1$$

$$\text{Hence } \frac{\sum_{-j}^{+j} m_j (1 + m_j x)}{\sum (1 + m_j x)} = \frac{0 + \frac{j(j+1)(2j+1)}{3} x}{(2j+1)+0} = \chi \frac{j(j+1)}{3} \quad \left. \right\}$$

materials where the Curie constant  $C = \frac{Ng^2\mu_0\mu_B^2}{K} \frac{j(j+1)}{3}$ .

The paramagnetic susceptibility is thus inversely proportional to the absolute temperature.

Curie's law is obeyed under generally prevailing conditions of low magnetization ( $\mu H < k_B T$ ), i.e., when only a relatively small fraction of atomic dipoles are aligned, with the magnetic field. Curie's law indicates that the Magnetization  $M$  depends on the applied field  $H$  (the stronger magnetic field aligns more dipoles) and the susceptibility  $\chi$ . However,  $\chi$  is inversely proportional to the temperature i.e., the magnetization decreases if the temperature is increased (increased thermal agitation prevents alignment of dipoles).

**Case 2:** If  $m_j g \mu_0 \mu_B H \gg KT$  i.e. the magnetic interaction energy is much greater than the thermal energy the exponent will be greater than 1.

Equation 1 can be written as

$$\mathbf{M} = Ng\mu_B \left[ \frac{\sum_{-j}^j m_j * \exp(m_j g \mu_0 \mu_B H / kT)}{\exp(m_j g \mu_0 \mu_B H / kT)} \right] = Ng\mu_B \frac{\sum_{-j}^j m_j * \exp(m_j x)}{\sum \exp(m_j x)} \quad \text{where } x = \frac{g\mu_0\mu_B H}{kT}$$

This can be simplified by taking  $a = xj$  to

$$\mathbf{M} = Ng\mu_B \mathbf{j} \left[ \frac{2j+1}{2j} \coth \left( \frac{2j+1}{2j} a \right) a - \frac{1}{2j} \coth \left( \frac{a}{2j} \right) \right] = Ng\mu_B \mathbf{j} \cdot \mathbf{B}_j(a)$$

where  $B_j(a) = \left[ \frac{2j+1}{2j} \coth\left(\frac{2j+1}{2j}\right)a - \frac{1}{2j} \coth\left(\frac{a}{2j}\right) \right]$  is the Brillouin function which describes the probability of all the dipoles to orienting in the direction of the external field.

When the dipoles are aligned completely in the direction of the external field, the magnetization of the material is saturated, and the saturation magnetization is given by  $M_s = Ng\mu_B$ .

Hence the magnetization can be written as  $M = M_s B_j(a)$ .

When  $j = \frac{1}{2}$  the Brillouin function reduces to  $\tanh(a)$ .

In the limit of large  $j$  the Brillouin function converges to the classical Langevin's function  $L(a) = \coth(a) - \frac{1}{a}$ .

[ $L(a)$  can be written as a series expansion in  $a$  as  $\frac{a}{3} - \frac{a^3}{45} + \frac{2a^5}{945} - \dots$ . For small values of  $a$ , the function then converges to  $\frac{a}{3}$ .]

For small values of  $a$  (large values of  $T$ ) the magnetization reduces to  $M = M_s \frac{a}{3}$  and the susceptibility is given by  $\chi = \frac{Ng^2 \mu_0 \mu_B^2}{3KT}$  which is similar to the Curie's theory of Paramagnetism.

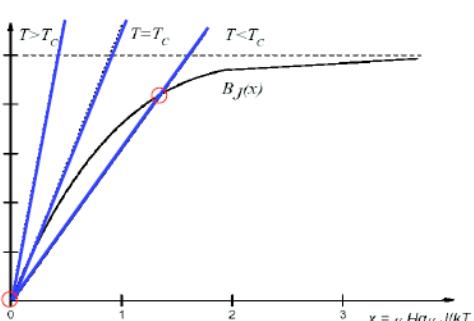
The variation of  $\frac{M}{M_s}$  is represented in the figure for three different cases of the temperature (as compared to  $T_c$  the Curie temperature of the material).

Examples of paramagnetic materials at room temperature include Aluminium (Al), Manganese (Mn), platinum (Pt), Oxygen (gas and liquid), and rare earth ions Ce, Nd.

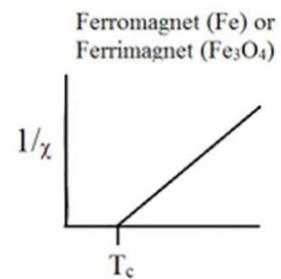
## 7. Weiss Molecular field concept.

The variation of  $\frac{1}{\chi}$  vs  $T$  is expected to be a straight line passing through the origin. However, some materials show a variation in this behaviour with the straight line showing a positive intercept  $T_c$  on the temperature axis.

Weiss in 1907 showed that this could be due to a molecular field which is the field at any point due to the neighbouring dipoles. If  $M$  is the magnetization in the material, then the magnetic field at any point is proportional to  $M$  and hence the field at any point in the material could have an additional contribution  $= \lambda M$ . This field has the tendency to align the dipoles in the direction of the field and hence would be a case of spontaneous magnetisation. Therefore, the Curie's law is modified as  $\frac{M}{H+\lambda M} = \frac{C}{T}$  which gives us  $\chi = \frac{C}{T-T_c}$  where  $T_c = \lambda C$  is the Curie temperature above which the materials show the paramagnetic behaviour. Below  $T_c$  the material behaves as a ferromagnetic material. However, most of the common materials have a low  $T_c$  and hence at normal temperatures does not show the spontaneous magnetization.

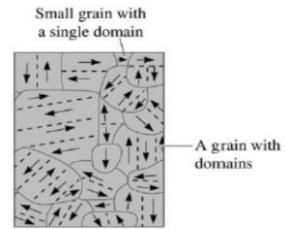


Pierre Weiss (1865–1940), French physicist deserves to be called the “Father of Modern Magnetism” because almost the whole theory of ferromagnetism is due to him, and his ideas also permeate the theory of ferrimagnetism. Most of his work was done at the University of Strasbourg.



## 8. Ferromagnetism

Ferromagnetism is the property by which certain materials are attracted by a magnet and form permanent magnets. Ferromagnetic materials have very high magnetic susceptibilities, ranging from 1000 up to 100,000. Ferromagnetic materials exhibit spontaneous magnetization and exhibit sharp hysteresis characteristics in the magnetisation versus magnetising field.

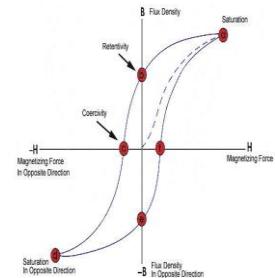


Ferromagnetism can be considered as a case of a Paramagnetic material with a high molecular field constant  $\lambda$  and a very high  $T_c$ .

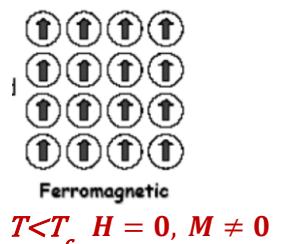
The local molecular field can result in a high ordering of spins in certain materials like Fe, Co, Ni etc, result in the materials being easily magnetised).

The presence of unpaired spins in the 3d shells of these materials gives a large dipole moment for the atom. (Cobalt has a  $T_c > 1000K$ , Fe has a  $T_c > 750K$  and Ni has a  $T_c > 350K$ )

In Ferromagnetic materials when an external magnetic field is applied the magnetic moments are aligned in the direction of the applied field and domains grow at the expense of their neighbours. Microscopic regions in which large numbers of dipoles are aligned are called magnetic domains. The unpaired electron spins to line up parallel with each other. This quantum mechanical interaction at the atomic level gives rise to long range order and creates magnetic domains. The alignment directions of the individual regions are random throughout the material. Hence the bulk of the material is usually unmagnetized or weakly magnetized in the absence of magnetic field.



The magnetisation of the material in the presence of an external magnetic field tends to exhibit the classic M-H hysteresis. When the external field is strong and all the spins are aligned the magnetisation shows a saturation value. When the external field is removed, sizable number of dipoles still maintains the alignment resulting in a net magnetization which is the retentivity of the material. Thus, the material gets permanently magnetized. This remnant magnetisation can be removed if a coercive field  $H_c$  is applied in the reverse direction. Since the material exhibits hysteresis, it is obvious that it has a memory of the previous experience of external fields and hence can be used as memory materials. The flipping of the magnetisation in opposite directions is achieved by applying a saturation magnetisation field  $H_s$  in the appropriate direction.



$$T < T_c \quad H = 0, \quad M \neq 0$$

All ferromagnets have a maximum temperature at which the thermal motion of the dipoles becomes violent, the alignment of dipole moments and spontaneous magnetization cannot be maintained. Phase change from ferromagnetic to paramagnetic behaviour with the usual weak magnetization occurs. This critical temperature is called as the Curie temperature. The magnetic susceptibility above the Curie temperature is given by  $\chi = \frac{C}{T-\theta}$  where  $\theta$  is the transition temperature constant.

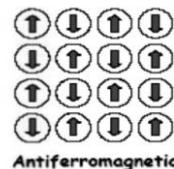
Ferromagnetic materials can be characterized by their Curie temperature in addition to their Permeability, Coercive field and Remnant Magnetization.

Apart from iron, other materials exhibiting ferromagnetic property are nickel, cobalt, some of the rare earths gadolinium, dysprosium, samarium and neodymium in alloys with cobalt. They have important

applications in fabrication of magnets, electromagnets, transformers; magnetic storage media e.g. tape recording, computer hard disks etc.

### 9. Anti-ferro magnetic materials

The magnetisation of a material also depends on the type of ordering that exist in some of the ordered materials. In the case of ferro magnetic materials it is seen that there is a long-range ordering of the magnetic dipoles that lead to strong magnetisation.

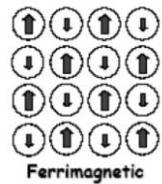


$$T < T_c \quad H = 0, \quad M = 0$$

The class of anti-ferro magnetic materials such as MnO, NiO, CoO etc in which the electron spins associated with the atoms at different crystallographic sites are ordered such that the net magnetisation of the material is zero below a certain temperature called as the Neel temperature  $T_N$ . Above the Neel temperature the materials behave as paramagnetic with the magnetic susceptibility inversely proportional to temperature.

### 10. Ferri magnetic materials

Ferri magnetic materials are a class of ordered structures in which the magnetic moments at crystal sites are anti parallel and unequal. These materials are treated as two sub lattices of a crystal with different magnetic moments and anti parallel alignments. Generally these materials contain cations of two or more types with different magnetic moments and hence show a net magnetisation not equal to zero. Examples of such materials are  $\text{NiFe}_2\text{O}_4$ ,  $\text{CoFe}_3\text{O}_4$ , and  $\text{BaFe}_{12}\text{O}_{19}$  etc.

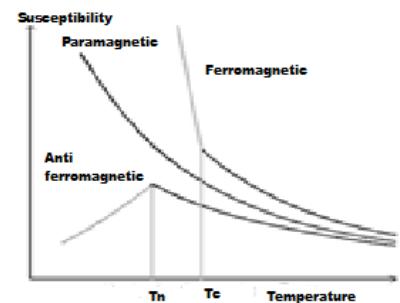


$$T < T_c \quad H = 0, \quad M \neq 0$$

Ferri magnetic materials like ferro magnetic materials show significant magnetisation below the transition temperatures. Above  $T_c$  the materials display paramagnetic behaviour.

### 11. Magnetic susceptibility vs temperature

The temperature dependence of the susceptibility for the Para, Ferro and anti-ferro magnetic materials are summarised as shown. For paramagnetic materials the susceptibility  $\chi_m$  varies monotonically as  $1/T$  following the Curie's law.

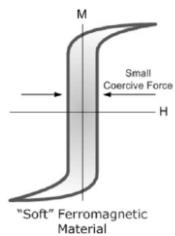


Ferromagnetic materials follow the Curie Weiss law and exhibit a paramagnetic behaviour above the Curie temperature.

Anti-ferromagnetic materials show an increase in susceptibility till the Neel temperature above which the material behaves as a paramagnetic material.

### 12. Soft and Hard Magnetic materials

Ferromagnetic materials can be classified as soft and hard materials depending on the nature of the hysteresis displayed by the material.

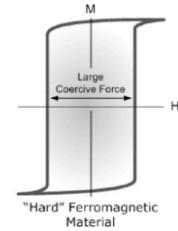


Soft magnetic materials are easily magnetisable and de-magnetisable. They are characterised by a small coercivity and large saturation magnetisation. The hysteresis loop is narrow and has low losses.

Soft magnetic materials find application in high frequency switching of the magnetisation and are used in transformers, motors and generators.

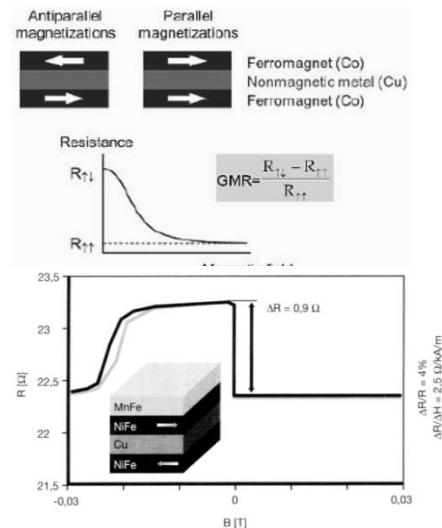
Hard magnetic materials on the other hand are difficult to magnetise and demagnetise. They exhibit a very high retentivity and require a large coercive field to demagnetise the material. The area under the hysteresis curve is large indicating the large amount of energy loss.

The high retentivity of the material makes it ideal for magnetic storage of information as in hard disk drives. The current capabilities are close to 1 Terra bits per square inch.



### 13. Giant Magneto Resistance device.

**scattering of electron is reduced when** Magneto resistance has been observed in layered magnetic materials where the resistance across the thickness of two magnetic layers (generally Cobalt) separated by a non magnetic layer (generally Copper) shows a dependence on the magnetisation states of the individual layers. The resistance to current flow depends on the direction of magnetisation of the two layers and can show large variations in the resistance. The effect has been attributed to the spin scattering of the electrons when they flow through the material. The scattering of electron is reduced when the magnetisation of the two layers is parallel. When the spin state of the two layers are anti parallel the scattering and hence the resistance increases.

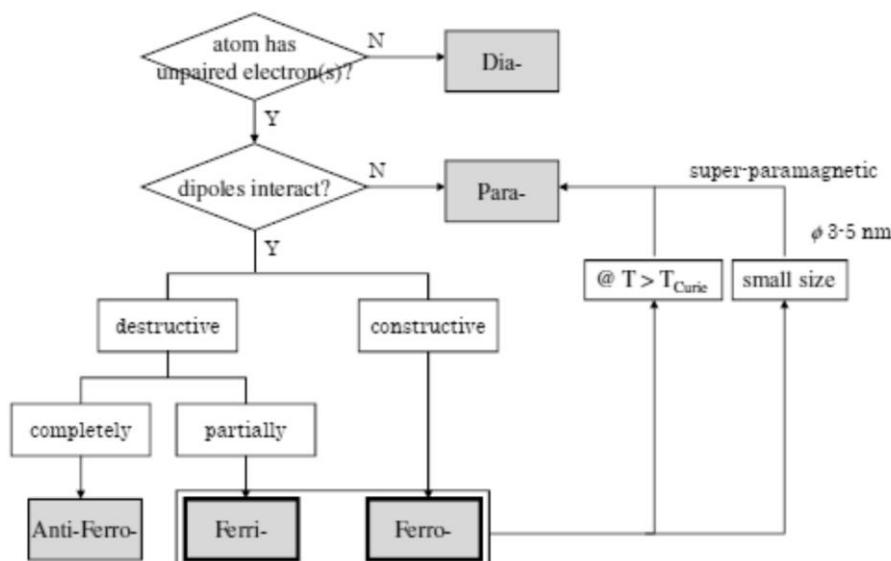


When the magnetic layers are in the range of 3 – 5nm with the separation layer about 25nm, it has been observed that the change in resistance can be as high as 50% of which is significant for any practical measurements and applications.

The Giant Magneto Resistor finds application in the read head of magnetic memories. One of the layers ferromagnetic (soft magnetic material) layer is pinned to an anti-ferro magnetic material and the other (soft magnetic material) free layer's spin orientation is flipped by the magnetisation of the domain (hard magnetic material) on the recording media.

### 14. General classification of magnetic materials

A general scheme for classifying materials according to the atomic characteristics is represented.



**Questions and Problem set**

1. Derive an expression for the Bohr Magneton and calculate the value.
2. Discuss the concepts of Larmor precession and gyromagnetic ratio.
3. Elaborate on two tests which can differentiate a paramagnetic material from a diamagnetic material
4. Discuss the parameters that distinguish ferro, antiferro and ferrimagnetic materials
5. Classify magnetic materials on the basis of the magnetic susceptibility.
6. Bring out the differences between soft and hard magnetic materials.
7. Write a note on applications of magnetic materials
8. Discuss the magnetic hysteresis of materials.
9. Discuss magnetic memory materials.
10. An electron in a hydrogen atom moves in a circular orbit of radius  $0.065\text{nm}$ . The electron makes  $10^{16}$  revolutions per second. Calculate the orbital magnetic moment.
11. The saturation magnetic induction of nickel is  $0.65 \text{ Wbm}^{-2}$ . If the density of nickel is  $8906 \text{ kgm}^{-3}$  and atomic weight is 514.7. Calculate the magnetic moment of nickel in Bohr magneton.

***Magnetism titbits***

- James Clerk Maxwell (1831–1879), Scottish physicist, who developed the classical theory of electromagnetic fields described by the set of equations known as Maxwell's equations.
- Pierre Curie (1859–1906) was a French physicist who worked extensively on magnetic materials. He and his wife, Marie (Skłodowska) Curie (1867–1934), later became famous for their research on radioactivity.

## **Contents**

- 1. Electric fields in dielectrics – concepts of polarization**
- 2. Electric field due to dipoles in the dielectric**
- 3. Polarization mechanisms**
- 4. Non-linear dielectrics – classification of non-centro symmetric systems**
  - a. Piezoelectric**
  - b. Pyroelectrics**
  - c. Ferroelectrics**
- 5. Solved Problems and practice problems**

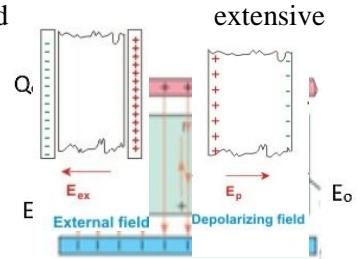
## Unit V Dielectrics

### Polarisation in dielectrics

Dielectrics are a class of material which respond to external electric fields, and find use in the electronics and electrical industry.

From our knowledge of capacitors, the dielectric constant of a material is

- $\epsilon_r = \frac{\text{capacitance of a parallel plate capacitor with the material}}{\text{capacitance of the capacitor without the material}} = \frac{C}{C_0}$
- $\epsilon_r = \frac{\text{field across a parallel plate capacitor without the material}}{\text{field across the capacitor with the material}} = \frac{E_0}{E}$



where  $E_0$  is the applied electric field and  $E$  is the net electric field across the dielectric.

An external electric field can cause the center of positive and negative charges in the crystal to shift from their mean position. This separation of charges results in creation of dipoles in the system. The net dipole moment created per unit volume is called the polarization  $\mathbf{P}$ . The polarization in the material is dependent on the net electric field experienced by the dielectric.

If  $E_0$  is the applied electric field applied to a parallel plate capacitor the surface charge density on the plates of the capacitor  $\sigma = \epsilon_0 E_0$

If a dielectric material is placed between the plates of the capacitor, the surface density of charge due to polarization  $\sigma_p = \epsilon_0 E'$  where  $E'$  is called the depolarization field.

The net electric field  $E$  between the plates is reduced by a factor which is the dielectric constant  $\epsilon_r$  of the material ie.,  $E =$

$$\frac{E_0}{\epsilon_r} \quad \text{or} \quad E_0 = \epsilon_r E$$

$$\text{The net electric field } E = E_0 - E' = \epsilon_r E - \frac{\sigma_p}{\epsilon_0}$$

$$\text{Simplifying } \sigma_p = \epsilon_0 \epsilon_r E - \epsilon_0 E = \epsilon_0 (\epsilon_r - 1) E$$

Hence the polarization in the material due to a net electric field is given by

$$\mathbf{P} = \sigma_p = \epsilon_0 (\epsilon_r - 1) E$$

The polarization of the material can also be written as

$\mathbf{P} = \epsilon_0 \chi \mathbf{E}$  where  $\chi$  is the dielectric susceptibility of the material and is a measure of the ability to create dipoles in the material. The polarization is linearly proportional to the applied electric field for pure dielectrics.

This gives us the relation between susceptibility and dielectric constant

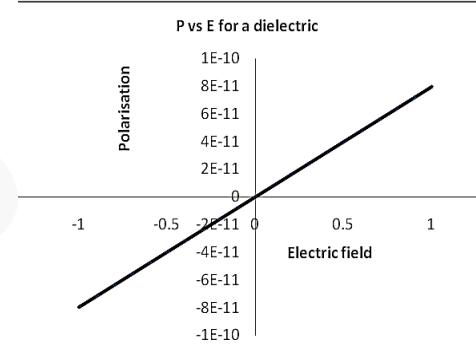
$$\chi = (\epsilon_r - 1) \quad \text{or} \quad \epsilon_r = 1 + \chi.$$

If  $N$  is the number of atoms per unit volume and  $\alpha_e$  is the polarisability of the individual dipoles then the polarization can be written as  $\mathbf{P} = \epsilon_0 \chi \mathbf{E} = N \alpha_e \mathbf{E}$ .

$$\text{Or } \chi = \frac{N \alpha_e}{\epsilon_0}$$

Polarization in dielectrics is thus proportional to the net electric field.

### Electric fields in a dielectric material



To understand the polarization mechanism in totality, it is essential to understand the components of the electric fields which exist in a real dielectric, apart from the applied electric field  $\mathbf{E}$  and the depolarization field  $\mathbf{E}'$ . In general the local electric field inside a dielectric material comprises of four components of electric field.

$$\mathbf{E}_{loc} = \mathbf{E}_o + \mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3$$

$\mathbf{E}_o$  is the external applied electric field ,

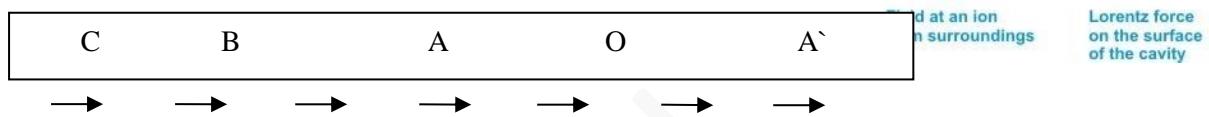
$\mathbf{E}_1$  is the depolarization field,

$\mathbf{E}_2$  is the Lorentz field on the surface of the spherical cavity (scooped out of the dielectric and

$\mathbf{E}_3$  is the field due to other dipoles lying within the sphere.

{ In the case of cubic structures the net Lorentz field can be shown to be zero. The electric field due to the dipoles inside the spherical cavity can be estimated as follows.

Consider a linear array of dipoles at A, B, C A` , B` and C` with dipole moment  $\mu$  at regular intervals of  $d$ .



The electric field at A and A` are equal in strength and direction and equal to

$$\mathbf{E}_A = \mathbf{E}_{A'} = \frac{2\mu}{4\pi\epsilon_0 d^3} \quad \text{and the net electric field } \mathbf{E}_{AA'} = \frac{\mu}{\pi\epsilon_0 d^3}.$$

The electric field at O due to the pair of dipoles equidistant from O can be written as

$\mathbf{E} = \mathbf{E}_{AA'} + \mathbf{E}_{BB'} + \mathbf{E}_{CC'} \dots \dots = \frac{\mu}{\pi\epsilon_0} \left( \frac{1}{d^3} + \frac{1}{(2d)^3} + \frac{1}{(3d)^3} \dots \dots \right) = \frac{\mu}{\pi\epsilon_0 d^3} \sum \frac{1}{n^3} = \frac{1.2 \mu}{\pi\epsilon_0 d^3} = \frac{\gamma P}{\epsilon_0}$  where  $\gamma$  is a constant that depends on the geometry of the material. From the series we can evaluate the contribution of the nearest neighbors and find that only first few pair of neighbors contributes significantly to the electric field at any site. ###

In the case of a dielectric with a cubic structure the effective field can be written  $\mathbf{E}_{in} = \frac{P}{3\epsilon_0}$

Thus the net electric field across the dielectrics will be greater by this factor and given by

$$E_{loc} = E + E_{in} = E + \frac{P}{3\epsilon_0}$$

From the definition of polarization we have  $P = N\alpha_e E$  loc  $= N\alpha_e \left( E + \frac{P}{3\epsilon_0} \right) = \epsilon_0(\epsilon_r - 1)E$

Solving this we get  $\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha_e}{3\epsilon_0}$ . This is the Clausius Mosotti relation which relates the macroscopic dielectric constant to the microscopic polarisability of the material.

It is obvious that the effective microscopic polarisability is greater when the internal fields are considered and should evolve in a more realistic dielectric constant of the material.

[ derivation of the Clausius Mosotti relation:

$$P = N\alpha_e \left( E + \frac{P}{3\epsilon_0} \right)$$

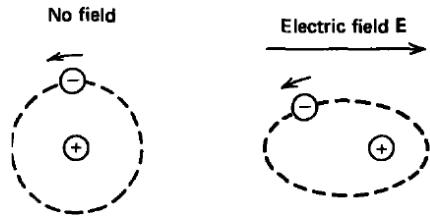
Rearranging terms we get  $P \left( 1 - \frac{N\alpha_e}{3\epsilon_0} \right) = N\alpha_e E$

$$P = \frac{N\alpha_e E}{\left( 1 - \frac{N\alpha_e}{3\epsilon_0} \right)} = \epsilon_0 (\epsilon_r - 1) E, \text{ simplifying} \quad \frac{N\alpha_e / \epsilon_0}{\left( 1 - \frac{N\alpha_e}{3\epsilon_0} \right)} = (\epsilon_r - 1) \quad \text{Taking the inverse}$$

$$\frac{\left( 1 - \frac{N\alpha_e}{3\epsilon_0} \right)}{N\alpha_e / \epsilon_0} = \frac{1}{\frac{N\alpha_e}{\epsilon_0}} - \frac{1}{3} = \frac{1}{(\epsilon_r - 1)} \quad \text{leading to} \quad \frac{1}{\frac{N\alpha_e}{\epsilon_0}} = \frac{1}{3} + \frac{1}{(\epsilon_r - 1)} = \frac{(\epsilon_r + 2)}{3(\epsilon_r - 1)} \quad \text{Hence } \frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha_e}{3\epsilon_0} \quad ]$$

## Polarisation mechanisms

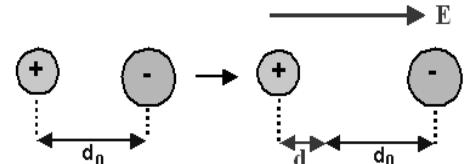
**Electronic polarization :** When an atom is subjected to an electric field  $E$ , the nucleus and the electron cloud will try to move in opposite directions. The nucleus moves in the direction of the applied field and the electron cloud in the direction opposite to that of the applied field. The centre of the negatively charged electron cloud no longer coincides with the positive nucleus and hence results in an induced dipole. The polarization produced due to this induced dipole is called "Electronic polarization".



The electronic polarizability is  $\alpha_e = 4\pi\epsilon_0 R^3$  where  $R$  is the radius of the atom. The electronic polarization is temperature independent since the size of the atom does not depend on temperature.

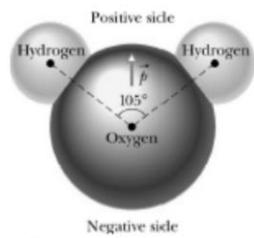
## Ionic Polarisation

Dielectric materials with ionic bonding there exists regular arrangement of positive and negative ions. Ions between any two bond is then a dipole. Because of the symmetric arrangement of the dipoles in the material, the net dipole moment in the material may be zero.



In the presence of an external electric field the elongation of the bond will result in an increased the dipole moment along the direction of the field. However when the ions are displaced from their equilibrium position, a restoring force in the form of the columbic force of attraction tends to constrain the bond elongation.

The displacement of the ions results in a net induced dipole moment per unit volume or the electric field induces polarization in the material. The ionic polarisability  $\alpha_i$  is independent of temperature and depends on the Young's modulus of the material.



## Orientational polarization:

Polar molecules have permanent dipole moments since the net charge centers are separated by a small distance. These dipoles can move and rotate freely (polar liquids - such as the water molecule). However due to the random motion of the molecules at normal temperatures, there is no net polarization in the material.

In the presence of an external field the dipoles tend to align in the direction of the field. This results in a net dipole moment for the material and is called orientational polarization.

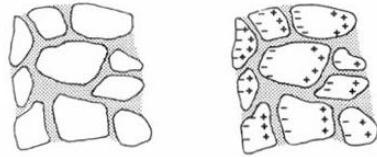
The polarisation is given by  $P = \frac{N\mu^2 E}{3kT}$

Where  $N$  is the no of dipoles per unit volume,  $\mu$  is the dipole moment of the individual molecules and  $T$  the temperature.

Increase in temperature increases the random motion of the dipoles and hence the orientational polarization is highly temperature dependent.

### Space charge limited polarisation

In general when two materials of different conducting phases meet at an interface, a potential barrier layer is formed resulting in an accumulation of charges of the opposite polarities on either sides of the interface. This can be modeled to be a polarization of charges in the bulk of the material. The width of the barrier is generally very small and can result in reasonably high capacitance. These are however very sensitive to voltages and frequencies and may not be effective at normal working conditions.

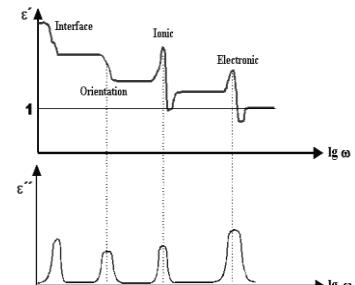


### Frequency dependence of dielectric constant.

The response of the dielectric constant to an applied ac electric field can be understood by considering the ability of the individual dipoles in the material to follow the external AC field. The dielectric constant of an ideal dielectric which has all mechanism contributing to the polarization can be expressed as

$$\epsilon_r = \epsilon_{sp} + \epsilon_{or} + \epsilon_{io} + \epsilon_e$$

The AC electric field induces the dipoles due to the individual polarization mechanisms have to align in the direction of the field. At low frequencies, the dipoles due to all mechanisms tend to align with the electric field easily. As the frequency of the applied electric field increases, the dipoles alignment tends to lag behind the field (depending on the inertia of the dipole). This results in an effective decrease in the polarization of the material as the frequency increases.



The AC response of the dielectric constant can be represented as  $\epsilon = \epsilon' + j\epsilon''$  where  $\epsilon'$  is the real part of the dielectric constant and  $\epsilon''$  is the imaginary part of the dielectric constant which describes the losses in the dielectric.

At low frequencies of about 100Hz, the contribution to the dielectric constant from the space charge polarization disappears and hence the dielectric constant decreases. Beyond this and up to about  $10^9$  Hz remains constant implying all the other three polarization mechanisms are active. At round  $10^9$  Hz (the microwave region) the orientation polarization stops responding to the electric field and the contribution from this mechanism to the dielectric constant becomes zero and the effective dielectric constant of the material decreases to a lower value.

At this point only two polarization mechanisms are contributing to the dielectric constant – the ionic and electronic polarization mechanisms.

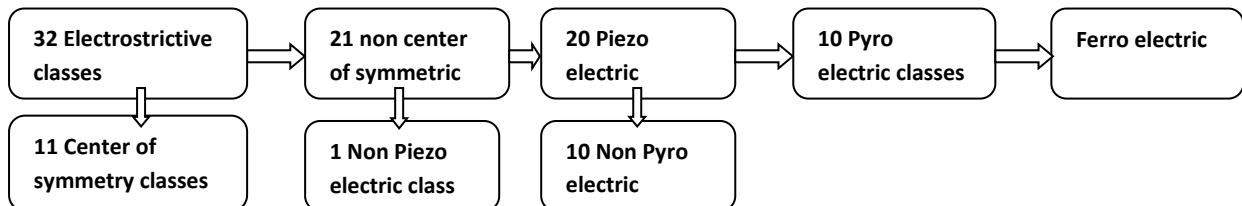
Around  $10^{13}$  Hz (far infra red) the frequency of the AC field is in close to the vibrational frequencies of the bond and resonance phenomena sets in. The dielectric constant shows an initial increase and exhibits a resonance type of behavior around the resonant frequency.

Beyond this range the dielectric constant is only due to the electronic polarization. As the frequency of the AC approaches  $10^{15}$  Hz - the visible range which corresponds to the visible absorption frequency and a resonant condition sets in with a behavior similar to the ionic range.

The material may be treated as transparent to frequencies  $> 10^{16}$  Hz and the dielectric constant should be that of vacuum or free space.

The dielectric loss  $\epsilon''$  represents the energy loss in the dipoles following the electric fields. As the frequency increases generally the inertia of the dipoles becomes significant and at particular frequency ranges the dipoles become inert to the increasing ac frequency. } } # # #

### Classification of non linear dielectric materials

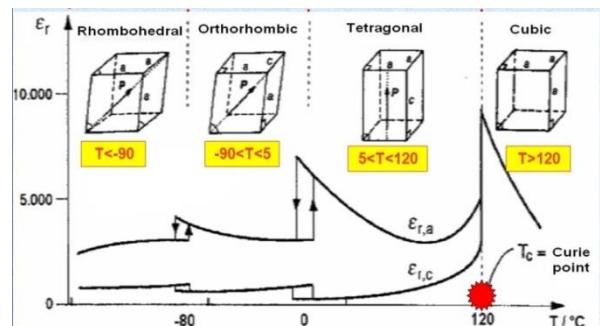
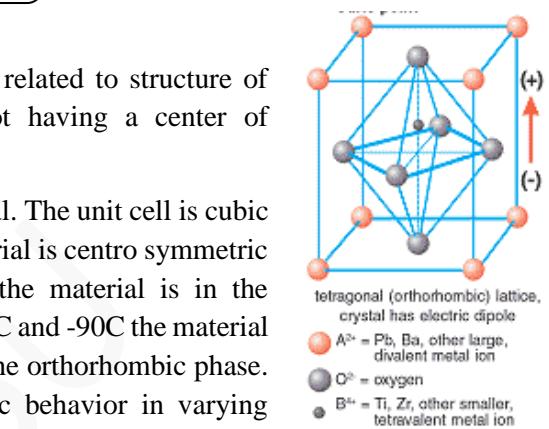


### Non Centro-symmetric system

Out of a total of 32 crystal point groups (see the course related to structure of materials), 21 are non-centrosymmetric *i.e.* crystals not having a center of symmetry.

BaTiO<sub>3</sub> is a good example of a non centro symmetric crystal. The unit cell is cubic above the curie temperature of about 120 C, when the material is centro symmetric and behaves as a paraelectric. Between 5C and 120C the material is in the tetragonal phase exhibiting ferroelectric behavior. Below 5C and -90C the material has a orthogonal phase and below -90C the material is in the orthorhombic phase. In all these phases also the material exhibit ferroelectric behavior in varying proportions.

These dipoles arise due to the fact that in the tetragonal unit cell of BaTiO<sub>3</sub>, the Ti<sup>4+</sup> cation is surrounded by six O<sup>2-</sup> anions in a slightly deformed octahedral configuration, and can occupy one of two asymmetrical sites. In either position, the Ti<sup>4+</sup> cation is not coincident with the negative charge center of the oxygen anions by a small fraction of an Angstrom, creating an electric dipole. The energy barrier between the two possible Ti atom positions is sufficiently low to permit motion of the atom between sites by the coercion of an electric field, and the material can thus be directionally polarized with ease.



Non centro symmetric crystals can respond to an external stimulus producing polarization or surface charges which show up as a potential across the element. However these properties are highly anisotropic and could be described as a tensor (which describes the direction dependent properties of materials). Piezoelectric behavior is the response of these crystals to external mechanical pressures; Pyroelectric behavior is the response to thermal changes and Ferroelectric behavior is a response of the material to external electric fields.

### Piezoelectric materials

Piezoelectric Effect is appearance of an electrical potential across some faces of some crystals when a pressure is applied to the crystal. Pierre Curie and his brother Jacques discovered the effect in 1880. Subsequently the inverse piezoelectric effect was observed as a distortion in the crystal when an electrical field is applied.

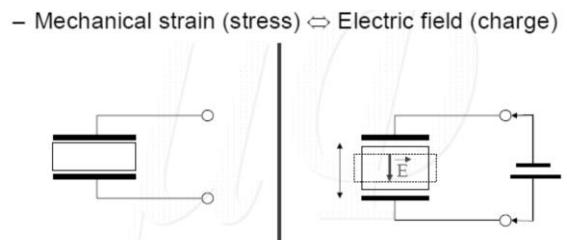
The term piezoelectricity refers to the fact that, when a crystal is strained, an electric field is produced within the substance. As a result of this field, a potential difference develops across the sample, and by measuring this potential one may determine the field. The inverse effect - that an applied field produces strain - has also been observed. It is explained by the displacement of ions, causing the electric polarization of the crystal's structural units. When an electrical field is applied, the ions are displaced by electrostatic forces, resulting in the mechanical deformation of the whole crystal.

The piezoelectric effect is very small. A field of  $10^3$  V/cm in quartz ( $\text{SiO}_2$ ) produces a strain of only  $10^{-7}$ . That is, a rod 1 cm long changes its length by  $10\text{\AA}$ . Conversely, even small strains can produce enormous electric fields.

The piezoelectric effect is often used to convert electrical energy into mechanical energy, and vice versa; i.e., these materials are used to make transducers. For instance, an electric signal applied to the end of a quartz rod generates a mechanical strain, which consequently leads to the propagation of a mechanical wave - a sound wave - down the rod.

Piezoelectric materials like PZT ( $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$ ), and Quartz find extensive application in electronics as sensors and actuators.

- Piezoelectric microbalances are used as very sensitive chemical and biological sensors.
- Atomic force and scanning tunneling microscopes for precision manipulation of sample at nano meter levels
- Transient pressure measurement to study explosives, internal combustion engines (knock sensors), and any other vibrations, accelerations, or impacts.
- Energy Harvesting from impact on the ground
- Electric igniters
- Transducers are used in electronic drum pads to detect the impact of the drummer's sticks.



### Pyroelectric materials

Pyroelectricity is the ability of certain materials to generate an electrical potential when they are heated or cooled. Non centrosymmetric crystals with a net spontaneous polarization can be sensitive to external temperatures.

The change in temperature modifies the positions of the atoms slightly within the crystal structure, such that the polarization of the material changes. This polarization change gives rise to a voltage across the crystal. If the temperature stays constant at its new value, the pyroelectric voltage gradually disappears due to leakage current (the leakage can be due to electrons moving through the crystal, ions moving through the air, current leaking through a voltmeter attached across the crystal, etc.).

The pyroelectric coefficient may be described as the change in the spontaneous polarization vector  $\mathbf{P}_s$  with temperature  $T$

$$\mathbf{p}_i = \frac{\partial \mathbf{P}_s}{\partial T} \quad \text{where } p_i (\text{Cm}^{-2}\text{K}^{-1}) \text{ is the vector for the pyroelectric coefficient.}$$

It can be used to create a flow of current in an external circuit connected to a device using pyroelectric materials. The effect has been known for many years, but it is only since about 1960 that its technological applications have been seriously considered.

These have been almost entirely in the field of the detection of electromagnetic radiation, especially in the two “atmospheric window” infrared (IR) bands of 3-5 pm and 8-14 pm. The ambient temperature operation of pyroelectric detectors, leading to low power consumption, low cost, compactness.

Pyroelectric detectors have found a huge range of applications in products ranging from fire alarms to intruder detectors, in instrumentation such as gas analysis and laser beam characterization and in military/paramilitary applications such as thermal imaging.

### **Ferroelectric materials**

Charge displacements in dielectric and para electric ceramics, such as  $\text{Al}_2\text{O}_3$ , mica,  $\text{TiO}_2$ , are totally reversible, as ions / electron cloud return to their original position once an applied field is removed, and the polarization effect is linear.

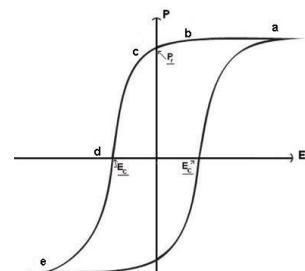
Ferroelectrics are a class of non-centro symmetric crystals which are also a subclass of the pyro electric / piezoelectric materials. These materials show a spontaneous polarization even in the absence of an electric field.

The spontaneous polarization observed in ferroelectric materials depends on the crystalline phase of the material (generally referred to as perovskites).  $\text{BaTiO}_3$  is a classic example of a perovskite material.

The dielectric susceptibility of the material is highly temperature dependent and is given by  $\chi = \frac{C}{T - T_c}$

for all  $T > T_c$  where C is a constant dependent on the material and  $T_c$  is the curie temperature. At temperature below  $T_c$ , the material shows spontaneous polarization and is classified as a ferroelectric material. At temperatures greater than  $T_c$ , the material is para electric with the susceptibility inversely proportional to temperature.

Ferroelectric dielectrics differ from dielectric materials in their response to external applied electric field. Ferroelectrics display a nonlinear response of polarization to changing electric fields and display a hysteresis in the P versus E variations. The hysteresis loop is caused by the existence of permanent electric dipoles in classes of materials, which develop spontaneously below the Curie temperature. The polarisation state of the ferroelectric material has a memory effect and hence is used extensively in DRAMs and SRAMs.



Ferro electric materials find numerous applications as sensors and actuators taking advantage of the temperature and field dependencies of the susceptibility (dielectric constant).

**Solved examples**

- 1. The surface density of charge of a parallel plate capacitor is  $7.2 \times 10^{-10} C m^{-2}$ . A dielectric medium with  $\epsilon_r = 12$  is introduced between the plates of the capacitor. Estimate the induced surface density of charge on the dielectric surface and the electric fields between the plates with and without the dielectric material.**

The electric field across the plates of the capacitor without dielectric  $E_o = \frac{\sigma_o}{\epsilon_0} = 81.35 V/m$

The electric field across the dielectric due to surface charges  $= E_p = \frac{\sigma_p}{\epsilon_0}$

$$\sigma_p = (\epsilon_r - 1) \frac{\sigma_o}{\epsilon_r} = 6.6 \times 10^{-10} C m^{-2}.$$

Electric field across dielectric  $= \frac{\sigma_p}{\epsilon_0} = 74.57 V/m$

Electric field across the plates with the dielectric  $= 6.78 V/m$

- 2. A dielectric medium with  $\epsilon_r = 25$  is introduced between the plates of the capacitor with surface density of charge on the plates equal to  $8.00 \times 10^{-10} C m^{-2}$ . Estimate, the electric fields between the plates with and without the dielectric material and the surface density of charge on the dielectric.**

The electric between the plates of the capacitor without the dielectric

$$E_o = \frac{\sigma_o}{\epsilon_0} = 90.40 V/m$$

The electric field between the plates with the dielectric  $= \frac{E_o}{\epsilon_r} = 3.62 V/m$

The electric field across the dielectric  $E' = 86.78 V/m$

The surface density of charge on the dielectric  $\sigma = E' * \epsilon_0 = 7.68 \times 10^{-10} C m^{-2}$

- 3. An elemental dielectric has  $\epsilon_r = 10$  and contains  $7.5 \times 10^{29} \text{ atoms } /m^3$ . Calculate the electronic polarisability of the material..**

$$P = \epsilon_0(\epsilon_r - 1)E = N\alpha_e E \quad \text{Given } \epsilon_r = 10$$

$$\alpha_e = \frac{\epsilon_0(\epsilon_r-1)}{N} = \frac{8.85 \times 10^{-12} \times 9}{7.5 \times 10^{29}} = 10.62 \times 10^{-41} F m^2$$

**Problem Set:**

- If the molecular dipoles in a  $10^{-3} m$  radius water drop are pointed in the same direction, calculate the polarisation of the water drop. Dipole moment of water molecule is  $6 \times 10^{-30} C m$ .
- Assuming that the polarisability of Kr atom is  $2.18 \times 10^{-40} F m^2$ , calculate its dielectric constant. Kr has  $2.7 \times 10^{25}$  atoms per unit volume at NTP.
- An elemental dielectric has  $\epsilon_r = 12$  and contains  $5 \times 10^{29} \text{ atoms } /m^3$ . Calculate the electronic polarisability of the material.
- Find the total polarisability of  $CO_2$  if its susceptibility is  $0.985 \times 10^{-3}$ . Density of  $CO_2$  is  $1.977 \text{ Kgm}^{-3}$ .
- On being polarised an oxygen atom shows a dipole moment of  $0.5 \times 10^{-22} C \cdot m$ . If the distance of the center of the -ve charge cloud from the nucleus is  $4 \times 10^{-17} m$ , calculate the polarisability of oxygen.

6. A parallel plate capacitor without a dielectric is charged such that the surface charge density on the plates is  $10^6 \text{ C-m}^{-2}$ . If a slab of a material with dielectric constant 10 is inserted between the plates, calculate the polarisation in the material and the electric field due to induced surface charge on the dielectric.
7. A dielectric material has one species having an atomic polarizability value of  $10^{-30} \text{ Cm}^2\text{V}^{-1}$ . It is found that when the dielectric sample is kept in a uniform electric field, the field reduces to one tenth of its original value. Estimate the number of atoms per unit volume of the material.
8. Electronic polarisability of Sulphur is  $3.28 \times 10^{-40} \text{ F-m}^2$ . Calculate the dielectric constant of Sulphur if the density and atomic weight of Sulphur are  $2.08 \times 10^3 \text{ kg-m}^{-3}$  and 32 respectively.

**Unit IV LASERS****Contents :**

1. Introduction – interaction of radiation with matter – Einstein's Coefficient
2. Conditions for laser action
  - a. Two level system
  - b. Three level system
  - c. Four level system
3. Basic requirement of a laser system
4. Round trip gain in a laser medium
5. Properties of LASERs.
6. Atomic LASER - He Ne LASER system
7. Molecular LASER – CO<sub>2</sub> LASER system
8. Semiconductor LASER – CO<sub>2</sub> LASER system

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### Introduction

LASER is the acronym for Light Amplification by Stimulated Emission of Radiation. Einstein analyzed the interaction of radiation with matter and formalized the rate equations for induced absorption and spontaneous emission. He also conceptualized stimulated emission as a probable emission mechanism emission from excited atoms. From the discussions that follow it will be evident that the process of stimulated emission is the key to a LASER system.

#### 1. Interaction of radiation with matter – Einstein's coefficients

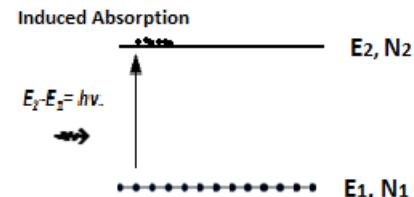
The interaction of radiation with matter can be explained by the three processes namely

- **Induced absorption (stimulated absorption )**

In the induced absorption process an atom in the ground state / lower energy state ( $E_1$ ) absorbs radiation and is excited to the higher state ( $E_2$ ). The rate of absorption is dependent on the population of the ground state  $N_1$  / lower energy state and the energy density of radiation ( $\rho(hv)$ ) of the appropriate frequency such that  $h\nu = E_2 - E_1$ .

$$\text{The rate of induced absorption } R_{ind\ abs} = B_{12} * N_1 * \rho(v)$$

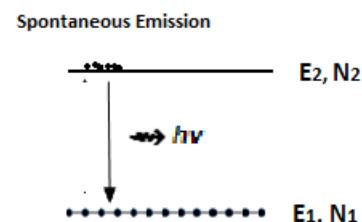
where  $B_{12}$  is the Einstein's coefficient for induced absorption.



- **spontaneous emission**

An atom in the higher energy / excited state cannot normally remain in the excited state for a long time and generally de-excites to the lower energy state spontaneously. The lifetimes of the excited states are generally of the order of nanoseconds. The rate of spontaneous emission is dependent on the population of atoms in the excited state  $N_2$  only and

$$R_{sp\ em} = A_{21} * N_2 \quad \text{where } A_{21} \text{ is the Einstein's coefficient for spontaneous emission.}$$

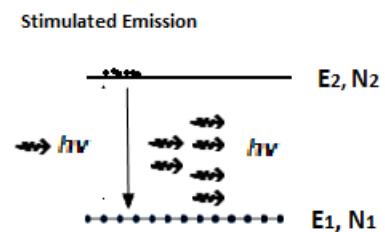


If the process of spontaneous emission is predominant we can infer that  $R_{sp\ em} = -\frac{dN_2}{dt} = A_{21} * N_2$ .

From this we can infer that  $N_2 = N_2(0)e^{-A_{21}t}$  and the Einstein's co-efficient for spontaneous emission can be understood to be  $A_{21} = \frac{1}{\tau}$  where  $\tau$  is the average life time of electrons in the upper energy state for spontaneous emission.

- **Stimulated emission.**

An atom in the excited state can have a life time in the excited state for longer periods of time of the order of milliseconds to few seconds. These states are referred to as Meta stable states. Such excited atoms have to be stimulated to return to the lower energy state with an external intervention in the form of a photon whose energy is equal to  $E_2 - E_1$ . In this process the energy of the excited atom is released as a photon whose characteristics remain the



same as that of the stimulating photon. This process sets in a chain of photon emission where all the photons are in the same state. The rate of stimulated emission is then dependent on the population of atoms in the excited state and the energy density of radiation is given by

$$R_{\text{stem}} = B_{21} * N_2 * \rho(\nu) \quad B_{21} \text{ is the Einstein's coefficient for stimulated emission.}$$

When the material is in thermal equilibrium with the radiation, the rate of absorption should be equal to the rates of emission due to different processes ie.,  $B_{12} * N_1 * \rho(\nu) = A_{21} * N_2 + B_{21} * N_2 * \rho(\nu)$

This gives

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

$$\rho(\nu) = \frac{A_{21} * N_2}{(B_{12} * N_1 - B_{21} * N_2)} = \frac{A_{21}/B_{21}}{\left(\frac{B_{12} * N_1}{B_{21} * N_2} - 1\right)}$$

The distribution of electrons in the energy states are described by the Maxwell Boltzmann distribution laws and are given by  $\frac{N_1}{N_2} = \exp^{\frac{(E_2 - E_1)}{kT}} = \exp^{\frac{hv}{kT}}$ . Substitution of this in the equation for energy density gives the expression for the energy density of radiation as

$$\rho(\nu) = \frac{A_{21} * N_2}{(B_{12} * N_1 - B_{21} * N_2)} = \frac{A_{21}/B_{21}}{\left(\frac{B_{12}}{B_{21}} \exp^{\frac{hv}{kT}} - 1\right)} \quad (1)$$

Comparing this with the Planck's expression for energy density of radiation at any frequency and temperature

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3} \frac{1}{\left(\exp^{\frac{hv}{kT}} - 1\right)} \quad (2)$$

Comparing term by term we observe that  $A_{21}/B_{21} = \frac{8\pi h\nu^3}{c^3}$  and  $\frac{B_{12}}{B_{21}} = 1$ . This implies that  $B_{12} = B_{21} = B$  i.e., the induced absorption coefficient is equal to the stimulated emission coefficient and the ratio of the coefficient of spontaneous emission to the coefficient of stimulated emission is proportional to  $\nu^3$ .

For a system to have a predominant stimulated photon emission, then the ratio of the rate of stimulated emission to the rate of spontaneous emission should be greater than 1.

Thus  $\frac{B * N_2 * \rho(\nu)}{A * N_2} = \frac{\rho(\nu)}{\frac{A}{B}} = \frac{1}{\left(\exp^{\frac{hv}{kT}} - 1\right)} \approx \exp^{-\frac{hv}{kT}} = \frac{N_2}{N_1}$ . (Since  $hv \gg kT$ ,  $\exp^{\frac{hv}{kT}} \gg 1$  for visible radiations at normal temperatures).

This implies that the rate of stimulated emission will be predominant over rate of spontaneous emission if and only if  $N_2 > N_1$  or the population of the higher energy state is higher than the lower energy state. This condition is referred to as the population inversion.

## 2. Conditions for the lasing action

### Two level systems

The basic requirement for light amplification to occur is that the stimulated emission is the predominant emission mechanism over the spontaneous emission mechanism (which is the natural response of a system).

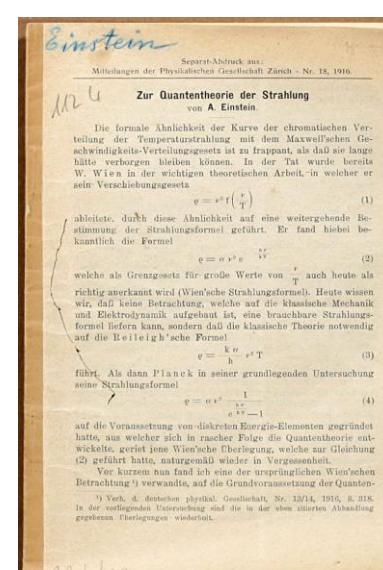
From the discussion it is evident that stimulated emission is possible when the upper energy state has a higher population of occupation than the lower energy state. For a two level laser system this requires  $N_2 > N_1$  or population inversion has to be established between the higher and lower energy states. But from the MB distribution function we find that

$$\frac{N_1}{N_2} = \exp \frac{hv}{kT} \gg 1.$$

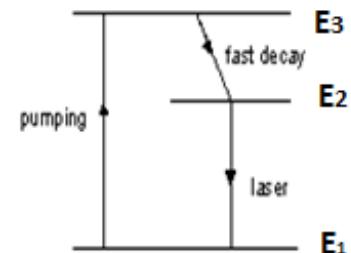
For a two level system in equilibrium this implies that T has to be negative if  $N_2$  has to be greater than  $N_1$ . Hence it is not possible to obtain population inversion between  $E_2$  and  $E_1$  in a two level system and it may not be possible to get a LASER beam from absorption and emission between two energy levels. The understanding is that it is not possible to get a LASER if the same levels are involved in both the emission and absorption process.

### b. Three level systems:

The introduction of an intermediate level between the ground state and the upper excited state can result in decoupling the emission process and absorption process levels. The absorption process is between the ground state  $E_1$  and the upper excited state  $E_3$ . The electrons from the upper energy state decays non-radiatively to the intermediate meta stable state  $E_2$ . If this state is a meta stable state (lifetime of the electrons  $\approx 10^{-3}$  seconds), electrons can accumulate in this state and the population of electrons in the meta stable state could be higher than the population of the ground state in a very short time resulting in a favorable condition for stimulated emission from  $E_2$  to  $E_1$ . However, the drawback is that the ground state is quickly depleted resulting in a discontinuous phenomenon of stimulated emission. Generally, three level systems give a pulsed LASER. This is because the ground state is still a common factor in the absorption and emission process.

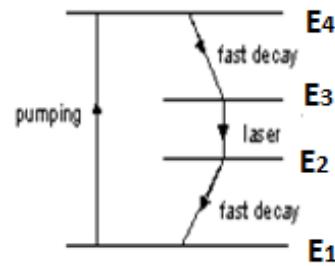


Einstein's original paper on radiations 1917.



### c. Four level systems:

A four level system can effectively decouple the absorption levels and the emission levels. In a four level system the absorption is between the lower (ground) state  $E_1$  and the higher excited state  $E_4$ . The electrons in the excited state decays non radiatively to the intermediate meta stable state  $E_3$ . The electrons are stimulated to transit to a lower energy state  $E_2$  (above  $E_1$ ).



Finally the electrons from the level  $E_2$  fall back to the ground state maintaining the population of the lower  $E_1$  so that the process of excitation can continue. The absorption is between  $E_1$  and  $E_4$  whereas the stimulated emission is between  $E_3$  and  $E_2$ . Thus the energy states in the two processes are completely decoupled. In this way the system can behave in a continuous mode and can produce a continuous LASER.

### 3. Basic requirements of a laser system

- I. **Active medium** – The active medium consists of the medium which possess the appropriate energy levels which are meta stable states. The presence of the meta stable states increases the probability of population inversion which is a prime condition for laser action. The active medium could be solids, liquids or gases depending on the type of lasers.
- II. **Energy pump** – The constituents of the active medium have to suitably excited to the lasing high energy state from an external energy source. The external energy sources could be optical, thermal, electrical or chemical depending on the type of lasers. In the case of gas lasers, generally an electrical discharge is a sufficient source for exciting the medium.
- III. **Resonating Cavity** – Once the lasing action is initiated it is essential that the stimulated emission in the desired wavelength is amplified to get a sustainable laser action of sufficient intensity. The design of the optical cavity is an important aspect of the laser system.

The optical cavity may be the active medium of a suitable dimension (in the case of a solid state laser system) or a suitable enclosure for the gas or liquid as the case may be.

The emitted photons are contained in the cavity through multiple reflections by highly aligned mirrors at the end of the cavity. The reflectivity of one of the mirrors could be close to 100% while the second mirror could be 90-98% reflective.

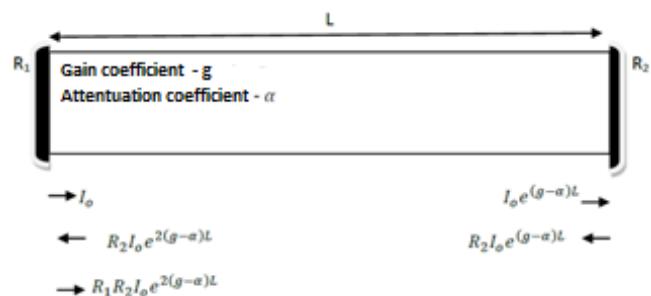
In general the optical cavity has to be a narrow region whose length in the direction of propagation is a half integer multiple of the desired wavelength.

This helps in the reflected beam to be in phase with the incident beam thus preventing photon loss due to destructive **interference**.

### 4. Round trip gain in a laser medium

The stimulated emission in the medium provides for gain with a optical feedback mechanism of reflecting mirrors on both ends of the cavity. This arrangement results in multiple travel of the trapped optical beam in the medium and ideally the beam should have a high intensity after few reflections. The gain of photons as the beam progresses is given by the intensity increasing as  $I = I_o e^{gx}$  where  $g$  is the gain coefficient.

However, there could be also losses in the medium due to absorption, scattering and the partial transmission from one of the mirrors. The reduction in the intensity due to scattering and absorption is described by  $I = I_o e^{-\alpha x}$  where  $\alpha$  is the loss coefficient.



In order to reach a steady-state with non zero intensity (oscillation) the gain due to stimulated emission must be sufficient to overcome these losses.

In general the intensity of the photon beam as it travels a distance  $x$  in the medium can be written as

$$I = I_0 e^{(g-\alpha)x}$$

Consider a beam of photons of intensity  $I_0$  originating from one of the cavity of length  $L$  at  $x=0$ .

One round trip of the photons is then the process where

- the photons starting from the face of the first mirror travel the length  $L$  to the second mirror
- gets reflected at the mirror with reflectivity  $R_2$
- travels back to the first mirror covering a distance of  $L$
- and reflected back from the mirror with reflectivity  $R_1$

The intensity of the beam after one round trip gain is  $I = I_0 R_1 R_2 e^{2(g_0 - \alpha)L}$

The amplification factor is then the ratio of the output intensity to the input intensity and should be equal to  $R_1 R_2 e^{2(g_0 - \alpha)L}$ .

If  $R_1 R_2 e^{2(g_0 - \alpha)L} > 1$ , oscillations can build up and the laser is said to be above the threshold. The threshold of laser oscillations is then defined by  $R_1 R_2 e^{2(g_{th} - \alpha)L} = 1$

$$g_{th} = \frac{1}{2L}(2\alpha L - \ln(R_1 R_2))$$

This implies that the gain of the system can be tuned with the length of the cavity and the reflection coefficients of the two mirrors.

## 5. Properties of LASERs.

The most important properties of a LASER are attributed to the stimulated emission of photons (BOSONS which display identical properties)

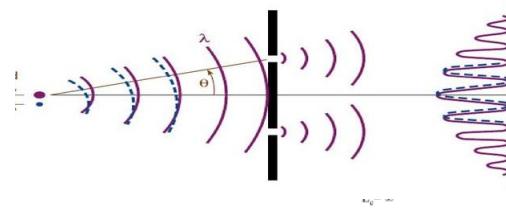
1. **Monochromaticity (spectral line broadening):** Light from a laser typically comes from an atomic transition with a single precise wavelength. So, the laser light has a single spectral color and is almost the purest monochromatic light available. However, the laser light is not truly monochromatic.

The emission line widths are also limited by the uncertainty principle which limits the accuracy of the energy ( $\Delta E$ ) of the photons emitted by electrons which spend times with a spread in time ( $\Delta t$ ). Generally, LASER line widths  $\Delta\lambda$  are very small of the order of  $10^{-6}$  Å as compared to 1 Å for ordinary monochromatic sources.

The spectral emission line has a finite width due to Doppler Effect of the moving atoms or molecules from which the transitions occur. Since the wavelength of the light is extremely small compared to the size of the laser cavities used, many resonant modes of the tiny spectral bandwidth can exist in the laser cavity.

Light source	Center Wavelength $\lambda_0$ (Å <sub>0</sub> )	FWHM Line width $\Delta\lambda_0$ (Å <sub>0</sub> )	FWHM line width $\Delta\nu$ (Hz)
Ordinary discharge lamp	5896	≈1	9X10 <sup>10</sup>
Cadmium low-pressure lamp	6438	≈0.013	9.4X10 <sup>8</sup>
Helium-neon laser	6328	≈10 <sup>-7</sup>	7.5X10 <sup>3</sup>

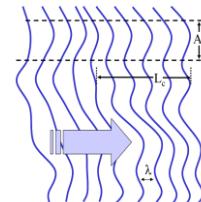
2. **Coherence** - Coherence is a unique property of laser light. In the stimulated emission process triggered by a common, the emitted photons are "in phase" or have a definite phase relation to each other. This coherence is essential to produce high quality interference, which is used to produce holograms.



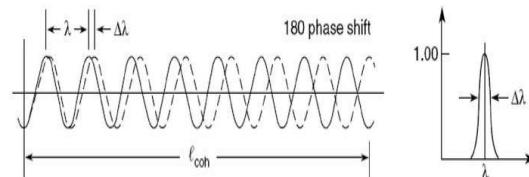
Ordinary light is incoherent because it comes from independent atoms, which emit on time scales of about  $10^{-8}$  seconds. There is a degree of coherence in sources like the mercury green line and some other useful spectral sources, but their coherence does not approach that of a laser.

Coherence can be of two types of temporal coherence and spatial coherence.

- **Temporal coherence** refers to the correlation between the field at a point and the field at the same point after an elapse of time. If the phase difference between the two fields is constant during the period (of the order of microseconds), the wave is said to have said to have temporal coherence. If the phase difference changes many times and in an irregular way during the period of observation, the wave is said to be non-coherent.



Temporal coherence is characteristic of a single beam of light. The temporal coherence is evaluated as  $\tau_c = \frac{1}{\Delta\nu}$  where  $\Delta\nu$  is the spread in the frequency of the Laser. The coherence length defines the largest distance for which interference can be well defined and is given by  $l_c = \tau_c \cdot c$  where  $c$  is the velocity of light.



The length in which the coherence exists may be of the order of kilometers for LASERS compared to few centimeters for ordinary light.

- **Spatial coherence** - Two fields at two different points of a wave front is said to be spatially coherent if they preserve a constant phase difference over any time  $t$ . Two beams of light originating from different parts of a source will have been emitted by different groups of atoms. Each beam will be time incoherent and will have random phase changes. Two such beams are said to be spatially incoherent and the interference pattern produced by these will have a poor visibility. When visibility of the interference pattern as a function of the size of the source then we have spatial coherence and is described by the coherence width  $l_w \approx \frac{\lambda D}{d}$ .

3. **Divergence** (directionality) – LASER is characterized by a very low divergence which ensures that the beam profile is small over long distances. The divergence of a LASER beam is given by  $\theta = \frac{\lambda_o}{\pi\omega_o}$  where  $\lambda_o$  is the wavelength, and  $\omega_o$  is the spot size. Typically, the divergence is of the order of mill radians ( $0.001^\circ$ ). A common lab laser beam of a wavelength of 532nm and a radius of 1mm on the surface of the earth would have a diameter of 6.50 km on the surface of the moon. ( $\theta = (2/\pi) * (532 \text{ e-9} / 2 * 10^{-3}) =$

$1.7 \times 10^{-4}$  this is then multiplied by the distance to the moon ( $3.844 \times 10^8$  m), which gives the spot size to be 65192 m.)

4. **Intensity** – The high intensity of a Laser arises out of the properties of monochromaticity, coherence and low divergence. Typically, very low power LASERs of about 1 to 2mW output with a beam diameter of 1 mm can result in an intensity of about  $10 \text{ kW/m}^2$  as against an intensity of  $10\text{W/m}^2$  produced by a 20W bulb.

## 6. Atomic LASER – He-Ne LASER system

**Active medium:** The He-Ne LASER is a atomic species laser where the active medium is the He-Ne gas mixture contained in a quartz tube of narrow diameter and maintained at a low pressure which forms the active medium.

**Energy pump:** The energy pump is enabled by maintaining an electrical discharge across the length of the Quartz tube by either a high voltage DC source or a RF source.

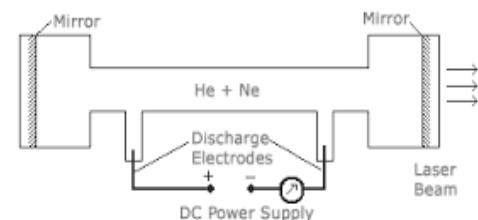
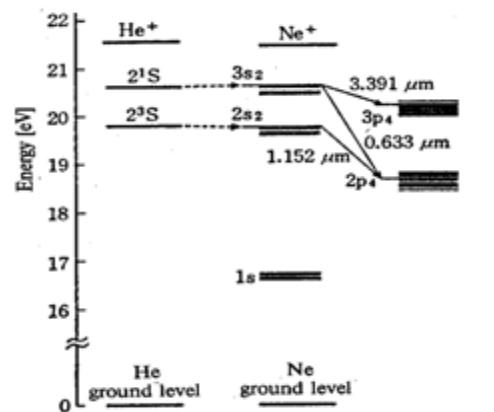
**Resonant cavity:** The cavity is the Quartz tube of appropriate lengths with reflecting mirrors on both ends of the axis of the tube. Additional polarisers may be placed in the path of the beam to ensure a polarized beam of LASER.

He and Ne mixed in the ratio of 10:1 is the active medium where the absorption levels are in the He atoms and the lasing levels are in the Ne atomic transitions. The He atoms are excited with an electrical discharge and the two excited states of helium atom, the  $2^3S$  and  $2^1S$  which are Meta stable. These excited He atoms transfer their energy to Ne atoms by collisions and the excites the Neon atoms to the  $2s_2$  and  $3s_2$  levels as the energy levels of these states are close to the He excited states. (This process is referred to resonant energy transfer.)

A large number of Ne atoms due to collision with He atoms get to the excited state create a population inversion with the ground state. The excited states of Ne are not meta stable and hence de-excites to the ground states through the intermediate states of  $3p$  and  $2p$ . The transition between the  $3s$  to the  $2p$  intermediate states gives the characteristic red laser of Ne with a wavelength of 632.8 nm. The transitions from the  $3s$  to  $3p$  and  $2s$  to  $2p$  lines give rise to radiations with wavelengths in the Infra red of 3.39 micrometers and 1.152 micrometers.

The transitions from the  $3p$  and  $2p$  levels to the  $1s$  intermediate level (close to the ground state) is non radiative. However the  $1s$  state is a Meta stable state and has to be quickly depopulated. This is achieved by making the tube narrow increasing the collision probability of the atoms with the sides of the walls of the tube.

Once in the ground state the Ne atoms are pumped back and the system gives a continuous output.



The cavity consists of reflecting mirrors and the path length adjusted for the visible radiation at 632.8 nm, which also suppress the IR radiations. Additionally some gases which have absorption in the Infra red are added in small quantities to suppress the IR radiations.

Light from the system can be partially polarized (the polarization state of the stimulating photon). The addition of Brewster's windows at the ends of the discharge tube before the reflecting mirrors would ensure that the emitted beam would be fully polarized in the plane of incidence. However the addition of the Brewster's window would eventually lead to a reduction in the output by a factor of 40% to 50%.

### 7. Molecular laser

Molecular vibrations in the infra red are very interesting in that the molecular excited states generally have lifetimes of the order of 1s to a few milli seconds. It would be therefore possible to excite the molecules to the higher energy state and make them relax to the ground state to get stimulated emission quite naturally if the population of the higher energy state can be managed to be greater than the lower energy states. The CO<sub>2</sub> laser is an example of a molecular laser where the Laser emission is in the infrared. Interestingly these are high power continuous wave lasers with the efficiencies reaching up to 40%.

#### Carbon dioxide laser

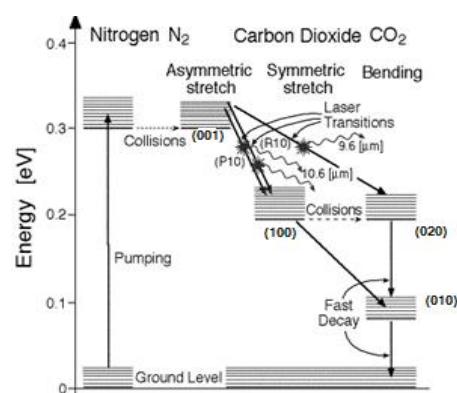
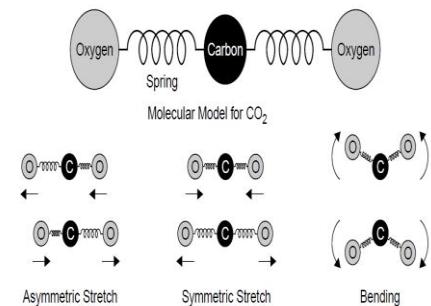
In the CO<sub>2</sub> molecule, the Oxygen atoms are bound to the Carbon atom by the bonding force which acts like a harmonic oscillator. Molecules can be excited to vibrate about their mean positions. Additionally, the molecules may rotate and spin because they are in a gaseous state. The rotational and vibrational states are quantized.

Transitions between vibrational energy states/levels results in photon emission in the infrared, while transitions between rotational states emit photons in the microwave region.

If the CO<sub>2</sub> molecules are excited and made to relax they emit in the infra red producing heat. This mode of emission could be mimicked to a **stimulated emission** if the population of molecules in the excited states is greater than the population in the ground state, thus creating a LASER with infra red wavelengths.

Carbon dioxide molecule has three possible vibrational states – an excited asymmetric stretch (001 state), a lower symmetric stretch (100 state) and bending states (020 and 010 states). The asymmetric stretch states have a higher life time (molecular excited states have higher life times of the order of 1ms to a fraction of a second) and higher energy than the symmetric and bending modes. An excited carbon dioxide molecule in the higher anti symmetric stretch state can relax into the symmetric stretch state giving a radiation at 10.6 μm (0.117eV) and into the bending mode with emission of IR at 9.6 μm (0.129 eV).

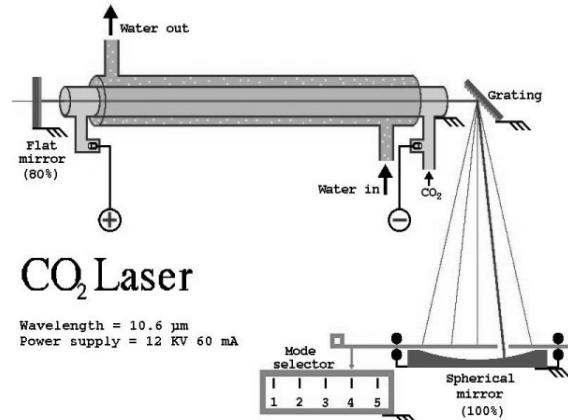
The carbon dioxide laser is a high power gas laser with immense industrial applications.



#### **Construction and Principle of Operation**

All lasers consist of three components: a gain (or laser) medium, an energy source (also known as a pump) and an optical resonating cavity. The three components of a Carbon dioxide laser system comprise of :

- **THE ACTIVE MEDIUM** - A mixture of carbon dioxide, nitrogen, and helium gases serve as the gain medium. Typical gas mixtures have an  $\text{CO}_2$ :  $\text{N}_2$ : He ratio of 1:2:8. The  $\text{N}_2$  molecules are excited with energy close to the excited states of  $\text{CO}_2$  which results in the excitation of  $\text{CO}_2$  to the asymmetric stretch mode.
- **THE ENERGY PUMP** - Electrical discharge current — serving as the laser pump — which excites the gas medium to higher energy states through the electrical discharge of the He gas, which collides with the  $\text{N}_2$  gas to excite them into the higher energy states.
- **OPTICAL CAVITY** - A specialized optical resonator. Because  $\text{CO}_2$  lasers operate solely within the infrared spectrum and can attain high power outputs, their optical components are typically made of specialized (and often expensive) materials such as Germanium, Zinc Selenide, Silver, Gold, and Diamond. Since the  $\text{CO}_2$  lasers work in the Infra red region all parts connected with the laser cavity have to have suitable infra red absorption coatings and an effective cooling system is required for the system as a whole. The hot helium atoms must then be cooled to maintain a population inversion (a sufficient difference between excited and lower energy atoms to produce optical gain) with the excited carbon dioxide molecule.



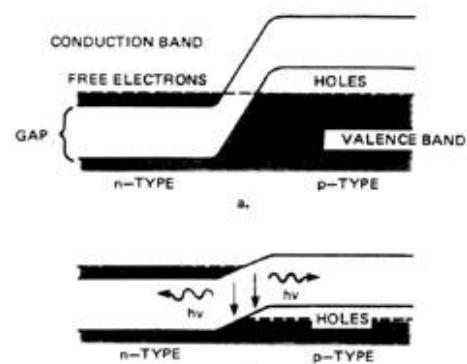
### 8. Semiconductor lasers - Homo junction

Light emitting diodes work on the principle of recombination of electron and holes in the depletion region of a pn junction diode which result in the emission of a photon. The photon emission is possible only if the semiconductor is of the direct band gap type such as GaAs, InP etc (Si and Ge have an indirect band gap and are not suitable for such applications). The photon emission is a case of spontaneous emission which is highly non coherent and has no directionality.

To convert a LED into a laser it is essential conditions of population inversion in the depletion region, stimulated emission and a resonating cavity are satisfied.

Semiconductor lasers use heavily doped direct band gap semiconductors like GaAs which is the active medium. The heavy doping results in an extremely thin depletion region and, moves the Fermi level of the n type into the conduction band and the Fermi level of the p type into the valence band.

Figure shows the depletion region of a heavily doped PN junction in the unbiased condition where the in electrons and holes are present in the “depletion region”, however they are not in a

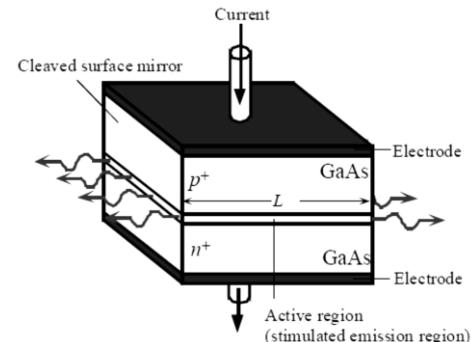


favorable state for recombination.

The energy pump in these devices is the large forward bias current when the PN junction is forward bias. The larger number of electrons in the n side and holes in the p side are in a favorable state for recombination in a narrow region referred to as the active region. This recombination result in the generation of photons in the action region. This emission is of the stimulated type. A suitably designed laser cavity with appropriate dimensions (proportional to  $\lambda/2$ ) and cleaving the surface carefully for maximum reflection at opposite ends, results in the emission of laser from the active region.

The homo junction lasers are not very efficient and require a very high forward current density of the order of  $10000 \text{ A cm}^{-2}$  at room temperature and hence are operated at very low temperatures or in the pulsed condition.

This is attributed to the low charge concentrations in the active region and not all the photons produced by the electron hole recombination are part of the laser output. This results in a device with extremely low efficiencies.



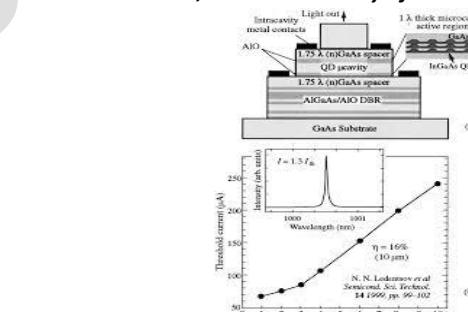
### Heterojunction lasers.

The problems in a homojunction laser can be overcome with the design of a hetero junction laser. Hetero-structures makes it possible to solve the problems in a homo junction laser since in hetero junctions the fundamental parameter of semiconductor crystals and devices like band gaps, effective masses of the charge carriers and their mobilities, refractive indices, etc could be effectively tailored.

The double heterojunction device ensures higher efficiency by

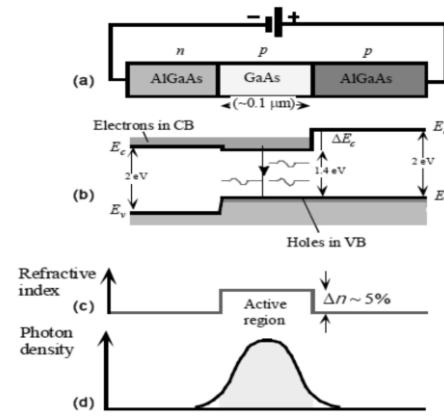
1. **Carrier confinement:** A double hetero structure diode has two junctions which are between two different band gap semiconductors (GaAs and AlGaAs). The GaAs active layer has a lower band gap than the AlGaAs layers on either side. This results in a population of electrons in the conduction band of the GaAs layer from the n type AlGaAs layer and a population of holes in the GaAs layer from the p type AlGaAs. The population of the electrons and hole in the GaAs layer can recombine in the forward bias condition resulting in

*Nobel Lecture: The double heterostructure concept and its applications in physics, electronics, and technology\* Zhores I. Alferov A. F. Ioffe Physico-Technical Institute, Russian Academy of Sciences, St. Petersburg 194021,*



Petersburg 194021,

Russian Federation (Published 22 October 2001)



stimulated emission of photons. This requires less current to establish the required concentration of electrons for population inversion.

2. **Photon confinement:** The other aspect of confining all the emitted photons to a narrow region can be achieved by constructing a dielectric waveguide around the optical gain region and increase the probability of stimulated emission. The n and p type AlGaAs on either side have lower refractive index than the GaAs region which result in an increase in the number of photons traveling along the cavity axis by total internal reflection.

Single hetero junction lasers require a current density of about  $1500 \text{ A cm}^{-2}$  whereas double hetero junction lasers operate at lower currents of  $600 \text{ A cm}^{-2}$ .

Practical hetero junction lasers however consist of many layers to improve the efficiency of the carrier and photon confinements and operate at much lower operating currents at room temperatures.

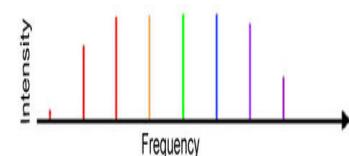
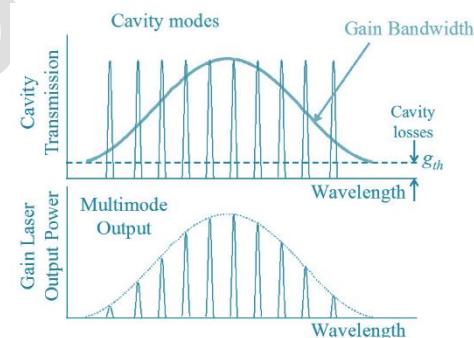
### Applications of Lasers

#### 1. Frequency comb.

A resonant cavity oscillator can support multiple wavelengths (frequencies). Given a cavity of length L (which is much greater than the wavelength of visible radiations) the resonant frequencies, which are referred to as the cavity modes, can be represented as shown.

In the case of a LASER the line width indicates that there are multiple frequencies in output as well. The gain curve of the laser gives the laser output in all the frequencies with a  $g_{th}$  greater than 1. The output then is a frequency comb, which has multiple applications as demonstrated by TW Hansch and J Hall, the Nobel Prize winners in 2005.

Optical Frequency combs (OFC) with mode locked femtosecond pulsed lasers are perfect time or frequency references. OFC also are found to be the most accurate time references and are the most stable clock references for integrated opto electronic systems. Laser spectroscopy using frequency combs have become a standard analytical tool in analysis of materials. These systems are used in a variety of astronomical measurements and is considered to be a potential standard clock reference.



#### 2. Principles of Holography

Information storage with light has been known from the days of photography where in the wavelength and intensity of light are recorded on a photographic plate or digitally on pixels. The photographic information storage has a limitation of being a 2D creation of the information of the object being photographed.

Fundamentally light is fully characterized by wavelength  $\lambda$ , phase  $\phi$  and intensity  $I$  at any point. Hence, capturing all the three parameters would result in storing all the information about an object on a medium or a digital medium. This is the fundamental idea of Holography.

Capturing phase information is best done with an interference. Interference requires two wavefronts - one is a reference beam (whose phase information is fixed) and the second is the wavefront reflected by the object, which carries the phase information from different points on an object. Thus, the object beam contains light from every point on the object carries all required information of wavelength, phase and intensity. When the two beams interfere, the resultant interference pattern has all information about all the points on the object.

The recording and reconstruction process can be explained in the language of Mathematics as follows. The complex amplitude of the reference wave can represented by

$$R_r(x, y) = R_o(x, y)^* e^{i\psi(x, y)}$$

where with real amplitude  $R_o(x, y)$  and phase  $\psi(x, y)$ .

The wave which originates from the reflection from a surface similarly is given by

$$O(x, y) = O_o(x, y)^* e^{i\phi(x, y)}$$

with real amplitude  $O_o(x, y)$  and phase  $\phi(x, y)$ .

The interference of the two waves on the holographic plate resulting in a complex interference pattern and the intensity distribution can be evaluated as

$$I(x, y) = [O(x, y) + R_r(x, y)]^2 = [O_o(x, y)]^2 + [R_r(x, y)]^2 + O(x, y) \cdot R_r(x, y)^* + O(x, y)^* \cdot R_r(x, y)$$

$$\text{Where the last term is } O(x, y) \cdot R_r(x, y)^* + O(x, y)^* \cdot R_r(x, y) = 2O_o(x, y)^* O_r(x, y)^* \cos(\psi(x, y) - \phi(x, y))$$

includes both the amplitude and phase of the object wave fronts, i.e.,  $O_o(x, y)$  and  $\phi(x, y)$ .

The reconstruction of the image will require the recorded holographic film and the reference source. The beam that is transmitted is sensitive to the intensity of the source.

The transmission function of optical recording devices including photographic film is sensitive to intensity. We will assume that the sensitivity is linear in intensity. The reference  $R_r(x, y)$  is assumed to be constant, and equal to  $A_r$ , which is a plane wave incident perpendicular to the hologram. The transmission function (also known as the hologram function) of such a device contains the stored information and can be written as

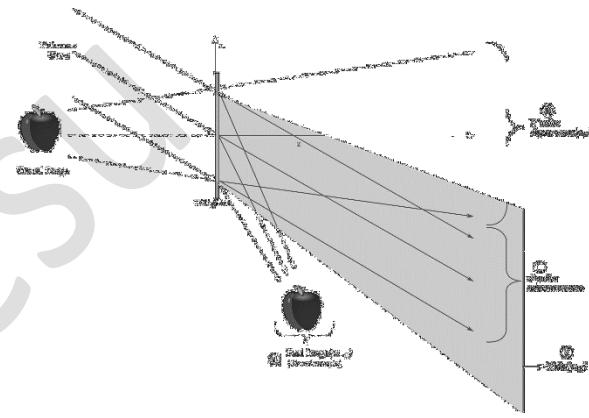
$$t(x, y) = t_0 + \beta \tau \{ [O_o(x, y)]^2 + [A_r(x, y)]^2 + O_o^* R_r + O_o R_r \}$$

where  $\beta$  and  $t_0$  are constants. The constant  $\beta$  is the slope of the amplitude transmittance versus exposure characteristic of the light sensitive material. For photographic emulsions  $\beta$  is negative.  $\tau$  is the exposure time and  $t_0$  is the amplitude transmission of the unexposed plate.  $t(x, y)$  is known as the hologram function.

If the hologram created as above, is illuminated by another reference wave  $R_p(x, y)$  as shown in the figure

The wave emanating from the hologram can be written as

$$\begin{aligned} U(x, y) &= [t(x, y) * R_p(x, y)] \\ &= [t_0 + \beta \tau \{ [O_o(x, y)]^2 + [A_r(x, y)]^2 + O_o^* R_r + O_o R_r \}] * R_p(x, y) \end{aligned}$$



## Unit IV : LASERS

$$R_t = U_1 + U_2 + U_3 + U_4$$

where,  $U_1 = (t_0 + \beta\tau[O_o(x, y)^2]) \cdot R_p(x, y)$

$$U_2 = \beta\tau[[A_r(x, y)]^2 \cdot R_p(x, y)]$$

$$U_3 = \beta\tau[OR_r^*] \cdot R_p(x, y)$$

$$U_4 = \beta\tau[O^*R_r] * R_p(x, y)$$

Suppose that  $R_r$  and  $R_p$  are the same and are constant, as in the case of a plane wave perpendicular to the direction of propagation. Then,  $U_3$  is proportional to  $O$ , and  $U_4$  is proportional to  $O^*$ .

The first term  $U_1$  refers to the intensity reduction of the reconstruction wave by the factor  $t_0 + \beta\tau|A_r(x, y)|^2$  during reconstruction.

The second term is small assuming that we choose  $A_0(x, y) < A_r(x, y)$  during recording. This term is distinguished from the first term by its spatial variation  $|A_0(x, y)|^2$ . The  $|A_0(x, y)|^2$  term contains low spatial frequencies which have small diffraction angles and create a so-called halo around the reconstruction wave. The size of the halo is given by the angular dimension of the object. These first two terms form the zeroth diffraction order in equation.

The third term  $U_3$  denotes the object wave  $U(x, y)$  multiplied with the constant factor  $\beta\tau R_r^2$ . An observer who registers this wave in his eye therefore sees the virtual image of the object (not present). This is the most important term and represents the first diffraction order. The wave travels divergent from the hologram thus creating a virtual image at the position of the original object. It is a virtual image because the wave is not converging to form a real image. This image cannot be captured on a screen. The intensity (square of amplitude) of the image does not depend on the sign of  $\beta$ . Therefore, it is unimportant whether the hologram is processed "positive" or "negative".

The fourth term  $U_4$  is essentially the complex conjugate of the object wave  $U^*$  except for a multiplicative term. This represents the -1 st diffraction order. Since it is complex conjugated wave, the phase changes its sign with respect to  $U(x, y)$ . As a consequence, the wave  $U^*(x, y)$  travels convergent and forms a real image. The conjugated real image  $U_4$  is usually located at the opposite side of the hologram with respect to  $U_3$ .  $U_3$  and  $U_4$  are called twin images or also represented as virtual and real images, respectively. All these reconstructed wavefronts are represented in Figure.

## Solved Numericals:

- 1. An emission system has two levels which gives rise to an emission wavelength of 546.1 nm. If the population of the lower state is  $4 \times 10^{22}$  at 600 K, estimate the population of the higher energy state.**

Let  $N_1$  and  $N_2$  be the populations of energy states  $E_1$  and  $E_2$ .

According to the Maxwell Boltzmann distribution  $\frac{N_1}{N_2} = \exp^{\frac{(E_2 - E_1)}{kT}}$ .

$$\text{Hence } N_2 = N_1 \exp^{\frac{-(E_2 - E_1)}{kT}} = N_1 \exp^{-\frac{hc}{\lambda kT}} = 8.088 \times 10^{-20}$$

- 2. The ratio of population between the high energy states to the lower energy state is  $5 \times 10^{-19}$  at 400K. Find the emission wavelength between two states and the ratio A/B.**

$$\text{Given } N_2/N_1 = 5 \times 10^{-19} \quad N_1/N_2 = 2 \times 10^{18} = e^{hv/kT}$$

$$\lambda = \frac{hc}{kT \ln \left( \frac{N_1}{N_2} \right)} = 854.56 \text{ nm}$$

$$\frac{A}{B} = \frac{8\pi h}{\lambda^3} = 2.667 \times 10^{-14}$$

- 3. The ratio of population of the upper excited state to the lower energy state in a system at 300K is found to be  $1.2 \times 10^{-19}$ . Find the wavelength of the radiation emitted and the energy density of radiation.**

$$\frac{N_1}{N_2} = \exp^{\frac{(E_2 - E_1)}{kT}} = \exp^{\frac{hc}{\lambda kT}}$$

$$\text{Wavelength } \lambda = 1.06 \times 10^{-6} \text{ m}$$

$$\rho(v) = \frac{8\pi hv^3}{c^3} \frac{1}{\left( \exp^{\frac{hv}{kT}} - 1 \right)} = 1.987 \times 10^{-33} \text{ Js/m}^3.$$

- 4. A laser emission from a certain laser has an output power of 10 milli watts. If the wavelength of the emission is 632.8nm, find the rate of emission of the stimulated photons.**

$$\text{Power of Laser } P = n \times hv = n \times h \times \frac{c}{\lambda} \text{ where } n \text{ is the rate of stimulated emission.}$$

$$n = \frac{P \times \lambda}{h \times c} = 3.18 \times 10^{16} \text{ per second}$$

**Problem set**

- 1 The ratio of the population of two energy levels is  $1.5 \times 10^{30}$ . The upper level corresponds to a meta stable state. Find the wavelength of light emitted at 330K (**Ans 628 nm**)
- 2 An hypothetical atom has energy levels uniformly separated by 1.2 ev. Find the ratio of the no of atoms in the 7th excited state to that in the 5th excited state. (**Ans:  $5.22 \times 10^{-41}$** )
- 3 A pulsed laser has a power of 1mW and lasts for 10 ns. If the no. of photons emitted per second is  $3.491 \times 10^7$ , calculate the wavelength of the photons. (**Ans: 693 nm**)
- 4 If  $R_1$  is the rate of stimulated emission and  $R_2$  is the rate of spontaneous emission between two energy levels, show that  $\lambda = hc / [kT \ln\{(R_2/R_1)+1\}]$ .
- 5 Find the ratio of the rate of stimulated emission to the rate of spontaneous emission for a system emitting a wavelength of 632.8 nm at 300K. (**Ans:  $1.11 \times 10^{-33}$** )
- 6 If  $B_{10} = 2.7 \times 10^{19} \text{ m}^3/\text{W}\cdot\text{s}^3$  for a particular atom, find the life time of the 1 to 0 transition at (a) 550nm and (b) 55nm (answer: (a)370ns (b) 0.37ns )
- 7 The energy levels in a two-level atom are separated by 2eV. There are  $3 \times 10^{18}$ atoms in the upper level and  $1.7 \times 10^{18}$  atoms in the ground level. The coefficient of stimulated emission is  $3.2 \times 10^5 \text{ m}^3/\text{W}\cdot\text{s}^3$  and the spectral radiance is  $4 \text{ W/m}^2\cdot\text{Hz}$ . Calculate the stimulated emission rate?
- 8 For an ordinary source, the coherence time  $\tau_c = 10^{-10}$  second. Obtain the degree of non-monochromaticity for wavelength  $\lambda_0 = 5400 \text{ \AA}$ .
- 9 Calculate the coherence length of a laser beam for which the band width  $\Delta v = 3000 \text{ Hz}$ .
- 10 The lifetime of transitions in a Na atoms emitting wavelength of 589.6nm is estimated to be 16.4ns. Calculate the Einstein's coefficients A and B. Calculate spectral broadening and the coherence length of radiations.
- 11 The spectral line width of a HeNe laser emitting 632.8 nm is  $10^{-16} \text{ m}$ . Calculate Einstein's coefficients A and B and the coherence length of radiations.
- 12 Calculate the threshold gain factor of a helium–neon laser, which has a loss factor of  $0.05 \text{ m}^{-1}$  if the configuration of the system is as follows:
  - (a) A 50-cm tube with one mirror 99% reflecting and the output coupler 90% reflecting
  - (b) A 20-cm tube with one mirror 99% reflecting and the output coupler 95% reflecting
  - (c) A 20-cm tube with one mirror 99% reflecting and the output coupler 97% reflectingComment on the results obtained.