Unit-1 Quantum Mechanics.

Quantum Mechanics:- (Microscopic)

" Science dealing with the behaviour of Matter & light on atomic & Subatomic Scale."

It attempts to describe the Properties of Molecule atoms and their Constituents (Electron, Protons, Neutrons and other Subatomic Particle).

Classical Mechanics:-

Branch of Physics deals with the Motion of object Smaller as well as large objects.

OR Classical Mechanics deals with the Motion of bodies Under the Influence of Force.

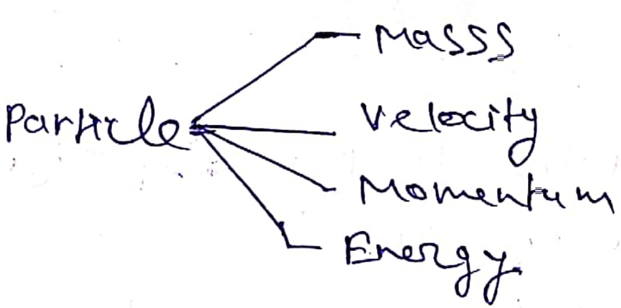
Classical Mechanics	Quantum Mechanics
I) Deals with Macroscopic objects	I) Deals with Microscopic objects
II) Based on Newton's Law of Motion.	II) Based on Schrodinger wave Equation.
III) In Classical Mechanics Behaviour of Particle can be completly known.	III) In Quantum Mechanics there is some Uncertainity in determination of Position and Momentum of Particle.
IV) Classical Mechanics deals with certainities	IV) Quantum Mechanics deals with Probablities.

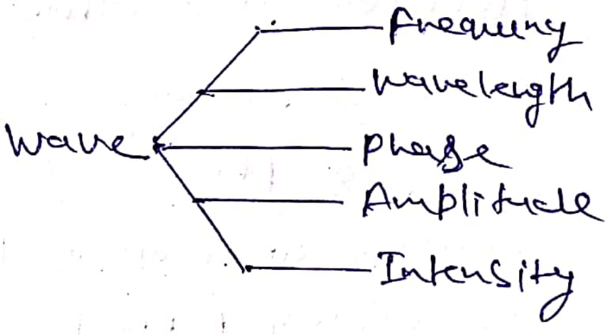
Wave Particle Duality :-

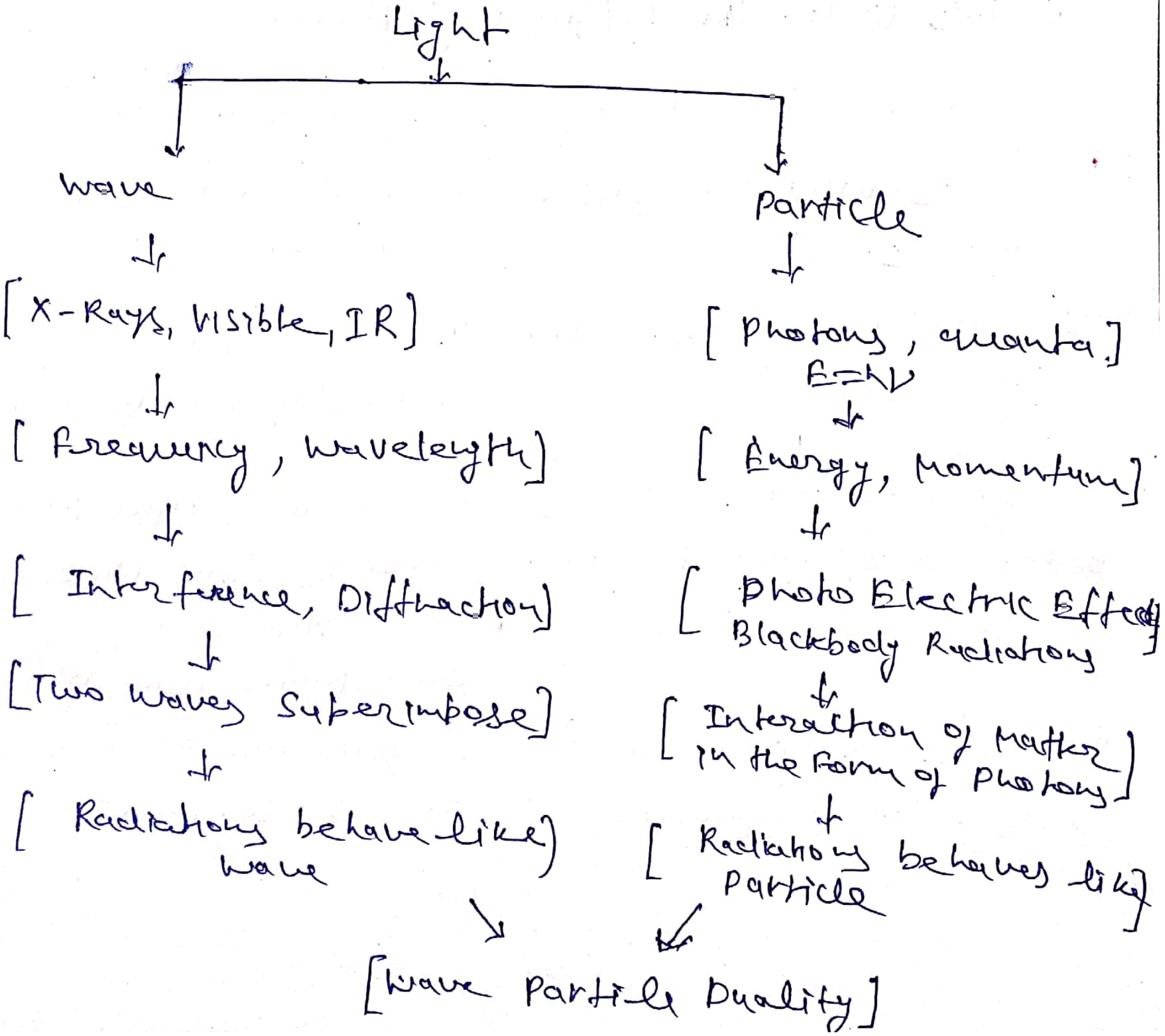
"Wave Particle Duality Describe the properties of ~~both~~ Photons and Subatomic Particles to exhibit the ~~Propertie~~ of properties of both waves & Particles"

OR

"It is the concept of Quantum Mechanics that every particle or entity may be described as a Particle or wave".







De Broglie Hypothesis:-

Light wave can act as a wave sometimes and as a Particle at other times this is known as de Broglie Hypothesis.

Matter waves:-

According to de Broglie Hypothesis any Moving Particle is associated with a wave. The wave associated with a Particle known as de Broglie waves or Matter waves.

The wavelength λ of Matter waves associated with a Particle moving with velocity v is inversely Proportional to the Magnitude of Momentum of Particle. Thus

$$\boxed{\lambda = \frac{h}{mv}} = \frac{h}{p} \quad (P = mv)$$

The relation $\lambda = \frac{h}{mv}$ is known as de-Broglie Equation and wavelength λ is called De-Broglie wavelength.

De-Broglie wavelength Associated with an accelerated Charge Particle:-

If a charge Particle, say an electron is accelerated by a Potential difference of V volts, then its Kinetic Energy is given by

$$K.E = eV$$

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

$$v = \sqrt{\frac{2eV}{m}}$$

Then electron wavelength is given by -

$$\lambda = \frac{h}{mv} = \frac{h}{m}\sqrt{\frac{m}{2eV}}$$

$$\boxed{\lambda = \frac{h}{\sqrt{2emV}}}$$

De Broglie wavelength Expressed in term of Kinetic Energy:-

If a Particle has K.E, Kinetic Energy

$$K.E = \frac{1}{2}mv^2$$

$$= \frac{1}{2}mv^2 \times \frac{m}{m}$$

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

$$P = \sqrt{2m(K.E)}$$

(Substituting value of h, m&e) $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(K.E)}} = \frac{12.28}{\sqrt{V}} A°$

De-Broglie wavelength Associated with a Particle in thermal Equilibrium:-

For a Particle in thermal Equilibrium at temperature T, then their kinetic Energy is given by.

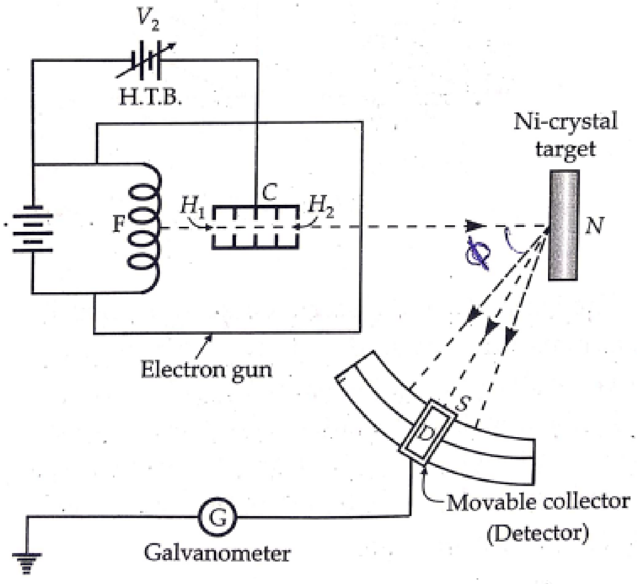
$$K.E = \frac{3}{2}KT$$

$$\lambda = \frac{h}{\sqrt{2m(K.E)}} = \frac{h}{\sqrt{3mKT}}$$

Davisson & Germer Experiment:-

(Experiment to show the Existance of Matter waves)

Davisson & Germer shows that electron beam can undergo diffraction when passed through an atomic crystal. It confirms the wave Nature of electron and De-Broglie wave length.



* In Experimental Arrangement of Davisson & Germer

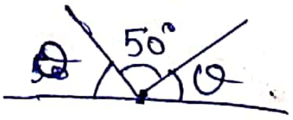
→ The Electron beam is generated from a hot Tungsten Filament F. The Filament is Connected to Variable voltage Source (V).

→ The electron emerges through an opening and falls normally on the surface of Nickel crystal.

→ The intensity of scattered electron can be measured by detector D in different direction. The dedector can be moved in Different Directions.

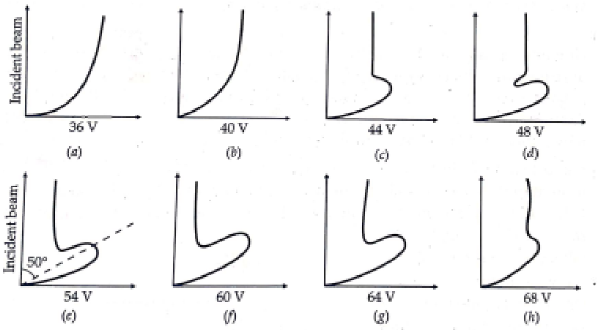
Note:-

$$\theta + 50 + \theta = 180^\circ$$
$$2\theta = 130^\circ$$
$$\boxed{\theta = 65^\circ}$$

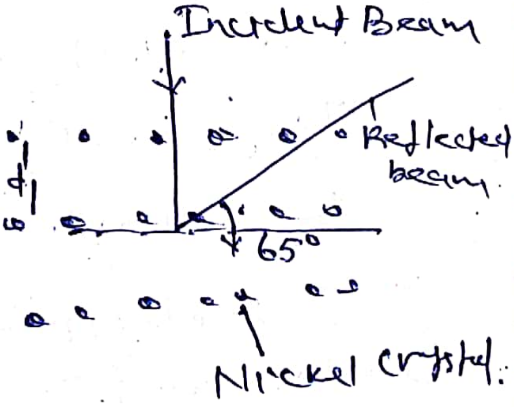


* First of all accelerating voltage V is given a low value and detector on the circular scale moved to various position and value of current was measured.

* The current (which measures the intensity of diffracted beam) is plotted against angle ϕ.. (ϕ is the angle between incident beam on the crystal and the beam entering in the detector).



* It is seen that bump begins to appear in the curve for 44-volt electron. With increasing potential (V) the bump becomes most prominent (Maximum Intense) for 54 volt at $\phi = 50°$.



* As Nickel is made up of crystal using Bragg's law of Diffraction wave length (λ) can be calculated

$\lambda = 2d \sin\theta$

$\lambda = 2 \times 0.91 A° \times \sin 65°$

$\boxed{\lambda = 1.65 A°}$ —①

($d = 0.91 A°$, d is the interplaner spacing).

The wavelength of electron can also be calculated from accelerating potential V using De-Broglie equation.

$$\boxed{\lambda = \frac{h}{\sqrt{2meV}}}$$

Note:-

$$\lambda = \frac{h}{p}$$

$$P = mV$$

$$p^2 = m^2 v^2 = m \times m v^2$$

$$= m \times 2E \quad \left(K.E = \frac{1}{2}mv^2\right)$$

$$\Rightarrow p^2 = 2mE$$

$$E = \frac{p^2}{2m} \Rightarrow \boxed{P = \sqrt{2mE}}$$

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}}$$

Hence

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 54 \times 1.6 \times 10^{-19}}}$$

(Substituting
$h = 6.6 \times 10^{-34}$
$m = 9.1 \times 10^{-31}$
$e = 1.6 \times 10^{-19}$)

∴ (Note $E = 54\,eV$
$= 54 \times 1.6 \times 10^{-19} J$)

$$\boxed{\lambda = 1.66\,Å} \quad -②$$

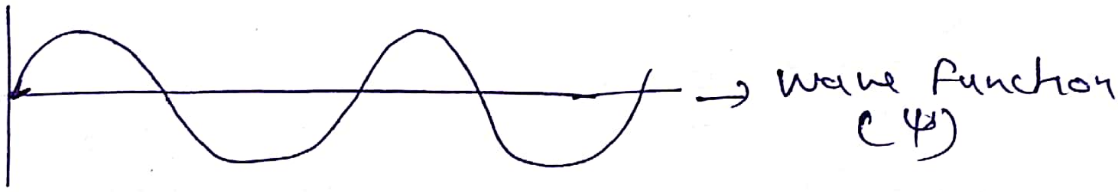
It is seen that the values obtained experimentally using Bragg's equation and De-Broglie equation agreed well. Therefore Davisson-Germer conclude that electrons exhibit diffraction properties.

Wave Function:- Function describing the Probability of Each Possible observation such as Position & Momentum.

Represented by (ψ) – Psi

$\psi(r,t)$

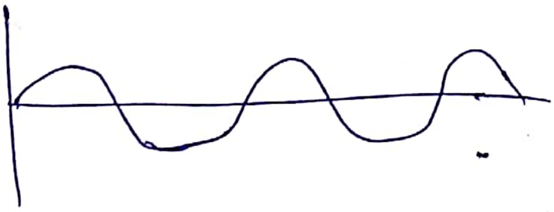
Position time



Note- A wave is Associated with a particle.

Characteristics:-

I) If a wave has higher Energy it Rotate with high Frequency.



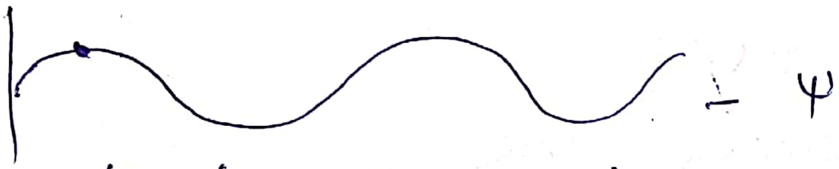
II) maximum Amplitude of a wave has maximum probability of finding the particle. ($\psi2$)

III) Momentum of a wave is inversly Proportional to wavelength.

$P \propto \frac{1}{\lambda}$ (P- Momentum)

Operator! An operator is a Mathematical operation on the wave function that produce another wave function.

Suppos ψ be any wave function



Then A(ψ) (operator of ψ)

$$\underset{\text{Operator}}{A}(\underset{\text{wave function.}}{\psi})$$

E.g- Hamiltonian operator (H)

Hamiltonian operator (H) represent total Energy of a system

$$\underset{\text{Hamiltonian}}{H} = \underset{\text{Kinetic Energy}}{T} + \underset{\text{Potential Energy}}{V}$$

Normalization of a wave Function.

~~Normalization~~. When the Probability of finding a particle is 1 then the function is said to be Normalize

$$\boxed{\int \psi^* \psi \, dx = 1}$$

Suppose ~~If~~ a function is not Normalize (1.1)

$$\int \psi^* \psi \, dx = N \quad (\neq 1)$$

then

$$\frac{1}{N} \int \psi^* \psi \, dx = 1$$

$$\boxed{\int \frac{\psi^*}{\sqrt{N}} \frac{\psi}{\sqrt{N}} \, dx = 1}$$

↓

Normalized

~~It~~ means Probability of finding Particle is 1

($\psi^* \psi$ – Represent Probability of finding Particle)
(Probability density)

2.5 Normalize the wave function

$\psi(x) = 0$ outside the box of size l

$\psi(x) = A \sin kx \quad 0 < x < l$

where $k = \frac{\pi}{l}$ **[GGSIPU, May 2012 (4 marks)]**

Hint : $$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1,$$

Here $$\psi(x) = A \sin kx = A \sin \frac{\pi x}{l} = \int_0^l A^2 \sin^2 \frac{\pi x}{l} dx = 1$$

From above expression, $A = \sqrt{\frac{2}{l}}$

Then $$\psi_n = \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l}$$

Wave Function & Probability Interpretation:-

Micro particles exhibit wave properties, quantity ψ represent a de broglie wave. This quantity (ψ) is called wave function.

ψ describe wave as a function of position & time. It is an observable quantity.

ψ^* is a complex valued function.

We can only know the probable value in a measurement

The probability cannot be negative.

Probability Interpretation of wave Function:-

$|\psi|^2$ (Square of magnitude of wave function), represent the probability of finding particle in that region.

probability of finding the particle ~~[illegible]~~ is proportional to $|\psi(x,y,z)|^2 dx\,dy\,dz$ at time t.

$$P \propto |\psi(x,y,z)|^2 dv$$

$|\psi|^2$ is called Probability density

ψ is Probability Amplitude.

Physical Interpretation of Wave Function ψ:

A satisfactory interpretation of wave function ψ associated with a moving particle was given by born in 1926. He postulated that square of magnitude of wave function $|\psi|^2$ at a particular point is proportional to probablity of finding the particle at that point.

Also

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

A wave function that obey this equation said to be normalized

Beside being normalized ψ must fulfill the following requirement.

I) ψ must be finite everywhere.

If ψ is ~~~~ infinite it would have infinite probablity of finding the particle at that point. This would voilate the uncertainity principle. Hence ψ must be finite.

II) ψ must be single valued:-

If ψ has ~~a~~ more than one value at any point, it would have more than one value of probablity of finding the particle at that point. Hence it must be single valued.

III) ψ must be continuous and have continuous first derivative everywhere:-

$d^2\psi/dx^2$ must be finite every where. This ~~possible~~ is so only if $d\psi/dx$ has no discontunity. Further $d\psi/dx$ as a continuous function implies that ψ too continus across boundary.

Heisenberg's Uncertainity Principle:-

This Principle was discovered by Heisenberg in 1927. It states that we can measure either position or momentum of a particle with any desired degree of accuracy (within limit of experimental Equipment). OR

It is impossible to measure both position and momentum simultaneously with accuracy.

$$\boxed{\Delta x \cdot \Delta P_x \geq \frac{h}{4\pi}}$$

Δx → Uncertainity in position.
ΔP → Uncertainity in Momentum.

Physical significance!

I) Uncertainity principle Explain why it is possible for Radiation and Matter to have dual (wave-particle) character.

II) It also make it clear that we can predict only the probable behaviour of quantum mechanical system not the Exact behaviour.

III) It helps in understanding many phenomenon like absence of electron within Nuclei, natural broadening of spectral lines etc.

Energy Momentum Uncertainity!-

The uncertainity relation for simultaneous measurement of Energy E & time t expressed as.

$$\cancel{\Delta E} \quad \Delta E.\Delta t \geq \frac{\hbar}{2} \qquad \left(\hbar = \frac{h}{2\pi}\right)$$

Derivation let us consider a microparticle moving with velocity v, Its kinetic Energy will be.

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

$$\Delta E = \Delta\left(\frac{1}{2}mv^2\right)$$

$$= mv\Delta v = v\Delta p$$

$$\left(v = \frac{\Delta x}{\Delta t}\right)$$

$$\Rightarrow \Delta E = \frac{\Delta x}{\Delta t}\Delta p$$

$$\Delta E.\Delta t = \Delta x.\Delta p$$

$$\boxed{\Delta E.\Delta t \geq \frac{\hbar}{2}}$$

~~ot~~ or $\boxed{\Delta x.\Delta p \geq \frac{\hbar}{2}}$

Example 1.5 *Find the smallest possible uncertainty in position of the electron moving with velocity* 3×10^{7} *m/s (Given* $h=6.63\times10^{-34}$ *Js,* $m_0=9.1\times10^{-31}$ *kg)* **[GGSIPU, May 2007 (2.5 marks)]**

Solution. Given $v=3\times10^{7}$ m/s

Let Δx_{min} be the minimum uncertainty in position of the electron and Δp the maximum uncertainty in the momentum of the electron.

Thus we have,

$$\Delta x_{\text{min}}\cdot\Delta p_{\text{max}}=\frac{h}{2\pi} \qquad ...(i)$$

or

$$\Delta p_{\text{max}}=p=mv$$

$$\Delta p_{\text{max}}=\frac{m_0 v}{\sqrt{1-\dfrac{v^2}{c^2}}} \qquad ...(ii)$$

$$\Delta x_{\text{min}}=\frac{h\sqrt{1-\dfrac{v^2}{c^2}}}{2\pi m_0 v}=\frac{6.63\times10^{-34}\sqrt{1-\left(\dfrac{3\times10^{7}}{3\times10^{8}}\right)^2}}{2\times3.14\times9.1\times10^{-31}\times3\times10^{7}}\text{ m}$$

$$=0.03867\times0.9949\times10^{-10}\text{ m}=3.8\times10^{-12}\text{ m}$$

Example 1.7 *Show that the uncertainty in the location of the particle is equal to de-Broglie wavelength the uncertainty in its velocity is equal to its velocity.* **[GGSIPU, April 2014 (2 marks)]**

Solution. Given $\Delta x=\lambda$,

Since we know that the uncertainty principle

$$\Delta x\,\Delta p_x=h \quad \text{or} \quad \lambda\Delta p_x=h$$

or $$\Delta p_x=\frac{h}{\lambda} \quad \text{or} \quad \Delta p_x=p$$

or $$m\Delta v_x=mv_x \quad \text{or} \quad \Delta v_x=v_x$$

p

1.23 A typical atomic nucleus is about 5 Fermi in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is part of nucleus. **[GGSIPU, Feb. 2012 (2 marks)]**

Hint : We know that 1 Fermi = 10^{-15} m

The uncertainty principle in electron's position is

$$\Delta x = 5 \times 10^{-15}\,\text{m}$$

$$\Delta p \geq \frac{\hbar}{\Delta x} = \frac{6.626 \times 10^{-34}\,\text{Js}}{2\pi \times 5 \times 10^{-15}\,\text{m}} = 2.11 \times 10^{-20}\ \text{kg m/s}$$

The momentum would also be of the same order if this is the uncertainty in it. This suggests that the kinetic energy of electron is far greater than its rest energy and it can be written as

KE = pc, so that

$$pc \geq (2.11 \times 20^{-20}\,\text{kg m/s}) \times (3 \times 10^{8}\ \text{m/s}) \geq 6.33 \times 10^{-12}\,\text{J} \geq 39\ \text{MeV}$$

Thus, the kinetic energy of an electron must exceed 39 MeV, for it to be a nucleus constituent. Experiments indicate that the electrons in an atom have only a function of this energy. Thus, we can conclude that the electrons are present in the nucleus.

1.24 An electron has a speed of $2 \times 10^{4}\,\text{ms}^{-1}$ within the accuracy 0.01%. Calculate the uncertainty in the position of the electron. **[GGSIPU, May 2017 (2.5 marks)]**

Hint : $\Delta x \Delta p_x = \Delta x (m \Delta v_x) = \dfrac{h}{n\pi}$

$$\Rightarrow \qquad \Delta x = \frac{h}{n\pi m \Delta v_x} = \frac{6.63 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times (2 \times 10^{4} \times 0.0001)} = 29\ \mu\text{m}$$

1.2 Calculate the de-Broglie wavelength of (*i*) a 46 g golf ball moving with velocity 30 m/s and (*ii*) an electron moving with velocity 10^7 m/s. Which one is measurable ? **[GGSIPU, May 2010 (2.5 marks)]**

Hint : $\lambda = \dfrac{h}{mv}$

(*i*) *For golf ball :* $\lambda = \dfrac{6.63\times10^{-34}}{46\times10^{-3}\times30} = 4.8\times10^{-34}\text{m}$ [Not measurable]

(*ii*) *For electron :* $\lambda = \dfrac{6.63\times10^{-34}}{9.1\times10^{-31}\times10^{7}} = 72\text{ nm}$ [measurable] .

1.5 A ball of mass 10^{-3} kg moves with a velocity of 10^{-2} ms^{-1}. What is the de-Broglie wavelength of the ball ?

Hint : $\lambda = \dfrac{h}{p} = \dfrac{h}{mv} = \dfrac{6.626\times10^{-34}\text{ Js}}{10^{-3}\text{kg}\times10^{-2}\text{ ms}^{-1}} = 6.626\times10^{-29}\text{ m}$

1.6 An electron and a proton have the same de Broglie wavelength. Prove that the energy of electron is greater. **[GGSIPU, April 2015 (2 marks)]**

Hint : $\lambda = \dfrac{h}{p} = \dfrac{h}{mv} = \dfrac{h}{\sqrt{2mE}}$ then $\lambda_e = \lambda_p \quad \Rightarrow \quad \dfrac{h}{\sqrt{2m_eE_e}} = \dfrac{h}{\sqrt{2m_pE_p}}$

$m_eE_e = m_pE_p \quad \Rightarrow \quad E_e = \dfrac{m_pE_p}{m_e}$ since $m_e < m_p$, so $E_e = \dfrac{m_pE_p}{m_e}$

1.7 An electron and a proton are moving with same velocity. Find the ratio of their (*i*) de Broglie wavelength, (*ii*) phase velocity and (*iii*) group velocity. **[GGSIPU, May 2015 (6 marks)]**

Hint : (*i*) $\dfrac{\lambda_e}{\lambda_p} = \dfrac{h}{m_ev_e}\times\dfrac{m_pv_p}{h} = \dfrac{m_p}{m_e}$

(*ii*) $\dfrac{v_{g_e}}{v_{g_p}} = \dfrac{v_e}{v_p} = 1$ and (*iii*) $v_pv_g = c^2$ so $\dfrac{v_{p_e}}{v_{p_p}} = \dfrac{v_e}{v_p} = 1$

1.8 Calculate the de Broglie wavelength of basket ball of mass 1 kg, moving at a speed of 10 ms^{-1}. Discuss the reason, why we cannot observe its wave nature. **[GGSIPU, May 2015 (4.5 marks)]**

Hint : $\lambda = \dfrac{h}{mv} = \dfrac{6.63\times10^{-34}}{10\times10} m = 6.63\times10^{-36}\text{m}$ which is not measurable.

1.13 Determine the de-Broglie wavelength of an electron having kinetic energy 2.0 eV [Given : mass of electron = 9.1×10^{-31} kg, $h = 6.63\times10^{-34}$J.s] **[GGSIPU, Feb. 2010 (2 marks)]**

Hint : $\lambda = \dfrac{hc}{\sqrt{K(K+2m_0c^2)}}$

$$= \frac{6.63\times10^{-34}\times3\times10^{8}}{[2.0\times1.6\times10^{-19}(2.0\times1.6\times10^{-19}+2\times9.1\times10^{-31}\times(3\times10^{8})^2]^{1/2}}$$

1.16 Find the phase and group velocities of an electron whose de-Broglie wavelength is 1.2 Å.

[GGSIPU, Feb. 2012 (5 marks)]

Hint : $m_0 c^2 = 511 \text{ keV}, \quad m_0 = 9.1 \times 10^{-31} \text{ kg}$

$$\frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \quad \Rightarrow \quad \frac{1}{2}mv^2 = \frac{h^2}{2m\,\lambda^2}$$

$$\Rightarrow \quad v = \frac{h}{m\lambda} = 6.07 \times 10^6 \text{ m/s}$$

$$v = v_g = 6.07 \times 10^6 \text{ m/s}$$

But $\quad v_p v_g = c^2$

$$\Rightarrow \quad v_p = \frac{c^2}{v_g} = \frac{(3\times10^8)^2}{6.07\times10^6} = 1.48\times10^{10} \text{ m/s.}$$

1.17 Calculate the de-Broglie wavelength of 40 keV electrons used in certain electron microscope.

[GGSIPU, May 2011 (2.5 marks)]

Hint : $E = 40 \text{ keV} = 4.0 \times 10^3 \times 1.6 \times 10^{-16} \text{ J} = 6.4 \times 10^{-15} \text{ J}$

$$E = \frac{1}{2}mv^2 \quad \text{or} \quad v = \sqrt{2E/m}$$

de-Broglie wavelength, $\lambda = \dfrac{h}{mv} = \dfrac{h}{\sqrt{2mE}} = 6.15 \times 10^{-15} \text{ m}$

1.18 Calculate the de-Broglie wavelength of an electron accelerated through a potential difference 100 V.

[GGSIPU, April 2011 (2 marks)]

Hint : $\lambda = \dfrac{h}{mv} = \dfrac{h}{\sqrt{2mE}} = \dfrac{1.228\times10^{-10}}{\sqrt{V}} = 1.228 \times 10^{-10} \text{ m} = 1.228 \text{ Å}$

1.19 A nuclear particle is confined to a nucleus of diameter 5×10^{-4} m. Calculate the minimum uncertainty in the momentum of the nucleon. Also calculate the minimum kinetic energy of the nucleon.

[GGSIPU, Feb. 2009 (2 marks)]

Hint : The diameter of nucleus $(\Delta x) = 5\times10^{-14}$ m

$\therefore \quad \Delta p \Delta x = \hbar$

$$\Rightarrow \quad \Delta p = \frac{\hbar}{\Delta x} = \frac{1.05\times10^{-34}}{5\times10^{-14}} \text{kg m s}^{-1} = 2.1\times10^{-2} \text{ kg m s}^{-1}$$

and the minimum K.E. of the nucleon $= \dfrac{p^2}{2m_0} = \dfrac{2.1\times10^{-21}}{2\times m_0}$ here m_0 = mass of nucleon.

Group velocity & Phase velocity:-

Phase velocity:- Velocity of individual wave forming wave packet is called Phase velocity.

According to de Broglie Hypothesis

If a Particle is in motion a wave is associated with it. Called Matter wave

Wavelength of wave $\boxed{\lambda = \frac{h}{mv}}$ —①

(where v is the velocity of Particle)
h- Placks constant
m- Mass of the Particle)

We have to calculate the velocity of wave

Velocity of wave ~~E~~

$\boxed{u = \nu\lambda}$ —② (ν- frequency)

Note
Extra

Note

$E = h\nu \Rightarrow \nu = \frac{E}{h}$.

But $E = mc^2$

$\boxed{\nu = \frac{mc^2}{h}}$ —③

⇒. Using ①③ in ②

$u = \nu\lambda = \frac{mc^2}{h} \times \frac{h}{mv} = \frac{c^2}{v} \Rightarrow \boxed{u = \frac{c^2}{v}}$ ④

velocity of wave

A plane wave travelling along x-axis is given by -

$$\psi = A\sin(\omega t - kx)$$

$$u = \nu\lambda$$

$$\left(\begin{aligned} \omega &= 2\pi\nu \\ k &= \frac{2\pi}{\lambda} \end{aligned}\right)$$

(where ω is Angular velocity
k - Propagation constant)

Now ~~ψ= 2A(Sin~~ $u = \frac{2\pi}{2\pi}\nu\lambda$

$$= \frac{\omega}{2\pi}\lambda = \frac{\omega}{k}$$

$$u = \frac{\omega}{k}$$

$$\boxed{v_p = \frac{\omega}{k}}$$ – Phase velocity.

Group Velocity :-

~~Group velocity~~ is The velocity of wave packet formed by the individual waves is called group velocity.

Superposition of wave is called wave packet. or wave group.

Let us consider a wave group which consist of two Component of equal amplitude a. but slightly different angular frequencies ω_1 & ω_2 and propagation constant k_1 & k_2. Displacement is given by.

$$y_1 = a\sin(\omega_1 t - k_1 x)$$

$$y_2 = a\sin(\omega_2 t - k_2 x)$$

Their superposition gives.

$$y = y_1 + y_2$$

$$= a\left[\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)\right]$$

Using

$$\left(\sin A + \sin B = 2\sin\frac{A+B}{2}\cos\frac{(A-B)}{2}\right)$$ we get.

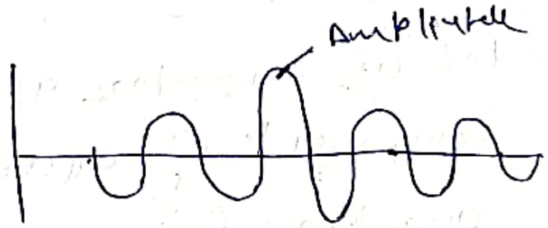
$$y = 2a\sin\left(\frac{(\omega_1 t - k_1 x + \omega_2 t - k_2 x)}{2}\right)\cos\left(\frac{\omega_1 t - k_1 x - \omega_2 t + k_2 x}{2}\right)$$

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

or $$y = \underbrace{2a\cos\left(\frac{(\omega_1-\omega_2)t}{2} - \frac{(k_1-k_2)x}{2}\right)}_{\text{Amplitude}} \sin\underbrace{\left[\frac{(\omega_1+\omega_2)t}{2} - \frac{(k_1+k_2)x}{2}\right]}_{\text{Angle}}$$

Note ($\psi = A\sin(\omega t - kx)$)

For Group velocity we use Amplitude velocity



where Amplitude A

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

∴ Group velocity $$V_g = \frac{\frac{\omega_1-\omega_2}{2}}{\frac{k_1-k_2}{2}} = \frac{\omega_1-\omega_2}{k_1-k_2}$$

$$\boxed{V_g = \frac{\Delta\omega}{\Delta k}}$$ — Group velocity

Relation between group velocity & Phase velocity :-

We have $V_p = \frac{\omega}{k} \Rightarrow \omega = (kV_p)$

$$V_g = \frac{d\omega}{dk} = \frac{d(kV_p)}{dk}$$

$$= V_p + k\frac{dV_p}{dk}$$

(Using $\boxed{k = \frac{2\pi}{\lambda}}$) $$V_g = V_p + \frac{2\pi}{\lambda}\frac{dV_p}{d(\frac{2\pi}{\lambda})}$$

$$V_g = v_p + \frac{1}{\lambda}\frac{dv_p}{d\left(\frac{1}{\lambda}\right)}$$

But $d\left(\frac{1}{\lambda}\right) = -\frac{1}{\lambda^2}d\lambda$, Therefore

$$\boxed{V_g = V_p - \lambda\frac{dv_p}{d\lambda}}$$

1.20 An electron has a de Broglie wavelength 2 pm. Find its kinetic energy, phase velocity and group velocity of its de Broglie wave. Rest mass energy of electron is 511 keV.

[GGSIPU, Feb. 2017 (3 marks)]

Hint : $m_0c^2 = 511\,\text{keV} \quad \Rightarrow \quad m_0 = 9.1\times10^{-31}\,\text{kg}$

$$\text{K.E.} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{1}{2}mv_g^2 \quad \Rightarrow \quad v_g = ? \quad \Rightarrow \quad v_pv_g = c^2 = ?$$

1.1 *Find the phase velocity and group velocity of the de-Broglie wave of an electron whose speed is 0.9c.*

[GGSIPU, Feb. 2009 (2 marks), May 2009 (2.5 marks) ; May 2019 (2.5 marks)

Hint : $v_pv_g = c^2$ and $v_g = 0.9c.$ Then $v_p = 3.33\times10^8\,\text{m/s}$.

Expectation values:- (Average value)

The average value of a large number of measurement of Physical quantity is represented by ~~large~~ Expectation value of a function $f(r)$.

$$\langle f(r)\rangle = \text{Average } f(r) = \overline{f(r)}$$

$$\boxed{\langle f(r)\rangle = \int \psi^*(r,t)\, f(r)\, \psi(r,t)\, d\tau}$$

Average value of position vector -

$$\langle \bar{r}\rangle = \int \psi^*(\bar{r},t)\, \bar{r}\, \psi(\bar{r},t)\, d\tau \quad -①$$

Average value of momentum.
(Expectation)

$$\langle P\rangle = \int \psi^* P \psi\, d\tau$$

$$\hat{p} = -i\hbar\nabla$$

$$\langle P\rangle = \int \psi^*(-i\hbar\nabla\psi)\, d\tau \quad -②$$

Expectation value of potential Energy V can be written as -

$$\langle V\rangle = \int \psi^*(r,t)\, V(r)\, \psi(r,t)\, d\tau \quad -③$$

Equⁿ ①, ② ③ are valid for Normalized wave Function. If wave function are not Normalized then average value function can be written as -

$$\langle f(r)\rangle = \frac{\int \psi^* f(r)\, \psi\, d\tau}{\int \psi^* \psi\, d\tau}$$

Eigen Values & Eigen Function

If there is some function f(x) which when operated on operator A gives the Equation

$$\boxed{\hat{A} f(x) = \lambda f(x)}$$

λ is constant and various possible value of λ are called eigen values of the operator and these functions are called Eigen Function.

$$\underset{\text{Operator}}{A}\ \underset{\text{Eigen Function}}{f(x)} = \underset{\text{Eigen. value}}{\lambda}\ f(x)$$

Note
Eigen values for matrices
$|A - \lambda I| = 0$

Suppose ψ be any wave function

Then AΨ (operation of ψ) =

where A is operator.

(Note An operator is a Mathematical operation on wave function that produce another wave function)

Thus " Eigen value Equation is that Equation in which operator operates on a function give the function multiplied by some constant" $\boxed{A f(x) = \lambda f(x)}$

***Example** 2.2 A particle limited to the x-axis has the wave function $\psi = ax$ between $x = 0$ and $x = 1$, $\psi = 0$ elsewhere. Find (a) the probability that particle can found between $x = 0.45$ and $x = 0.55$. (b) The expectation value $\langle x \rangle$ of the particle's position.* **[GGSIPU, May 2014 (3 marks), Feb. 2008, April 2007, Feb. 2012 (2 marks)]**

Solution. (*a*) The probability is

$$\int_{x_1}^{x_2} |\psi|^2\, dx = a^2 \int_{0.45}^{0.55} x^2\, dx = a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55} = 0.0251\, a^2$$

(*b*) The expectation value of the particle's position is

$$\langle x \rangle = \int_0^1 x|\psi|^2 dx = a^2 \int_0^1 x^3\, dx = a^2 \left[\frac{x^4}{4}\right]_0^1 = \frac{a^2}{4}$$

2.13 The eigenfunctions for a particle in a 1-*D* box are given by $\psi(x) = \sqrt{\frac{2}{a}} \sin\frac{m\pi x}{a}$. Find the expectation values of (*i*) position and (*ii*) momentum in the *n*th quantum state.

[GGSIPU, May 2016 (4 marks)]

Hint : (*i*) $\langle x \rangle = \int_{-\infty}^{\infty} \psi_n^* x \psi_n dx = \frac{2}{a}\int_0^a x \sin^2\frac{n\pi x}{a} dx$

Integrating by parts, we get : $\langle x \rangle = \frac{a}{2}$.

This result is as expected ; the probability density $\psi^*\psi$ is symmetric about $\langle x \rangle = \frac{a}{2}$, indicating that the particle spends as much time to the left of the center as to the right.

(*ii*) $$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi_n^* \left(i\hbar \frac{d}{dx}\right) \psi_n dx = \frac{2i\hbar}{a}\int_0^a \sin\frac{d}{dx}\left(\sin\frac{n\pi x}{a}\right) dx$$

$$= -\frac{2i\hbar}{a}\frac{n\pi}{a}\int_0^a \sin\frac{n\pi x}{a}\cos\frac{n\pi x}{a} dx = -\frac{i\hbar n\pi}{a^2}\int_0^a \sin\frac{2n\pi x}{a} dx$$

Solving the integral, we get $\langle p_x \rangle = 0$.

Again the result is expected. The particle moves back and forth, spending half its time moving towards the left and half its time moving towards the right. Thus, the average momentum must be zero.

Schrodinger Time dependent Equation in one Dimensio

Schrodinger Presented the wave Equation describing the Properties of electron in the form of equation called Schrodinger wave Equation to calculate the Probablities of electron at different places around Nucleus in the atom

OR.

It is a differential Equation for de-Broglie waves associated with particle and describing motion of particle.

$$\boxed{i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi}$$

m – Mass of electron
V – Potential Energy with refrence to Nucleus
ψ – wave function.

Derivation:- Equation of a particle moving freely in positive x direction is.

$$\psi = Ae^{-i(\omega t - kx)} \quad ①$$

Note

$\omega = 2\pi\nu$, $E = h\nu$
$\nu = E/h$
$$\boxed{\omega = \frac{2\pi E}{h}}$$

$k = \frac{2\pi}{\lambda}$, $\lambda = \frac{h}{p}$
$$\boxed{k = 2\pi\frac{p}{h}}$$

where A – Amplitude , k – Propagation constant
ω – Constant Angular Frequency.

Now substituting value of ω & k in Equation ①

$$\psi = Ae^{-i(\omega t - kx)}$$

$$\psi = Ae^{-i\left(\frac{2\pi Et}{h} - \frac{2\pi px}{h}\right)}$$

$$\psi = Ae^{-i\left(\frac{2\pi}{h}(Et-Px)\right)}$$

Using $\hbar = \frac{h}{2\pi}$ here $\hbar$ is Modified form of Planck's constant.

$$\Rightarrow \quad \psi = Ae^{-\frac{i}{\hbar}(Et-Px)}$$

$$= Ae^{\frac{i}{\hbar}(Px-Et)} \quad —②$$

Now Differentiating ② wrt x

$$\frac{d\psi}{dx} = Ae^{\frac{i}{\hbar}(Px-Et)}\frac{d}{dx}\frac{i}{\hbar}(Px-Et)$$

(Note using $\frac{d}{dx}e^{y} = e^{y}\frac{dy}{dx}$)

$$= \psi\frac{iP}{\hbar} \quad \text{from ②}$$

$$\Rightarrow \quad P\psi = \frac{\hbar}{i}\frac{d\psi}{dx} \quad —③$$

Now Differentiating wrt t

$$\frac{d\psi}{dt} = A\left(-\frac{iE}{\hbar}\right)e^{\frac{i}{\hbar}(Px-Et)}$$

$$= -\frac{iE}{\hbar}\psi \quad \text{from ②}$$

$$\Rightarrow \quad E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt} = \hbar i\frac{d\psi}{dt} \quad —④$$

Now Total Energy

E = Kinetic Energy + Potential Energy

$$E = \frac{1}{2}mv^2 \times \frac{m}{m} + V$$

$$\boxed{E = \frac{p^2}{2m} + V}$$

$$E(\psi) = \frac{p^2}{2m}(\psi) + V(\psi) \quad —⑤$$

Now Substituting value of ③ & ④ in ⑤
we get

$$i\hbar\frac{d\psi}{dt} = \frac{\left(\frac{\hbar^2}{i^2}\frac{d^2\psi}{dx^2}\right)}{2m} + V(\psi).$$

$$\Rightarrow \boxed{i\hbar \frac{d\psi}{dt} = \left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(\psi)\right)} \quad — ⑥$$

Time dependent Schrodinger wave Equation.

Time Independent ~~Schronger~~ Schrodinger Equation

We have Equation of a Particle moving freely in positive x direction.

$$\psi = Ae^{-i(\omega t - kx)}$$

$$\left(\text{Using } \omega = \frac{2\pi E}{h} \ \& \ k = \frac{2\pi p}{h}\right)$$

$$\psi(x,t) = Ae^{-i\frac{2\pi}{h}(Et - px)}$$

$$= Ae^{i\frac{2\pi}{h}(px - Et)}$$

$$= A\left(e^{\frac{2\pi i px}{h}}\right)\left(e^{-\frac{2\pi i Et}{h}}\right)$$

Again we have. — ①

$$\psi = Ae^{-i(\omega t - kx)}$$

For time independent $t=0$

$$\psi(x) = Ae^{-i(-kx)}$$

$$= Ae^{-i\left(-\frac{2\pi p}{h}x\right)}$$

$$\psi(x) = Ae^{\frac{2\pi i px}{h}}$$

— ②

Substituting ② in ① we get.

$$\psi(x,t) = \phi(x)\, e^{-2\pi i E t/h}. \quad -(A)$$

Differentiating wrt t

$$\frac{d\psi}{dt} = \phi(x)\, e^{-\frac{2\pi i E t}{h}} \left(-\frac{2\pi i E}{h}\right) \quad -(B)$$

Differenting wrt x

$$\frac{d\psi}{dx} = e^{-\frac{2\pi i E t}{h}} \frac{d\phi}{dx}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = e^{-\frac{2\pi i E t}{h}} \frac{d^2\phi}{dx^2} \quad -(C)$$

Substituting value of A, B, C in ⑤

From ⑤ we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = i\hbar\,\frac{d\psi}{dt}$$

$$\Rightarrow -\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} + V\psi = \frac{ih}{2\pi}\frac{d\psi}{dt}$$

$$\Rightarrow -\frac{h^2}{8\pi^2 m}\left(e^{-\frac{2\pi i E t}{h}}\frac{d^2\phi}{dx^2}\right) + V\left(\phi(x)\, e^{-\frac{2\pi i E t}{h}}\right)$$

$$= \frac{i\cancel{h}}{\cancel{2\pi}}\, \underbrace{\phi(x)\, e^{-\frac{2\pi i E t}{h}}} \left(\frac{-\cancel{2\pi} i E t}{\cancel{h}}\right)$$

$$\Rightarrow \cancel{e^{-\frac{2\pi i E t}{h}}}\left(-\frac{h^2}{8\pi^2 m}\frac{d^2\phi}{dx^2} + V\phi\right) = \cancel{e^{-\frac{2\pi i E t}{h}}}\, E\phi$$

$$\Rightarrow \boxed{\frac{d^2\phi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\phi = 0}$$

↓

Time independent Schrodinger Equⁿ

The Free Particle!-

The Particle is said to be a free Particle when it is moving in space without being subjected to any External force in any Region of space and its Potential Energy is constant ($V =$ constant).

Then time-Independent Schrodinger wave Equation for free Particle is given as-

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

$V=0$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}E\psi = 0$$

Note

Kinetic Energy $= \frac{1}{2}mv^2$

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

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

$p = \sqrt{2mE}$

propagation constant

$k = \frac{2\pi}{\lambda}$

$= \frac{2\pi p}{h}$

$k = \frac{2\pi\sqrt{2mE}}{h}$

on squaring

$$\boxed{k^2 = \frac{8\pi^2 mE}{h^2}}$$

Hence

$$\boxed{\frac{d^2\psi}{dx^2} + k^2\psi = 0} \quad ①$$

where $k^2 = \frac{8\pi^2 mE}{h^2}$

a) Wave Function:→ General Solution of Equation ① is given by

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

b) Energy:→ Energy of Particle is given by-

We have $k^2 = \frac{8\pi^2 mE}{h^2}$

(using $\hbar = \frac{h}{2\pi}$)

$$\boxed{E = \frac{h^2k^2}{8\pi^2 m} = \frac{\hbar^2 k^2}{2m}}$$

c) Momentum:- $\psi = Ae^{-i(\omega t - kx)}$

$$\left(\begin{array}{ll} \omega = 2\pi\nu & k = \frac{2\pi}{\lambda} \\ \quad = \frac{2\pi E}{h} & \quad = \frac{2\pi P}{h} \end{array} \right)$$

$$\psi = Ae^{-i\left(\frac{2\pi}{h}(Et - Px)\right)}$$

using $\left(\hbar = \frac{h}{2\pi}\right)$

$$= Ae^{\frac{i}{\hbar}}(Et - Px)$$

$$= Ae^{\frac{i}{\hbar}}(Px - Et)$$

$$\frac{d\psi}{dx} = A\frac{iP}{h}e^{\left(\frac{i}{\hbar}(Px - Et)\right)}$$

$$= \frac{iP\psi}{\hbar}$$

$$\Rightarrow \boxed{P\psi = \frac{\hbar}{i}\frac{d\psi}{dx}}$$

d) Position of particle:- Probablity of finding the particle is given by -

$$P\,dx = \psi^*(x,t)\,\psi(x,t)$$

The Probablity density P for the position of particle with definite value of momentum is constant over x-Axis.

Particle in a Rigid one Dimensional box (Infinite Square well Potential):

Let us consider a particle restricted to move along x-axis between ($x=0$ and $x=L$), ~~by~~

Suppose Potential Energy V of the Particle is zero inside the box, but rises to infinity outside.

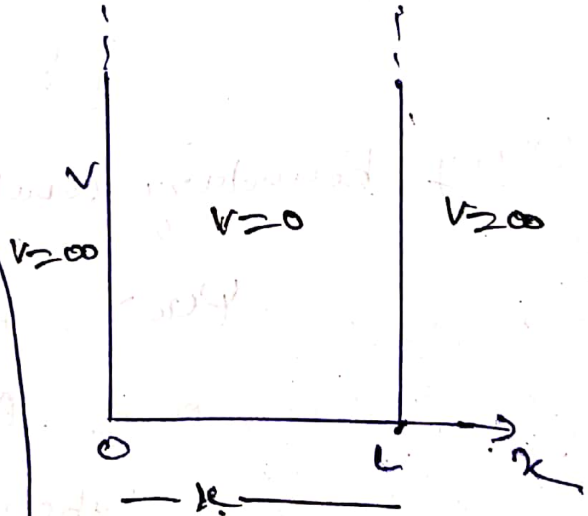
that is $\quad V=0$ for $(0 \le x \le L)$ - Inside box

$V = \infty$ for $(x<0$ & $x>L)$ - outside the box

In such case the Particle is said to be moving in an infinitely deep Square well Potential

Schrodinger Equation for the Particle within box is -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi = 0 \quad — ①$$



$V=0$ (Inside the box).

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m(E-V)\psi}{h^2} = 0$$

Substitute $V=0$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi = 0$$

Suppose $\quad \frac{8\pi^2 mE}{h^2} = k^2 \quad — ②$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad — ③$$

General Solution of differential Equation is of the form -

$$\psi(x) = A\sin kx + B\cos kx \quad \text{—④}$$

Where the constant A & B are to be determined by boundary conditions. Therefore, the wavefunction ψ must be zero outside the box.

ψ must also be zero at the walls ($x=0$, $x=L$ at walls)

Using the boundary condition $\psi=0$ at $x=0$ in ④

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

$$0 = A\sin k(0) + B\cos k(0)$$

$$0 = 0 + B(1)$$

$$\boxed{B=0} \underset{\text{in ④}}{\Rightarrow} \boxed{\psi(x) = A\sin kx} \text{—⑤}$$

Using boundary condition $\psi(x)=0$ at $x=L$ in ④

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

$$0 = A\sin k(L) + B\cos k(L)$$

Substituting $B=0$

$$0 = A\sin kL + 0$$

$$A\sin kL = 0$$

$$\sin kL = 0$$

~~$\sin kL = n\pi$~~ $(n = 1, 2, 3 \text{———})$

$$\sin kL = \sin n\pi$$

$$kL = n\pi$$

$$\boxed{k = \frac{n\pi}{L}}$$

Substituting $k = \frac{n\pi}{L}$ in (5)

$$\Rightarrow \boxed{\psi(x) = A\sin\left(\frac{n\pi x}{L}\right)} \quad \text{—(6)}$$

Now for Energy we have

$$k^2 = \frac{8\pi^2 mE}{h^2} \quad (\text{by } ②)$$

$$\Rightarrow E = \frac{k^2h^2}{8\pi^2 m}$$

Substituting $k = \frac{n\pi}{L}$

$$\boxed{E = \frac{n^2h^2}{8mL^2}} \quad (n = 1, 2, 3 ---)$$

Thus we see that in a potential well the particle can not have an arbitary Energy but can have only certain Energy values corresponding to n = 1, 2, 3 ---) these are Eigen values of the particle in the well and correspond to energy level of the system.

$$E_n = \frac{n^2h^2}{8mL^2}$$

Ground state Energy (n=1)

$$E_1 = \frac{h^2}{8mL^2}$$

First Excited State Energy (n=2)

$$E_2 = \frac{4h^2}{8mL^2}$$

We have calculated the values of Energy

Now we will find the solution of wave function in Equation ⑥ and value of A

From ⑥ we have

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

Where A → Normalization factor ~~or~~
Normalization Constant

To find the value of A we will use Normalization condition.

$$\boxed{\int_0^L \psi\psi^* dx = 1}$$

↓

Normalization condition

$$\Rightarrow \int_0^L \left(A\sin\left(\frac{n\pi x}{L}\right)\right)\left(A\sin\left(\frac{n\pi x}{L}\right)\right)dx = 1$$

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

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

$$\left(\begin{aligned} \text{using } & \cos 2\theta = 1 - 2\sin^2\theta \\ & 2\sin^2\theta = 1 - \cos 2\theta \\ & \sin^2\theta = \frac{1-\cos 2\theta}{2} \end{aligned}\right)$$

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

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

$$\Rightarrow \frac{A^2}{2}\left[L-0\right] = 1$$

$$A^2 = \frac{2}{L}$$

$$\boxed{A = \sqrt{\frac{2}{L}}}$$

in ⑥ $$\boxed{\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)} \; *$$

↓

Solution of wave function

Plotting of wave function :-

First three Eigen function ψ_1, ψ_2, ψ_3 together with the Probability densities $|\psi_1|^2, |\psi_2|^2, |\psi_3|^2$ are shown in figure

we have $\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

1) $n=1$ for ground state

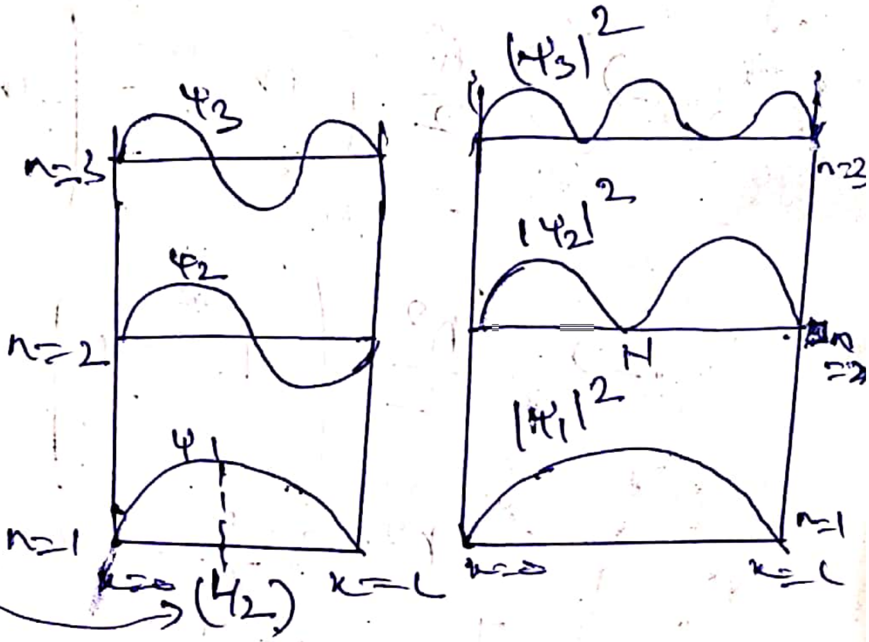
$$\psi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

- Maximum value of ~~sin~~ $\psi = \sin 90° = \sin\left(\frac{\pi}{2}\right)$

$$\Rightarrow \sin\left(\frac{n\pi}{L}\right) = \sin\left(\frac{\pi}{2}\right) = 1$$

$$\frac{\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = \frac{L}{2}}$$



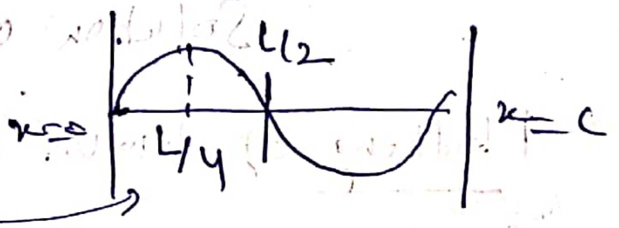
II) n=2

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

$$\sin\left(\frac{2\pi x}{L}\right) = \sin\frac{\pi}{2}$$

$$\frac{2\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = \frac{L}{4}}$$



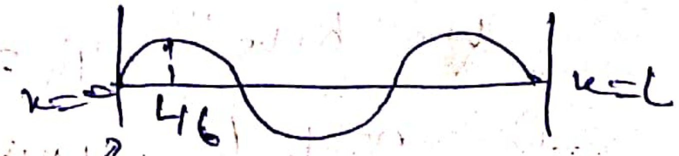
III) n=3

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

$$\sin\left(\frac{3\pi x}{L}\right) = \sin\frac{\pi}{2}$$

$$\frac{3\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = L/6}$$



2.9 Consider a particle confined in one-dimensional box of width l. Find the probability that the particle is found between $x = 0$ and $x = l/n$ when it is in nth state. **[GGSIPU, April 2015 (2 marks)]**

Hint : $\psi_n(x) = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$

$$p = \int_{x_1}^{x_2} |\psi_n(x)|^2 \, dx = \frac{2}{l} \int_{x_1}^{x_2} \sin \frac{n\pi x}{l} dx$$

$$= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1 = 0}^{x_2 = l/n} = \left[\frac{1}{n} - \frac{1}{2n\pi} \sin \frac{2n\pi l}{nl} \right] = \frac{1}{n}.$$

2.10 An electron is contrained to mvoe in a one dimensional box of length 0.1 nm. Find the first three energy eigen values and the corresponding de Broglie wavelengths.

[GGSIPU, May 2015 (4 marks)]

Hint : $E_n = \frac{n^2 h^2}{8ml^2} \quad \Rightarrow \quad E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2}$

$$E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2 \times (1.6 \times 10^{-19})} \text{eV} = 37.5\, n^2 \text{eV}$$

Then $E_1 = 37.5$ eV, $E_2 = 150$ eV, $E_3 = 337.5$ eV

For de Broglie wavelength $\lambda_n = \frac{h}{\sqrt{2mE_n}}$

2.11 Find the probability that a particle trapped in a box 'L' wide can be found between 0.45 L and 0.55 L for the first excited state. **[GGSIPU, May 2015 (4 marks)]**

Hint : $\psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$; $P = \int_{x_1}^{x_2} |\psi_n(x)|^2 \, dx = \frac{2}{l} \int_{x_1}^{x_2} \sin \frac{2n\pi x}{l} dx$

$$= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1}^{x_2}$$

Now $x_1 = 0.45$ L and $x_2 = 0.55\, l$ and $n = 2$ for first excited state, on solving it we get $P = 9.8\%$.

2.12 The wave function for a particle in a 1-D box is given by $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$. Show that the wave function for two different states are orthonormal.

[GGSIPU, May 2016 (3 marks)]

Hint : For the eigenfunctions in the mth and nth states, $m \neq n$, to be orthogonal, we must have

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = 0$$

For the given wavefunction, $\psi_m(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$, then $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = \frac{2}{a} \int_0^a \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a} dx$$

Therefore $$= \frac{2}{a} \left[\int_0^a \cos \frac{(m-n)\pi x}{a} dx - \int_0^a \cos \frac{(m+n)\pi x}{a} dx \right]$$

2.8 An electron is in a box of 0.01 nm. Find its permitted energy.

[GGSIPU, Feb. 2013, (2 marks) ; May 2008 (2.5 marks

Hint :

$$E_n = \frac{n^2h^2}{8ml^2} = \frac{n^2\times(6.626\times10^{-34})^2}{8\times9.1\times10^{-22}(0.01\times10^{-9})^2}$$

$$= 6\times10^{-16}\, n^2\ \text{J} = \frac{6\times10^{-16}}{1.6\times10^{-19}}\ \text{eV} = \frac{60000}{16}\, n^2\ \text{eV}$$

For $n = 1, 2, 3, \ldots$ the energy eigen value $E_1, E_2, E_3, \ldots$

$E_1 = 3750$ eV, $E_2 = 15000$ eV, $E_3 = 33750$ eV, …

2.13 The eigenfunctions for a particle in a 1-*D* box are given by $\psi(x) = \sqrt{\frac{2}{a}}\sin\frac{m\pi x}{a}$. Find the expectation values of (*i*) position and (*ii*) momentum in the *n*th quantum state.

[GGSIPU, May 2016 (4 marks)]

Hint : (*i*)

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi_n^* x\psi_n\,dx = \frac{2}{a}\int_0^a x\sin^2\frac{n\pi x}{a}\,dx$$

Integrating by parts, we get : $\langle x\rangle = \frac{a}{2}$.

This result is as expected ; the probability density $\psi^*\psi$ is symmetric about $\langle x\rangle = \frac{a}{2}$, indicating that the particle spends as much time to the left of the center as to the right.

(*ii*)

$$\langle p_x\rangle = \int_{-\infty}^{\infty}\psi_n^*\left(i\hbar\frac{d}{dx}\right)\psi_n\,dx = \frac{2i\hbar}{a}\int_0^a \sin\frac{d}{dx}\left(\sin\frac{n\pi x}{a}\right)dx$$

$$= -\frac{2i\hbar}{a}\frac{n\pi}{a}\int_0^a \sin\frac{n\pi x}{a}\cos\frac{n\pi x}{a}\,dx = -\frac{i\hbar n\pi}{a^2}\int_0^a \sin\frac{2n\pi x}{a}\,dx$$

Solving the integral, we get $\langle p_x\rangle = 0$.

Again the result is expected. The particle moves back and forth, spending half its time moving towards the left and half its time moving towards the right. Thus, the average momentum must be zero.

2.4 For an electron in a one-dimensional box of width 2 Å, calculate the separation between the lowes two levels in eV.

[GGSIPU, June 2013 (4.5 marks)]

Hint : $$E_n = \frac{n^2h^2}{8ml^2}$$

$$\Rightarrow \quad E_1 = \frac{1\times(6.63\times10^{-34})^2}{8\times9.1\times10^{-31}\times(2\times10^{-10})^2} = 2.273\times10^{-19}\,\text{J} = 1.42\text{ eV}$$

2.17 An electron is confined to move between two rigid walls separate by 2×10^{-9} m. Find the de Broglie wavelengths representing the first three allowed energy states of the electron.

[GGSIPU, May 2017 (4 marks)]

Hint : $$E_n = \frac{n^2h^2}{8ml^2} \quad \Rightarrow \quad \frac{hc}{\lambda_n} = \frac{n^2h^2}{8ml^2} \quad \Rightarrow \lambda_n = \frac{c}{n^2h}\times 8ml^2$$

$$\lambda_1 = \frac{3\times10^8}{(6.62\times10^{-34})}\times8\times(9.1\times10^{-31})\times(2\times10^{-9})^2 = 1.32\times10^{-5}\text{ m}$$

$$\lambda_2 = \frac{3\times10^8}{4\times(6.62\times10^{-34})}\times8\times(9.1\times10^{-31})\times(2\times10^{-9})^2 = 3.3\times10^{-6}\text{ m}$$

$$\lambda_3 = \frac{3\times10^8}{9\times(6.62\times10^{-34})}\times8\times(9.1\times10^{-31})\times(2\times10^{-9})^2 = 1.47\times10^{-6}\text{ m}$$

Problem 2.8 *The wave function of a certain particle is* $\psi = A\cos^2 x$ *for* $-\frac{\pi}{2} < x < \frac{\pi}{2}$

(a) Find the value of A (b) Find the probability that the particle be found between $x = 0$ *and* $x = \frac{\pi}{4}$.

[GGSIPU, Feb. 2012, (5 marks) reappear]

Solution. As $\psi = A\cos^2 x \quad -\frac{\pi}{2} < x < \frac{\pi}{2}$

(a) $$\int_{-\pi/2}^{\pi/2} |\psi|^2\,dx = 1$$

$$\Rightarrow \quad 2A^2\int_0^{\pi/2}\cos^4 x\,dx = 1 \quad \text{or} \quad 2A^2\frac{3\pi}{16} = 1$$

$$\frac{3\pi}{8}A^2 = 1 \quad \therefore \quad A = \sqrt{\frac{8}{3\pi}}$$

(b) $$P = \int_0^{\pi/4} |\psi|^2\,dx = A^2\int_0^{\pi/4}\cos^4 x\,dx \text{ as } A = \sqrt{\frac{8}{3\pi}}$$

$$P = \frac{8}{3\pi}\int_0^{\pi/4}\cos^4 x\,dx = 0.462$$

Schrodinger wave Equation for finite well:-

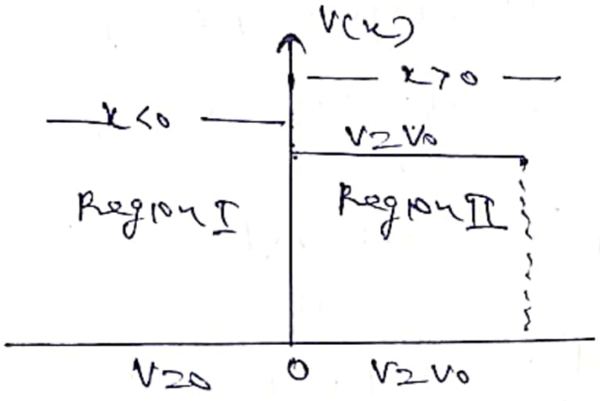
(Step barrier / Potential barrier & tunnel Effect).

1) Step barrier / Potential barrier.

When a particle approaches a region in which entrace of particle is opposed by some force then then region is said to form a barrier for a particle

Note:- Potential barrier is also a system used to identify incident, reflected & transmitted matter waves.

Let us consider a particle moving along x-axis from left to right and meeting a barrier of height V_0 let E be the total Energy of particle and V be the value of constant potential



we have two different region supported by discontinuous change of potential -

Region I : $x<0 \Rightarrow V=0$

$x>0 \Rightarrow V=V_0$

Behaviour of particle can be described in quantum mechanics as if energy of particle -

i) If $(E < V_0)$

Then there is a probality that the particle will be reflected back from the barrier

ii) If $(E > V_0)$

Then there is a probality that it will penetrate through the barrier.

Such behaviour of particle is impossible from the classical view point. It follow Schrodinger wave Equation

a) Region I

Let us consider the region $x < 0$ time independent Schrodinger wave Equation is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

$(V = 0$ in the region $x < 0)$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0$$

Let $K_1^2 = \frac{8\pi^2 m E}{h^2}$

$$\Rightarrow \frac{d^2\psi}{dx^2} + K_1^2\psi = 0 \quad — ①$$

b) Region II

Schrodinger wave Equation is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2}{h^2}(E-V_0)\psi = 0$$

$$\frac{d^2\psi}{dx^2} + K_2^2\psi = 0$$

where $K_2^2 = \frac{8\pi^2 m}{h^2}(E-V_0)$ — ②

Solution of Differential Equation ① + ② are-

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x}$$

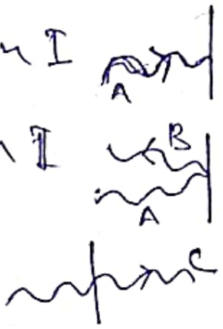
where-

A - Amplitude of incident wave in Region I

B - Amplitude of reflected wave in Region I

C - Amplitude of wave Penetrate the barrier in Region II

D - No Particle can flow to left hence D=0



Now In order to be a Proper wave Function ψ Must be Finite + Continuous every where on X-Axis. It means at boundary (x=0) wave function inside + outside Must have same values.

Hence ψ_1, ψ_2 + its derivatives Must be continuous at the boundary (x=0)

$$~~\psi(x)=~~ \psi_1 = \psi_2 \quad (\text{at } x=0)$$

$$\Rightarrow \quad Ae^{ik_1x} + Be^{-ik_1x} = Ce^{ik_2x}$$

Substituting x=0

$$\Rightarrow \quad A+B = C \qquad \text{—③}$$

Also its derivatives Must be continuous at x=0

$$\Rightarrow \quad \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$\frac{d}{dx}\left(Ae^{ik_1x} + Be^{-ik_1x}\right) = \frac{d}{dx}\left(Ce^{ik_2x}\right)$$

$$\Rightarrow \quad Aik_1e^{ik_1x} ~~+~~ - Bik_1e^{-ik_1x} = Cie^{ik_2x}$$

Now At x=0 we have

$$Aik_1 - Bik_1 = Cik_2$$

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$$\Rightarrow (A-B) = \frac{k_2}{k_1} C \quad -④$$

on solving ③ & ④ we get

$$2B = \left(1 - \frac{k_2}{k_1}\right) C$$

(Note
For solving
Add ③ + ④
& Subtract ③ − ④)

$$= \frac{k_1 - k_2}{k_1} \times \frac{2k_1}{k_1 + k_2} \times A$$

$$\Rightarrow \boxed{B = \left(\frac{k_1 + k_2}{k_1 - k_2}\right) A}$$

Also $$2A = \left(1 + \frac{k_2}{k_1}\right) C$$

$$\Rightarrow \boxed{A = \frac{k_1 + k_2}{2k_1} C}$$

Now Substituting value of A in ③ we get $$\boxed{C = \frac{2k_1}{k_1 + k_2} A}.$$

Now Case I For $E < V_0$

Probablity density is given by

$$(J_x) = \frac{\hbar}{2im}\left(\psi_1^* \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx}\right)$$

we have $$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\psi_1^* = Ae^{-ik_1x} + Be^{ik_1x}$$

$$\Rightarrow (J_x) = \frac{\hbar}{2im}\left[\left(Ae^{-ik_1x} + Be^{ik_1x}\right) \times \frac{d}{dx}\left(Ae^{ik_1x} + Be^{-ik_1x}\right)\right.$$
$$\left. - \left[\left(Ae^{ik_1x} + Be^{-ik_1x}\right) \times \frac{d}{dx}\left(Ae^{-ik_1x} + Be^{ik_1x}\right)\right)\right.$$

$$= \frac{\hbar}{2im}\left[\left(Ae^{-ikx} + Be^{ikx}\right) \times (ik_1)\left(Ae^{ik_1x} - Be^{-ik_1x}\right)\right]$$
$$- \left[\left(Ae^{ik_1x} + Be^{-ik_1x}\right) \times (-ik_1)\left(Ae^{-ik_1x} - Be^{ik_1x}\right)\right]$$

$$= \frac{k_1 \hbar}{m}\left(A^2 - B^2\right)$$

Here A^2 represent Magnitude of incident current

B^2 - Magnitude of Reflected current

Reflectance coefficient = $\frac{\text{Magnitude of Reflected Current}}{\text{Magnitude of incident Current}}$

$$R = \frac{B^2}{A^2}$$
$$= \frac{\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 A^2}{A^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

Case - II Region II

~~$\psi_2 = ce^{i}$~~ $\psi_2 = ce^{ik_2x}$

$\psi_2^* = ce^{-ik_2x}$

$$J_x = \frac{\hbar}{2im}\left(\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}\right)$$
$$= \frac{\hbar}{2im}\left[ce^{-k_2x}\frac{d}{dx}\left(ce^{+ik_2x}\right) - \left(ce^{+ik_2x}\frac{d}{dx}\left(e^{-ik_2x}\right)\right)\right]$$
$$= \frac{\hbar}{2im}\left(C \times C\,(ik_2) - C \times C\, ik_2\right)$$

$$\boxed{J = 0}$$

Now Transmittance coefficient =

$$\frac{\text{Magnitude of Transmittance current}}{\text{Magnitude of incident current}}$$

$$= \frac{C^2}{A^2}$$

$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 \cancel{A^2}}{\cancel{A^2}} \times \frac{k_2}{k_1}$$

$$\boxed{T = \frac{4k_1 k_2}{(k_1+k_2)^2}}$$

Also According to definition $\boxed{R+T=1}$ can be varified.

Tunneling Effect:

"When a Particle is able to cross the Potential barrier even when ~~the~~ its Energy is less than the barrier height ($E<V_0$) then this Phenomenon is called Tunnel Effect"

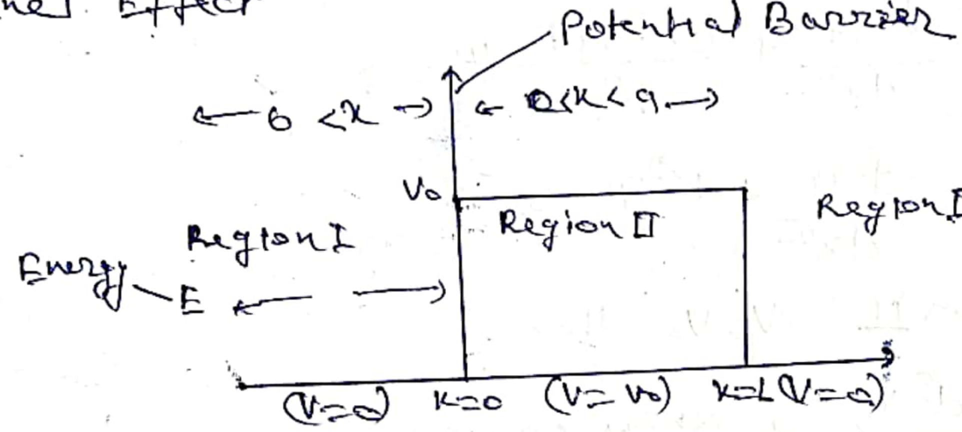


Figure represent a Potential barrier of height V_0 & thickness L. let us consider a Particle moving along x Axis from left to Right and moving a Rectangular Potential barrier of height V_0 and length L.

We have three different Region Seprated by discontinuous change of Potential Energy.

→ Potential Energy is zero in the region I & III for $x<0$ & $x>L$

→ Potential Energy is V_0 in the Region II.

If $E<V_0$ according to quantum Mechanics. Still there is a finite chance for the electron to leak the other side of Barrier. Hence the electron is tunneled through the potential barrier. This Phenomenon Called Tunneling.

The Schrodinger wave Equation for a particle along X-Axis is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

In Region I V=0 then

$$\frac{d^2\psi_1}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + \frac{K^2}{h^2}\psi_1 = 0 \quad -①$$

$$\left(k^2 = \frac{8\pi^2 mE}{h^2} \quad k = \sqrt{\frac{2mE}{\hbar}} \right.$$

In Region II V=Vo then

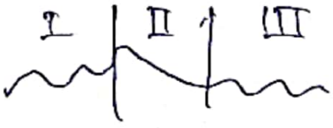
$$\frac{d^2\psi_2}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V_0)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \frac{8\pi^2 m}{h^2}(V_0-E)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0 \quad -②$$

$$\beta = \sqrt{\frac{8\pi^2 m}{h^2}(V_0-E)} = \sqrt{\frac{2m(V_0-E)}{\hbar}}$$

(Note:- In Region II waves is decaying Exponentially so Negative value of E in (Vo−E) is used Hence solution of this Equn (ψ_2) doesn't give i (iota) term)



Region -III V=0 then

$$\frac{d^2\psi_3}{dx^2} + K^2\psi_3 = 0 \quad -③$$

Solution of Equation ① , ② & ③ will be

$$\psi_1 = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2 = Ce^{\beta x} + De^{-\beta x}$$

$$\psi_3 = Ge^{ikx} + He^{-ikx}$$

$$= Ge^{ikx}$$

$H=0$ because no wave travel back from infinity

Applying boundary conditions to particle

1) At $x=0$ $\psi_1 = \psi_2$

$$Ae^{ikx} + Be^{-ikx} = Ce^{\beta x} + De^{-\beta x}$$

At $x=0$

$$A+B = C+D \quad -④$$

we also have -

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$ikAe^{ikx} - ikBe^{-ikx} = \beta Ce^{\beta x} - \beta De^{-\beta x}$$

at $x=0$

$$ik(A-B) = \beta(C-D)$$

$$A-B = \frac{\beta}{ik}(C-D) \quad -⑤$$

From equation ④ & ⑤ we get

$$A = \frac{1}{2}\left[\left(1+\frac{\beta}{ik}\right)C + \left(1-\frac{\beta}{ik}\right)D\right] \quad -⑥$$

$$B = \frac{1}{2}\left[\left(1-\frac{\beta}{ik}\right)C + \left(1+\frac{\beta}{ik}\right)D\right) \quad -⑦$$

At $x=0$ we have

$$\psi_2 = \psi_3$$

$$Ce^{\beta x} + De^{-\beta x} = Ge^{ikx}$$

At $x=a$

$$\Rightarrow Ce^{\beta a} + De^{-\beta a} = Ge^{ika} \quad ⑧$$

Also we have -

$$\frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}$$

$$C\beta e^{\beta x} - D\beta e^{-\beta x} = Gik e^{ikx}$$

At $x=a$

$$Ce^{\beta a} - De^{\beta a} = \frac{ik}{\beta} Ge^{ika} \quad ⑨$$

From eqn ⑧ and ⑨

$$C = \frac{1}{2}\left(1 + \frac{ik}{\beta}\right)e^{-\beta a} Ge^{ika}$$

$$D = \frac{1}{2}\left(1 - \frac{ik}{\beta}\right)e^{\beta a} Ge^{ika}$$

Put the value of C & D in eqn ⑥

From ⑥ we have -

$$A = \frac{1}{2}\left(\left(1 + \frac{\beta}{ik}\right)C + \left(1 - \frac{\beta}{ik}\right)D\right)$$

$$A = \frac{1}{4}\left(\left(1 + \frac{\beta}{ik}\right)\left(1 + \frac{ik}{\beta}\right)e^{-\beta a}Ge^{ika}\right) + \frac{1}{4}\left(\left(1 - \frac{\beta}{ik}\right)\left(1 - \frac{ik}{\beta}\right)e^{\beta a}Ge^{ika}\right)$$

$$A = \frac{G}{4}e^{ika}\left(\left(1 + \frac{ik}{\beta} + \frac{\beta}{ik} + \cancel{\frac{\beta ik}{\beta ik}}\right)e^{-\beta a} + \left(1 - \frac{ik}{\beta} - \frac{\beta}{ik} - \cancel{\frac{ik\beta}{ik\beta}}\right)e^{\beta a}\right]$$

$$= \frac{G}{4}e^{ika}\left(\left(2 + \frac{ik}{\beta} + \frac{\beta}{ik}\right)e^{-\beta a} + \left(2 - \frac{ik}{\beta} - \frac{\beta}{ik}\right)e^{\beta a}\right)$$

$$A = \frac{G}{4}e^{ika}\left[2\left(e^{-\beta a}+e^{\beta a}\right)+\left(\frac{\beta}{ik}+\frac{ik}{\beta}\right)e^{-\beta a}-\left(\frac{\beta}{ik}+\frac{ik}{\beta}\right)e^{\beta a}\right]$$

$$= \frac{G}{4}e^{ika}\left(2\frac{\left(e^{-\beta a}+e^{\beta a}\right)}{2}+\left(\frac{\beta}{ik}+\frac{ik}{\beta}\right)\cdot\left(e^{-\beta a}-e^{\beta a}\right)\right)$$

$$= \frac{G}{4}e^{ika}\left(2\frac{\left(e^{-\beta a}+e^{\beta a}\right)}{2}+2\left(\frac{\beta}{ik}+\frac{ik}{\beta}\right)\left(\frac{e^{\beta a}-e^{\beta a}}{2}\right)\right]$$

$$= \left[\cosh\beta a+\frac{i}{2}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh\beta a\right]Ge^{ika}$$

$$\Rightarrow \frac{A}{G} = \left[\cosh\beta a+\frac{i}{2}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh\beta a\right]e^{ika} \quad \text{— ⑩}$$

we have Transmittance coefficient (T)

$$(T) = \frac{\text{Magnitude of Transmitted wave}}{\text{Magnitude of incident wave}} = \left(\frac{G^2}{A^2}\right)$$

From ⑩

$$\left|\frac{A^*A}{G^*G}\right| = \left|\frac{A}{G}\right|^2 = \frac{1}{T} = \cosh^2\beta a+\frac{1}{4}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)^2\sinh^2\beta a$$

$$= 1+\left(1+\frac{1}{4}\left(\frac{\beta}{k}-\frac{k}{\beta}\right)^2\right)\sinh^2\beta a$$

$$= 1+\left[\frac{1}{4}\left(4+\left(\frac{\beta}{k}-\frac{k}{\beta}\right)^2\right)\right]\sinh^2\beta a \quad \text{— ⑪}$$

~~$\sin^2 h+\cos^2 h$~~
Using
~~$\sin^2 x+\cos^2 x=1$~~
$(a+ib)(a-ib) = (a^2+b^2)$
$(\cos^2 h-\sin^2 h=1)$

we have $k = \frac{\sqrt{2mE}}{\hbar}$ & $\beta = \frac{\sqrt{2m(V_0-E)}}{\hbar}$

$$\Rightarrow \frac{\beta}{k}-\frac{k}{\beta} = \sqrt{\frac{V_0-E}{E}}-\sqrt{\frac{E}{V_0-E}} = \frac{V_0-E-E}{\sqrt{E(V_0-E)}} = \frac{V_0-2E}{\sqrt{E(V_0-E)}}$$

Now $$\left(\frac{\beta}{k}-\frac{k}{\beta}\right)^2+4 = \frac{(V_0-2E)^2}{E(V_0-E)}+4 = \frac{V_0^2+4E^2-4EV_0+4EV_0-4E^2}{E(V_0-E)}$$

$$= \frac{V_0^2}{E(V_0-E)}$$

$$\Rightarrow \quad \frac{1}{T} = 1 + \frac{1}{4}\left[\frac{V_0^2}{E(V_0 - E)}\right] \sinh^2 \beta a$$

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}} \sinh^2 \beta a$$

Also $\sinh^2 \beta a = \left(\frac{e^{\beta a} - e^{-\beta a}}{2}\right)^2 = e^{\frac{2\beta a}{4}}$

$$\Rightarrow \quad \boxed{T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}} \times e^{\frac{2\beta a}{4}}}$$

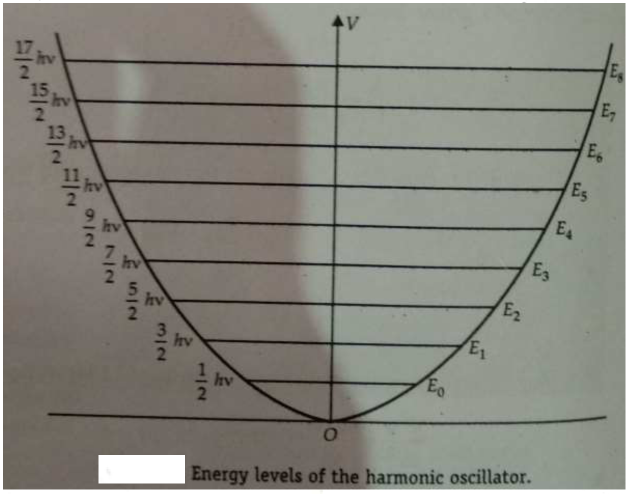
$\downarrow$

Transmission coefficient.

Simple Harmonic oscillator + Zero Point Energy:-

A Simple harmonic oscillator is a particle performing one dimensional motion under restoring force F which is proportional to particle displacement x from Equilibrium position.

The plot of V against x is a parabola and we may describe that the particle being a periodic potential well. If E be the total Energy of particle. It oscillate back & forth. from center.



Energy levels of the harmonic oscillator.

Now Force is proportional to particle displacement x from Equilibrium position

$$F \propto -x$$

$$F = -kx$$

Potential Energy of harmonic oscillator is.

$$V(x) = -\int_0^x F(x)\,dx$$

$$= \int_0^x kx\,dx$$

$$V(x) = \frac{1}{2}kx^2$$

$k = m\omega^2$

$$V(x) = \frac{1}{2}m\omega^2x^2 = 2\pi^2 m\nu^2x^2 \quad \text{—①}$$

Schrodinger wave Equation for particle motion is given by

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m(E-V)}{h^2}\psi = 0$$

Substituting value of ①

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - 2\pi^2 m v^2 x^2)\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \left(\frac{8\pi^2 m E}{h^2} - \frac{16\pi^4 m^2 v^2 x^2}{h^2}\right)\psi = 0$$

Let $\frac{8\pi^2 m E}{h^2} = \alpha$ and $\frac{4\pi^2 m v}{h} = \beta$

$$\beta^2 = \frac{16\pi^4 m^2 v^2}{h^2}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + (\alpha - \beta^2 x^2)\psi = 0 \quad \text{—②}$$

Let $y = \sqrt{\beta}x$

on Sq. $y^2 = \beta x^2$

$$x^2 = \frac{y^2}{\beta}$$

In ② $\frac{d^2\psi}{dx^2} + \left(\alpha - \beta^{\cancel{2}} \times \frac{y^2}{\cancel{\beta}}\right)\psi = 0$

$$\frac{d^2\psi}{dx^2} + (\alpha - \beta y^2) = 0 \quad \text{—③}$$

Now we have $y = \sqrt{\beta}x$

$$\frac{d\psi}{dx} = \frac{d\psi}{dy} \times \frac{dy}{dx} = \frac{d\psi}{dy} \times \sqrt{\beta}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = \beta\frac{d^2\psi}{dy^2}$$

Substituting in ③

$$\Rightarrow \beta\frac{d^2\psi}{dy^2} + (\alpha - \beta y^2)\psi = 0$$

$$\frac{d^2\psi}{dy^2} + \left(\frac{\alpha}{\beta} - y^2\right)\psi = 0 \quad \text{—④}$$

The Solution of Equation ④

will Satisfy the condition $\frac{\alpha}{\beta} = (2n+1)$

$$\alpha = \frac{8\pi^2 mE}{h^2} \qquad \beta = \frac{4\pi^2 m\nu}{h}.$$

$$\frac{\frac{8\pi^2 mE}{h^2}}{\frac{4\pi^2 m\nu}{h}} = (2n+1)$$

$$\Rightarrow E = \frac{h\nu}{2}(2n+1)$$

$$\boxed{E_n = h\nu\left(n+\frac{1}{2}\right)}$$

The lowest value of Energy which oscillation can take for n=0 is

$$\boxed{E_0 = \frac{1}{2}h\nu}$$

- This level is ground State. The Energy E_0 is called Zero Point Energy.
- A very Significant result that E_0 is never zero but has a lowest or Minimum value.
- A harmonic oscillator approaches this value as the temperature approaches 0K. This energy called zero point Energy.
- The Existance of zero point Energy is a consequence of Uncertainity Principle. At ~~T=0K~~ T=0K Position & Momentum can be determined Precisely.

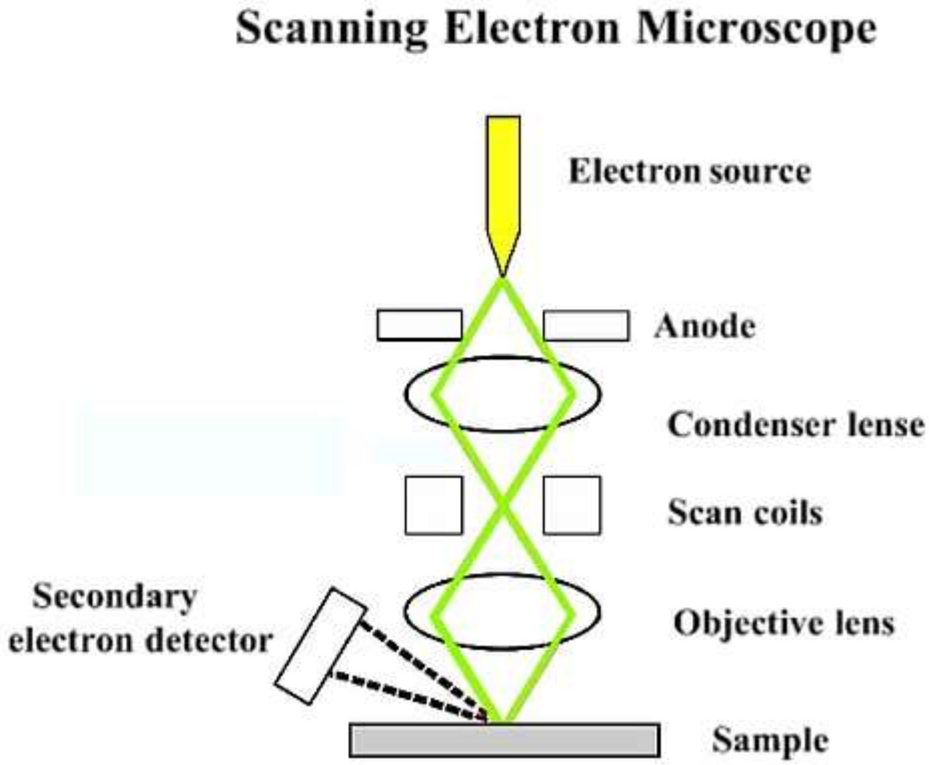
Scanning electron microscopes

Scanning electron microscopes (SEMs) have become powerful and versatile tools for material characterization, especially in recent years, as the size of materials used in various applications.

Electron microscopes use electrons for imaging in a similar way that light microscopes use visible light. SEMs use the electrons that are reflected or knocked off the near-surface region of a sample to create an image. Since the wavelength of electrons is much smaller than that of light, the resolution of SEMs is superior to that of a light microscope.

How SEMs work

In scanning electron microscopy, the electron beam scans the sample in a raster pattern. First, electrons are generated at the top of the column by the **electron source**.



Basic components of an SEM

Due to very narrow electron beam SEM Micrograph have large depth of field giving structure of sample.
The scan coil produces a magnetic field which deflect the electron beam in a controlled way.
Varying voltage is applied to the coil of the cathode ray tube which produce pattern of light.
When the electron beam hit the sample, it produces secondary electron.
The entire electron column needs to be under vacuum. Like all components of an electron microscope, the electron source is sealed inside a special chamber to preserve vacuum and protect it against contamination, vibrations, and noise.
Advantages: 1. Bulk/powder samples can be used
2. Provide much greater depth of view so it can produce image that can represent 3D structure of sample.

UNIT-2 QUANTUM STATISTICS

Statistics:- Collection and analysis of Data is known as Statistics.

Quantum Statistics:- A Statistical Description of a system of Particle that obey Rules of quantum Mechanics.

Mechanics:- Science concerned with the Motion of bodies Under Action of force.

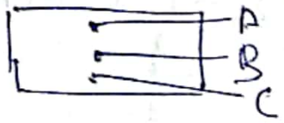
Quantum Mechanics:- Deals with smallest thing in Universe.

Eg. Electron, Proton, Neutron etc.

Classical Statistics & Quantum Statistics:-

Classical Statistics:- In classical Statistics all Particle in a System are considered Distinguishable. Means individual Particle in a system can be tracked. As a result changing the Position of any two Particle leads to completly different Configuration

Eg.



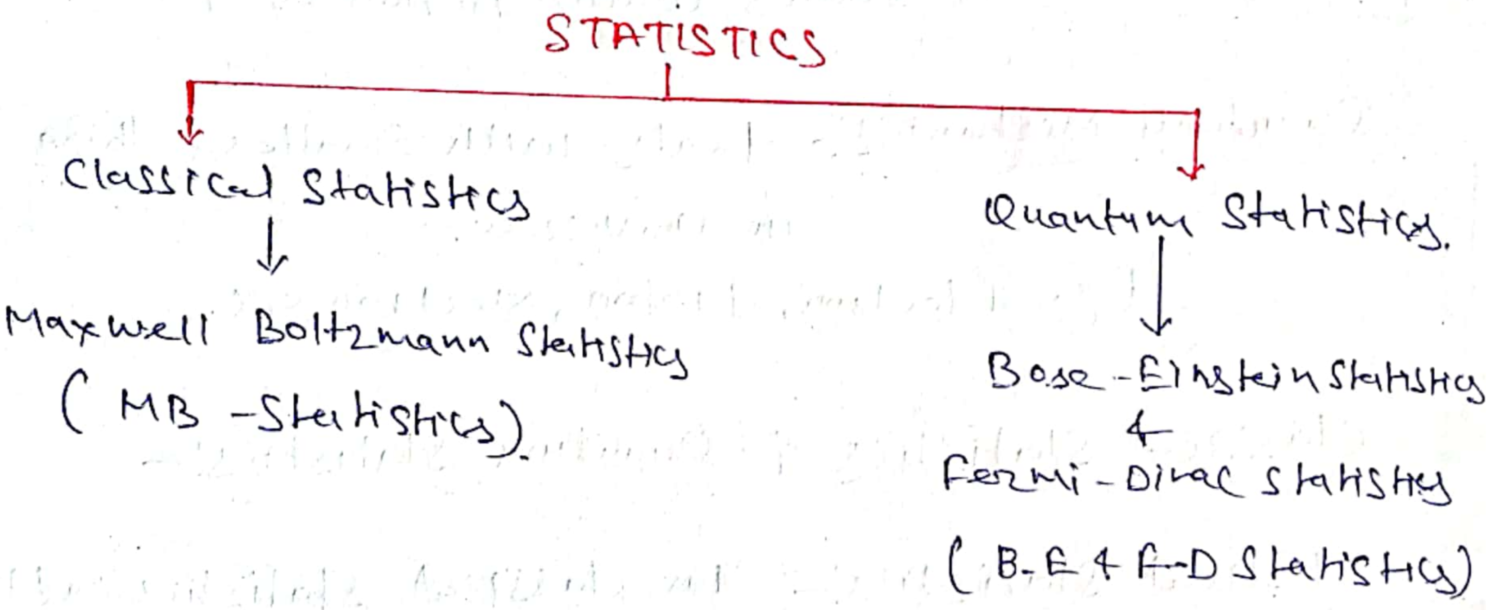
(A, B, C are Distinguishable Particle inside a System)

Quantum Statistics:- In quantum statistics, all particles in a system are considered indistinguishable. Ie we can't lable the Particle. Interchanging the Particle doesn't change the system.

Note:- Abbly on Non- observable.

Eg. -

(A, A, A are indistinguishable Particle in a System)



Examples.

I) M-B Statistics:- Gas Molecule

II) B-E Statistics:- Photons or Bosons.

III) F.D Statistics:- Electrons

3.11 COMPARISON OF MAXWELL-BOLTZMANN, BOSE-EINSTEIN AND FERMI-DIRAC STATISTICS

	Particular	**M.B. Statistics**	**B.E. Statistics**	**F.D. Statistics**
1.	*Nature of particles*	Particles are identical but distinguishable.	Particles are identical but indistinguishable.	Particles are identical but indistinguishable.
2.	*Size of the phase cell*	The available volume of the phase space cell can be small as we like and can even approach zero.	Minimum size of the available phase space volume is of the order of h^3, where h is the Planck's constant.	Minimum size of the available phase space volume is of the order of h^3.
3.	*Number of phase cells*	The phase space can be divided into any large number of cells of our choice.	The phase space can be divided into number of cells whose number is limited as the phase space volume of each cell cannot be less than h^3.	The phase space can be divided into the number of cells, whose number is limited as the phase space volume of each cell cannot be less than h^3.
4.	*Number of particles in a cell*	Any number of particles can occupy a single phase space cell.	Any number of particles can occupy a single phase cell.	A phase space cell cannot accommodate more than one particle.
5.	*Macrostates and microstates*	A macrostate can have more than one microstates.	Each macrostate has one microstate.	Each macrostate has one microstate.
6.	*Energy*	Continuous distribution of energy is assumed.	Energy is quantized.	Energy is quantized.
7.	*Spin*	The particles are spinless.	The particles have integral spin.	The particles have half integral spin.
8.	*Occupation index*	$\frac{1}{e^{\alpha+\beta E_i}}$	$\frac{1}{e^{\alpha+\beta E_i}-1}$	$\frac{1}{e^{\alpha+\beta E_i}+1}$
9.	*Total energy*	$\frac{3}{2}Nk_BT$	$\frac{3}{2}Nk_BT\left(1-\frac{1}{2^{5/2}e^{-\alpha}}\right)$	$\frac{3}{2}Nk_BT\left(1+\frac{1}{2^{5/2}e^{-\alpha}}\right)$
10.	*Wave function*		Symmetric under interchange of the coordinates of any two *Bosons*.	Antisymmetric on interchange of the coordinates of any two *Fermions*.

Emissive Power:-

Emissive power of a body at a given temperature is the quantity of Radiant energy emitted by the body per Unit time per Unit area of the body at that temperature.

Emissivity (ε)

Emissivity is defined as the Ratio of Energy Radiated from a Material surface to the Radiated Energy of Perfectly black body at that temperature.

Stefan's Boltzmann law:-

It State that total Radiations Emitted from a black body Per Unit area is Proportional to fourth power of its absolute temperature.

(Absolute Temperature - Temperature of Black body)

$$E \propto T^4$$

$$E = \sigma T^4$$

where σ - Stefan's constant

$\sigma = 5.67 \times 10^{-8}$ W/m²-K⁴

$$E = \frac{Q}{At}$$

$$Q = At \times E$$

$$Q = At \times (\sigma T^4)$$

Q - Amount of heat Emitted by a black body.

Black body Radiation Spectrum:-

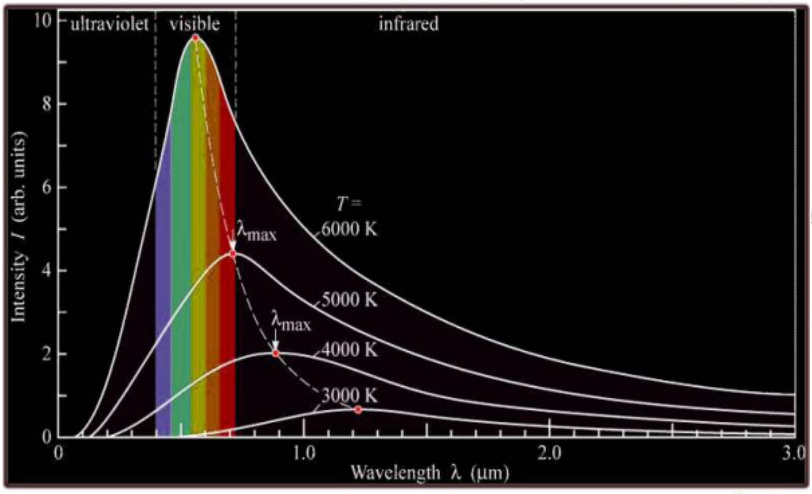
In Practice there is not perfect blackbodies, Scientist made a blackbody in laboratory by taking hollow Sphere & drilling a Small hole in it, which can absorb 99% of Radiations.

Inner Surface was coated with carbonblack when Radiations entering inside hit the wall of Sphere and get absorbed 99%.

Remaining radiations reflected back and collide with wall again.

Due to Absorption of heat its temperature inside increase and it Starts emitting Radiations from Narrow hole. This is called blackbody Radiations.

When radiations from black body traced on a graph Classical Mechanics fails to Explain Graph:



I) The blackbody radiation Spectrum is not having Uniform distribution of Energy wrt wavelength.

II) At a given temperature different wavelength Radiations have different energies.

III) Total Energy of Radiations at any temperature is given by area Under curve. The are is is directly proportional to fourth power of its absolute temperature $E \propto T^4$ (Stefan's law)

iv) The wavelength corresponding to maximum energy shift towards shorter wavelength with increase in temperature. $\lambda_m T =$ constant (Weins Displacement law)

λ_m - wavelength corresponds to maximum Energy.

Weins Displacement law:-

Weins displacement law is the relationship between temperature of a blackbody and wavelength at which it emit light.

Weins Displacement law state that the blackbody Radiation curve for different temperature peaks at a wavelength is inversly proportional to temperature.

$$\lambda_m \propto \frac{1}{T}$$

$$\lambda_m = \frac{b}{T}$$

b – weins constant

b = 2.898×10^{-3} Meter-kelvin.(MK)

Drawbacks:-

This law is applicable only for short wavelength region & for high temperature of the source of Radiations.

It fails to Explain decrease in Energy for longer wavelength.

Rayleigh Jeans law:-

Rayleigh Jeans law Express the Energy distribution in the Spectrum as a function of Temperature.

$$\boxed{E_\nu d\nu = \frac{8\pi \nu^2 KT}{c^3} d\nu}$$

According to this law Radiation Emitted by a Particle in a blackbody travel as a wave-

Average Energy Per Unit Vibration = KT

K - Boltzmann constant

T- Temperature.

In term of wavelength Energy density within the Range λ & $\lambda + d\lambda$ is .

Note

$\nu = \frac{c}{\lambda}$

$d\nu = -\frac{c}{\lambda^2} d\lambda$

Since increase in frequency correspond to decrease in wavelength

$E_\nu d\nu = -E_\lambda d\lambda$

In ①

$$E_\lambda d\lambda = \frac{8\pi \left(\frac{c}{\lambda}\right)^2 KT}{c^3} \times \left(\frac{c}{\lambda^2}\right) d\lambda$$

$$\boxed{E_\lambda d\lambda = \frac{8\pi KT}{\lambda^4} d\lambda}$$

↓

In term of wavelength.

Draw backs:-

Rayleigh Jeans law agree Experimental Results at large wave length (low frequencies). But strongly Disagree at shorter Wavelength (High frequencies).

Plancks law of Radiations

After failure of weins law & Rayleigh law "Planck's introduced an entirely new idea to explain the distribution of Energy among various wavelength of blackbody Radiations!"

Following Assumptions were Made-

I) Blackbody is Made up of large Number of oscilating Particles. These Particle vibrates in possible frequencies.

II) Atoms of the walls of Uniform temperature behaves as oscilator each with characteristic frequency of oscillation.

III) An oscilator can have discrete Energy given by-

$$E = nh\nu$$

ν - frequency of oscilator.
h - Plancks constant
n - an Integer quantum Number.

IV) An oscilator do not emit or Absorb energy continuously but only in Jump.

Let N be the total Number of oscilators & E be the total Energy of these oscillators, then Average Energy is given by

$$\bar{E} = \frac{E}{N}$$

Now let $N_0, N_1, N_2 --- N_n$ be the Number of oscillator having energies $0, h\nu, 2h\nu \_\_ nh\nu$.

By Max distribution formula we have

$$N_n = N_0 e^{-nh\nu/KT}$$

According to Maxwell Boltzmann Distribution law - Number of oscillator (N_n) with Energy (E_n) is given by.

$$N_n = N e^{-E_n/KT}$$

Average Energy of oscillator is given by -

$$\langle E\rangle = \frac{\sum_{n=0}^{\infty} E_n N_n}{\sum_{n=0}^{\infty} N_n}$$

$$= \sum_{n=0}^{\infty} \frac{E_n \cancel{N} e^{-E_n KT}}{\cancel{N} e^{-E_n/KT}}$$

$$= \sum_{n=0}^{\infty} \frac{nh\nu\, e^{-nh\nu/KT}}{e^{-nh\nu/KT}}$$

$$= \frac{0 + h\nu e^{-h\nu/KT} + 2h\nu e^{-2h\nu/KT} + ----}{1 + e^{-h\nu/KT} + e^{-2h\nu/KT} + ----}$$

let $e^{-h\nu/KT} = x$

$$\Rightarrow \quad \langle E\rangle = \frac{h\nu x\,(1+2x+3x^2 ----)}{1+x+x^2 ----}$$

$$= \frac{h\nu x\,(1-x)^{-2}}{(1-x)^{-1}}$$

$$= \frac{h\nu x}{(1-x)}$$

$$= \frac{h\nu e^{-h\nu/KT}}{(1-e^{-h\nu/KT})}$$

$$\boxed{E = \frac{h\nu}{e^{h\nu/KT}-1}} \leftarrow (1)$$

Average Energy of Planck's oscillation

Plancks Radiatioy Formula:-

Number of oscillation in the frequency Range v & $v+dv$ are Estimated to be -

$$\frac{8\pi v^2 dv}{c^3}$$

The Energy density of Radiations E_v in the frequency Range v & $v+dv$ is related to average Energy of oscillator as given by.

$$E_v dv = \frac{8\pi v^2 dv}{c^3} \times \underline{E}$$

(From ①)

$$= \frac{8\pi v^2 dv}{c^3} \times \frac{hv}{e^{hv/kT}-1}$$

$$\boxed{E_v dv = \frac{8\pi h v^3}{c^3} \cdot \frac{1}{e^{hv/kT}-1} dv} \quad -②$$

$\downarrow$

Plancks Radiation law.

In term of wavelength:-

Note $v = c/\lambda$

$dv = -\frac{c}{\lambda^2} d\lambda$

Since increase in frequency correspond to decrease in wavelength $E_\lambda d\lambda = - E_v dv$

in ②

$$E_\lambda d\lambda = \frac{8\pi h \left(\frac{c}{\lambda}\right)^3 \left(\frac{c}{\lambda^2}\right) d\lambda}{c^3 \times e^{hc/\lambda kT} - 1}$$

$$\boxed{E_\lambda d\lambda = \frac{8\pi h c}{\lambda^5} \cdot \frac{d\lambda}{e^{hc/\lambda kT}-1}} \quad -③$$

* Imp

Weins law and Rayleigh law from Plancks law!

Weins law and Rayleigh can be derived from Plancks law:-

From Plancks law we have (by ③)

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{d\lambda}{e^{hc/\lambda KT}-1}$$

i) When wave length λ is very small then. $e^{hc/\lambda KT} \gg 1$ So Plancks formula can be (③) written as- (Eqn ③)

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} e^{-hc/\lambda KT} d\lambda$$

Putting $8\pi hc = A$ & $\frac{hc}{K} = B$ we have

$$\boxed{u_\lambda d\lambda = \frac{A}{\lambda^5} e^{-B/\lambda T} d\lambda}$$

↓

Weins law.

ii) When λ is very large then.

$$e^{hc/\lambda KT} = 1 + \frac{hc}{\lambda KT}$$

So Equation ③ can be written as-

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5\left(1+\frac{hc}{\lambda KT}-1\right)} d\lambda$$

$$\boxed{u_\lambda d\lambda = \frac{8\pi KT}{\lambda^4} d\lambda}$$

↓

Rayleigh Jeans law.

Photo electric Effect

"When a beam of light of suitable frequency falls on a metal plate slow moving electrons are emitted from the metal surface. This phenomenon is called Photoelectric Effect"

Some of the basic features of photoelectric effect are-

I) The lowest frequency of light which can emit photoelectron from a material is called threshold frequency of that material. (ν_0)

II) Photoelectric current or Number of Photoelectrons emitted per second is directly proportional to the intensity of incident light.

III) Velocity of photoelectron is completely independent on intensity of incident light but depend on its frequency.

IV) The Negative Potential V_0 at which the photoelectric current is reduced to zero called stopping potential or cut off potential.

When light of frequency ν falls on metallic surface a part of its energy is used to librate the electron from the surface known as work function and rest energy is carried by emitted electron as kinetic Energy.

$$h\nu = \underbrace{\tfrac{1}{2}mv^2}_{\text{Kinetic Energy}} + \underbrace{\phi_0}_{\text{work Function.}}$$

$$h\nu = \tfrac{1}{2}mv^2 + h\nu_0$$

(ν_0 - Threshold Frequency)

$$\boxed{\tfrac{1}{2}mv^2 = h(\nu - \nu_0)}$$ - Einstein Photo electric Equation.

Concept of Statistical Mechanics:

Microstate: A State of a System where all the Parameter of a ~~System~~ Particle are Specifred.
Many Micro State exist for each of the System, and there are many Parameter for each State.

Macrostate: Any State of a System that describe the actual observation of ~~the~~ its Microscopic Statistical Properties.

Phase Space: Phase Space refers to the Plotting of both Particle momentum & Position on two dimension graph.
If we want to define the State of a Particle in Phase Space coordinate System, then we require Position (3D) & momentum (3D)
Thus Phase Space is a Six dimensional coordinate consisting of 3 Dimensions of Position and 3 Dimension of Momentum.

Position Space:- Three dimensional Space in which Position (location) of a Particle is Specifred. ~~by~~ Eg. Small volume element (dv) in Position Space is given by - $dV = dx dy dz$

Momentum Space: Three dimensional Space in which Momentum of Particle is Specifred by Momentum Coordinates P_x, P_y, P_z.

Cells in Phase Space :- cell in Phase space corresponding to a state of a system which can be labeled with some Number. A cell is a sub-compartment. Each compartment is divided into large number of cells. in such a way that each cell is of same size.

Gas Molecules! Identical Particles of any spins & can be Distinguished.

Bosons!- Identical Particles of 0 or Integral spins & can't be distinguished.

Fermions!- Identical Particles of odd half integral spins & can't be Distinguished.

Failure of classical Statistics: (M-B Statistics)

classical Statistics fails to Explain-

I) observed energy distribution of Electron in a Metals.

II) observed Energy Distribution of Photons inside an Enclosure.

Thats why we Need Quantum Statistics

Classical Statistics (Maxwell - Boltzmann Statistics)

"Maxwell Boltzmann law gives distribution of total Energy of a system having identical but distinguishable particle." It is mostly used in kinetic theory of gas to find various aspects such as molecular velocity, probable speed of molecule of gas etc.

Assumption of M-B Statistics.

I) All the particles which obey M-B statistics are known as Maxons & are Identical & Distinguishable

II) chosen volume has large number of cells and volume of each phase space is Extremely small.

III) There is no limit on number of particle in a cell.

IV) Total number of particle and total Energy remains constant in the system.

V) The state of each particle is specified by position and momentum coordinates.

VI) Energy is continuous.

probality F(E) that a boson occupy a state of Energy E is given by -

$$\boxed{F(E) = A\exp^{-E/KT}}$$

Maxwell Boltzman Distribution law:-

"Maxwell Boltzman distribution law gives how the total Energy of a System is distributed among various member of a System having identical Distinguishable Particle"

Let us consider an assembly of N Molecule in Phase Space. Let us divide Phase space into number of cells 1, 2, --- k, which contain Number of Particle n_1, n_2 --- n_k respectively in Equilbrium. Also suppose Energy of N Molecule are limited to $E_1, E_2 --- E_k$ within sequence of Energy level.

Note (
N - Molecule
1, 2, 3 --- k - Number of cells.
n_1, n_2 --- n_k - Number of Particle in a cell)

As the Molecule are moving continuously in many different ways and obey Fundamental Postulates of Statistical Mechanics as -

① Total Number of Molecule is constant

$$N = n_1 + n_2 --- n_k = \text{const.}$$

$$\delta N = \delta n_1 + \delta n_2 --- \delta n_k = 0$$

~~$\sum_i \epsilon_i \delta n_i = 0$~~ $\Sigma \delta n_i = 0$ —— ①

② Total Energy of System is constant.

$$E = \epsilon_1 n_1 + \epsilon_2 n_2 --- \epsilon_i n_i --- \epsilon_k n_k = \text{const.}$$

~~Bose Einstein Statistics~~

$$\delta E = E_1 \delta n_1 + E_2 \delta n_2 \text{ ——— } \delta E_k n_k = 0$$

$$\sum_i E \delta n_i = 0 \quad \text{—} ②$$

③ When a gas is in Equilibrium Probablity is Maximum.

ie $\delta P = 0$

$\delta \log P = 0$ —③

Now considering

g_i - Number of Energy level each having Energy E_i

n_i - Number of ~~Molecule~~ Particles having Energy E_i

Then Probablity P for Distribution is given by -

$$P = \frac{N!}{n_1!\, n_2!\, n_3! \text{ ---- } n_k!} (g_1)^{n_1} (g_2)^{n_2} \text{ ---- } (g_k)^{n_k}$$

$$P = \frac{N!}{n_1!\, n_2!\, n_3! \text{———} n_k!} (g_1)^{n_1} (g_2)^{n_2} \text{———} (g_k)^{n_k}$$

$$P = \frac{\sum_{i=1}^{k} (g_i)^{n_i} N!}{\sum_{i=1}^{k} n_i!}$$

Taking log on both side

$$\log P = \log N! + \sum_i \log (g_i)^{n_i} - \sum_i \log n_i!$$

$$\log P = \log N! + \sum_i n_i \log g_i - \sum_i \log n_i!$$

(Using Stirling Approximation
$\log N! = N \log N - N$)

$$\Rightarrow \log P = N \log N - N + \sum_i n_i \log g_i - \sum_i n_i \log n_i - \sum_i n_i$$

(Using $\sum_i n_i = N$ i.e total Number of Particle
$\sum_i n_i = N$)

$$= N \log N - \cancel{N} + \sum_i n_i \log g_i - \sum_i n_i \log n_i + \cancel{N}$$

$$\log P = N \log N - \sum n_i \log n_i + \sum_i n_i \log g_i$$

(Now Differentiating both side
and Considering N & g_i as constant)

$$\delta \log P = 0 - \left(\sum_i n_i \delta(\log n_i) + \sum_i \log n_i \delta n_i \right) + \sum_i \log g_i \delta n_i$$

$$\delta \log P = 0 - \sum_i \cancel{n_i} \frac{1}{\cancel{n_i}} \delta n_i - \sum_i \log n_i \delta n_i + \sum_i \log g_i \delta n_i = 0$$

$$= 0 - 0 - \sum_i \log n_i \delta n_i + \sum_i \log g_i \delta n_i$$

(using $\sum_i \delta n_i$ = Total Number of Molecule = 0)

$$= -\left(\sum_i \log \frac{n_i}{g_i} \delta n_i \right)$$

(Now Substituting $\delta \log P$ = Total probablity = 0.)

$$\Rightarrow \sum_i \log \frac{n_i}{g_i} \delta n_i = 0 \quad — ④$$

Multipliying ① by $-\alpha$ ② by $-\beta$ and Adding ①, ②, ④

$$\sum_i \log \frac{n_i}{g_i} \delta n_i + \sum_i \alpha \delta n_i + \sum_i \beta \delta \epsilon_i n_i = 0$$

$$\sum_i \left(\log \frac{n_i}{g_i} + \alpha + \beta \epsilon_i \right) \delta n_i = 0$$

$$\Rightarrow \log \frac{n_i}{g_i} + \alpha + \beta \epsilon_i = 0$$

$$\log \frac{n_i}{g_i} = -\alpha - \beta \epsilon_i$$

$$\frac{n_i}{g_i} = e^{-\alpha - \beta \epsilon_i}$$

$$n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i}} = g_i e^{-\alpha} e^{-\beta \epsilon_i}$$

taking $A = e^{-\alpha}$ $\boxed{n_i = g_i A e^{-\beta \epsilon_i}}$

Bose-Einstein Statistics:-

"Bose Einstein Statistics (B.E Statistics) determine the statistical distribution of identical indistinguishable particles (Boson) over the Energy State"

Basic Postulates:-

I) All the particles which obey B.E Statics are known as Bosons. Bosons are identical & indistinguishable particles.

II) Bosons obey Uncertainity Principle

III) Size of cell can't be less than h^3, where h is the Plancks constant

IV) The wave function representing Boson do overlap slightly and are symmetric.

V) The bosons don't obey Pauli Exclusion Principle

VI) Energy states are discrete.

VII) Number of Phase cells is comparable with Number of particles.

VIII) Bose-Einstein Statistics is applicable to Number of Particle with Itegral spin angular Momentum in unit of $\left(\frac{h}{2\pi}\right)$

Let us consider a system consisting of n independent and indistinguishable particle. Let there be n_1, n_2, n_3 --- n_i + --- n_k particles having mean energy E_1, E_2 --- E_k respectively. in compartment numbered as 1, 2, 3 - i --- k. containing g_1, g_2 --- g_i -- g_k cells respectively.

Note (N - Total Number of particles
n_1, n_2, n_3 --- n_k -- Number of particles in a cell
g_1, g_2, g_3 ~~g_i~~ -- g_k - cells.)

Now these particles obey fundamental postulates of quantum statistics as-

① Total Number of particles is constant

$$N = n_1 + n_2 \text{ ----- } n_k = \text{constant}$$

$$\delta N = \delta n_1 + \delta n_2 \text{ --- } \delta n_k = \text{constant} = 0$$

$$\Rightarrow \boxed{\Sigma \delta n_i = 0} \quad - ①$$

② Total Energy of system is constant

$$E = E_1 n_1 + E_2 n_2 \text{ --- } E_i n_i \text{ --- } E_k n_k = \text{constant}$$

$$\delta E = E_1 \delta n_1 + E_2 \delta n_2 \text{ --- } E_i \delta n_i \text{ --- } E_k \delta n_k = 0$$

$$\Rightarrow \boxed{\sum_i E \delta n_i = 0} \quad - ②$$

③ Distribution of particles is constant. (Thermodynamic Probablity)

$$\text{i.e. } \delta W = 0$$

$$\boxed{\delta \log W = 0} \quad ③$$

Hence the Number of ways in which n_i Particles are to be distributed in g_i cells in ith compartment is given by-

$$W = \frac{(n_i+g_i-1)!}{n!\,(g_i-1)!}$$

Total Number of Arrangements is -

$$W = \sum_{i=1}^{K} \frac{(n_i+g_i-1)!}{n!\,(g_i-1)!} = \sum_{i=1}^{K} \frac{(n_i+g_i)!}{n_i!\,g_i!}$$

Taking log on both sides.

$$\log W = \sum_{i=1}^{K} \left(\log (n_i+g_i)! - \log n_i! - \log g_i! \right)$$

(Using sterling Approximation.

$$\log N! = N\log N - N \,)$$

$$\log W = \sum_{i=1}^{K} \Big((n_i+g_i)\log(n_i+g_i) - \cancel{(n_i+g_i)} - n_i\log n_i + \cancel{n_i} - g_i\log g_i + \cancel{g_i} \Big)$$

$$\log W = \sum_{i=1}^{K} \Big(n_i\log(n_i+g_i) + g_i\log(n_i+g_i) - n_i\log n_i - g_i\log g_i \Big)$$

Now ~~taking log~~ Differentiating on both side & considering g_i as constant

$$\delta(\log W) = \sum_{i=1}^{K} \Big(n_i\,\delta\log(n_i+g_i) + \log(n_i+g_i)\,\delta n_i + g_i\,\delta\log(n_i+g_i) - (n_i\,\delta\log n_i + \log n_i\,\delta n_i) + 0 \Big)$$

$$\Rightarrow 0 = \sum_{i=1}^{K} \Big(n_i\,\delta\log(n_i+g_i) + g_i\,\delta\log(n_i+g_i) + \log(n_i+g_i)\,\delta n_i - n_i\,\delta\log n_i + \log n_i\,\delta n_i \Big)$$

$$\Rightarrow 0 = \sum_{i=1}^{k} \Big((n_i+g_i)\,\delta \log(n_i+g_i) + \log(n_i+g_i)\,\delta n_i - n_i\,\delta \log n_i - \log n_i\,\delta n_i$$

$$\Rightarrow 0 = \sum_{i=1}^{k} \Big(\cancel{(n_i+g_i)} \times \frac{1}{\cancel{(n_i+g_i)}}\,\delta n_i + \delta n_i \log(n_i+g_i) - \cancel{n_i} \times \frac{1}{\cancel{n_i}}\,\delta n_i - \delta n_i \log n_i \Big)$$

$$\Rightarrow \quad 0 = \sum_{i=1}^{k} \Big(\delta n_i \log(n_i+g_i) - \delta n_i \log n_i \Big)$$

$$\Rightarrow \quad -\sum_{i=1}^{k} \Big(\log n_i - \log(n_i+g_i) \Big)\delta n_i = 0$$

$$\Rightarrow \quad \sum_{i=1}^{k} \log\left(\frac{n_i}{n_i+g_i}\right)\delta n_i = 0 \quad \text{—④}$$

Now Multiplying ① by α & ② by β
Then Adding ①, ② & ④

$$\Rightarrow \quad \sum_{i=1}^{k} \Big(\log\left(\frac{n_i}{n_i+g_i}\right) + \alpha\,\delta n_i + \beta E_i\,\delta n_i \Big) = 0$$

$$\Rightarrow \quad \log\left(\frac{n_i}{n_i+g_i}\right) + \alpha + \beta E_i = 0$$

$$\log\left(\frac{n_i}{n_i+g_i}\right) = -\alpha - \beta E_i$$

$$\left(\frac{n_i}{n_i+g_i}\right) = e^{-\alpha-\beta E_i} = e^{-(\alpha+\beta E_i)}$$

$$\frac{n_i+g_i}{n_i} = e^{(\alpha+\beta E_i)}$$

$$1 + \frac{g_i}{n_i} = e^{(\alpha+\beta E_i)}$$

$$\Rightarrow \boxed{n_i = \frac{g_i}{e^{\alpha+\beta E_i} - 1}}$$

Fermi Dirac Statistics:

Fermi dirac describe distribution of particles in a system. (identical indistinguishable particles) that obey Pauli Exclusion Principle.

Basic postulates:-

i) All the particles which obey Fermi-dirac statistics known as Fermions.

ii) Fermions obey Uncertainity principle.

iii) Fermions obey Pauli Exclusive principle.

iv) Fermi Dirac distribution law is represented by -

$$\boxed{n_i = \frac{g_i}{e^{\alpha} e^{\epsilon_i/kT} + 1}}$$

Let us consider a system of n independent and indistinguishable Particles. Let the compartment be Marked 1, 2.---i--k and their Mean energy values be represented by $E_1, E_2 - E_i -- E_k$. g_1 containing g_1, g_2-- -- $g_i - g_k$ cells. Total Number of Particles in the System is $n = n_1 + n_2 -- n_i --- n_k$.

Now these Particles obey Fundamental Postulates of quantum Statistics. as -

① Total Number of Particles is constant

$$N = n_1 + n_2 ---- n_k = \text{constant}$$

$$\delta N = \delta n_1 + \delta_2 -- \delta n_k = \text{constant} = 0$$

$$\Rightarrow \boxed{\Sigma \delta n_i = 0} \quad -①$$

② Total Energy of system is constant

$$E = E_1 n_1 + E_2 n_2 ---- E_i n_i -- E_k n_k = \text{constant}$$

$$\delta E = E_1 \delta n_1 + E_2 \delta n_2 - E_1 \delta n_i --- E_k \delta n_k = 0$$

$$\Rightarrow \boxed{\sum_i E_i \delta n_i = 0} \quad -②$$

③ Distribution of particle (Thermodynamic Probability) is constant

ie $\delta W = 0$

$$\boxed{\delta \log W = 0} \quad -③$$

∴ Hence the Number of ways in which ni particles. Can be distributed in gi cells in ith compartment is -

$$W = \sum_{i=1}^{k} \frac{g_i!}{n_i!\,(g_i-n_i)!}$$

Taking log on both sides.

$$\log W = \sum_{i=1}^{k} \left(\log g_i! - \log n_i! - \log (g_i-n_i)! \right)$$

(Using Sterling Approximation. $\log N! = N\log N - N$)

$$\log W = \sum_{i=1}^{k} \Big(g_i \log g_i - g_i - (n_i \log n_i - n_i) - \big((g_i-n_i)\log(g_i-n_i) - (g_i-n_i) \big)\Big)$$

$$\Rightarrow \log W = \sum_{i=1}^{k} \Big(g_i \log g_i - \cancel{g_i} - n_i \log n_i + \cancel{n_i} - (g_i-n_i)\log(g_i-n_i) + \cancel{g_i} - \cancel{n_i} \Big)$$

$$\Rightarrow \log W = \sum_{i=1}^{k} \left(g_i \log g_i - n_i \log n_i - (g_i-n_i)\log(g_i-n_i) \right)$$

(Now Differentiating both sides and considering g_i as constant as g_i is Number of cells which is constant)

$$\Rightarrow \delta \log W = \sum_{i=1}^{k} \Big(0 - (n_i\, \delta \log n_i + \log n_i\, \delta n_i) - \big((g_i-n_i)\, \delta \log(g_i-n_i) + \log(g_i-n_i)\, \delta(g_i-n_i) \big)\Big)$$

$$0 = \sum_{i=1}^{k} \Big(0 - (n_i \times \frac{1}{n_i} \delta n_i + \log n_i\, \delta n_i) - \Big(\big((g_i-n_i) \times \frac{1}{(g_i-n_i)} (-\delta n_i)\big) + \log(g_i-n_i)(-\delta n_i) \Big)\Big)$$

$$0 = \sum_{i=1}^{k} \left(0 - 0 - \log n_i\, \delta n_i - 0 + \log (g_i-n_i)\, \delta n_i \right.$$

$$0 = \sum_{i=1}^{k} -\left(-\log (g_i-n_i)\, \delta n_i + \log n_i\, \delta n_i \right) \quad \text{—④}$$

∴ Multiplying ① by α ② by β and Adding ① + ② + ④

$$\Rightarrow \sum_{i=1}^{k} \left(\log\left(\frac{n_i}{g_i - n_i}\right) + \alpha \delta n_i + \beta \delta \epsilon_i n_i \right) = 0$$

$$\Rightarrow \sum_{i=1}^{k} \left(\log\left(\frac{n_i}{g_i - n_i}\right) + \alpha + \beta E_i \right) \delta n_i = 0$$

$$\Rightarrow \cancel{\sum_{i=1}^{k}} \log \frac{n_i}{g_i - n_i} = -\alpha - \beta E_i$$

$$\frac{n_i}{g_i - n_i} = e^{-\alpha - \beta \epsilon_i} = e^{-(\alpha + \beta \epsilon_i)}$$

$$\frac{g_i - n_i}{n_i} = e^{\alpha + \beta \epsilon_i}$$

$$\frac{g_i}{n_i} - 1 = e^{\alpha + \beta \epsilon_i}$$

$$\frac{g_i}{n_i} = e^{\alpha + \beta \epsilon_i} + 1$$

$$\boxed{n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i} + 1}}$$

Applications of Quantum Statistics:-

i) Maxwell Boltzmann (M-B) Statistics:-

Application:- Molecular speed and Energies of an ideal gas.

ii) Bose-Einstein (B-E) Statistics:-

Application- Black body spectrum.

iii) Fermi-Dirac (F-D Statistics).

Application:- Free Electron Theory.

Application of Maxwell's Boltzmann Statistics:-

(a) Molecular Speed and Energy of an ideal gas.

Let us consider an ideal gas in a container of volume V then according to Maxwell Boltzmann Distribution law The number of Molecule in the ith cell of Energy E_i will be

$$n_i = g_i e^{-(\alpha + \beta E_i)}$$

$$n_i = \frac{g_i}{e^{(\alpha + \beta E_i)}}$$

Substitute $\beta = \frac{1}{K_B T}$

$$\Rightarrow \quad n_i = \frac{g_i}{e^{(\alpha + E_i/K_B T)}} = g_i e^{-\alpha} e^{-E_i/K_B T}$$

Considering continuous Distribution of Molecular energies

$$n(E)\, d(E) = g(E)\, e^{-\alpha} e^{-(E/K_B T)} dE \qquad ①$$

Now a Molecule of Energy E has Momentum P whose Magnitude is

$$P = \sqrt{2mE}$$

let us consider a volume of Spherical cell in a Momentum space of radius P and thickness dP. volume of this spherical cell is $4\pi P^2 dP$

Now

$$g(P)\, d(P) = \text{Number of cell in Momentum range } P \text{ to } P+dP$$
$$= 4\pi P^2 dP$$
$$= B P^2 dP$$

where B is some constant.

Since Each Magnitude of Momentum P correspond to Energy E

Now $g(E)\, d(E) =$ Number of Energy State

$$= g(P)\, d(P)$$
$$= B P^2 dP$$

But $p^2 = 2mE$ and $dP = \frac{2m\,dE}{\sqrt{2mE}}$

we have

$$g(E)\,d(E) = BP^2\,dP$$

$$= B \times \cancel{2mE} \times \frac{2m\,dE}{\cancel{\sqrt{2mE}}}$$

$$= B \times \sqrt{2mE} \times 2m\,dE$$

$$= B\,(2m)^{3/2} \times E^{1/2}\,dE \quad ②$$

Substituting ② in ①

From ① $$n(E)\,d(E) = g(E)\,e^{-\alpha}\,e^{-(E/k_BT)}\,dE$$

$$= B\,(2m)^{3/2}\,E^{1/2} \times e^{-\alpha}\,e^{-(E/k_BT)}\,dE$$

let $B\,(2m)^{3/2}\,e^{-\alpha} = \text{constant} = C$

$$\Rightarrow n(E)\,d(E) = C\sqrt{E}\,e^{-(E/k_BT)}\,dE \quad ③$$

Now to find C make the condition that total No. of molecule is N.

$$N = \int_0^\infty n(E)\,dE = C\int_0^\infty \sqrt{E}\,e^{-(E/k_BT)}\,dE$$

using $\int_0^\infty \sqrt{x}\,e^{-ax}\,dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$

$$\Rightarrow N = C\,\frac{1}{2(1/k_BT)}\sqrt{\frac{\pi}{(1/k_BT)}} = C \times \frac{\sqrt{\pi}}{2} \times (k_BT)^{3/2}$$

$$\Rightarrow C = \frac{2\pi N}{(\pi k_BT)^{3/2}}$$

Put value of C in ③ ④

$$\boxed{\Rightarrow n(E)\,d(E) = \frac{2\pi N}{(\pi k_BT)^{3/2}} \times \sqrt{E}\,e^{-(E/k_BT)}\,dE}$$

* Now total Energy of the system is -

$$E = \int_0^\infty E n(E) dE = \frac{2\pi N}{(\pi k_B T)^{3/2}} \int_0^\infty E^{3/2} e^{-E/k_B T} dE$$

$$= \frac{2\pi N}{(\pi k_B T)^{3/2}} \times \frac{3}{4} (k_B T)^2 \sqrt{\pi k_B T}$$

$$\left(\text{using } \int_0^\infty \sqrt{x} e^{-ax} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}} \right)$$

$$\boxed{E = \frac{3}{2} k_B T}$$

b) Maxwell Boltzmann velocity Distribution.

Now Number of Molecule with velocity v & v+dv is.

Substituting $E = \frac{1}{2} mv^2$, $dE = mv dv$. in ④

we get

$$\boxed{n(v)\, d(v) = \frac{(\sqrt{2}\, \pi N m^{3/2})}{(\pi k_B T)^{3/2}} v^2 e^{-mv^2/2k_B T} dv}$$

Some Molecular Speeds:-

1) **Mean or Average Speed:-** Average speed of all the Molecules.

$$V_{avg} = \sqrt{\frac{8KT}{\pi m}}$$

2) **Root Mean Square Speed:-** Mean speed of Square of all the Molecule.

$$V_{rms} = \sqrt{\frac{3KT}{m}}$$

3) **Most Probable Speed:-** Speed posses by Maximum number of Molecule.

$$V_{mp} = \sqrt{\frac{2KT}{m}}$$

Relation between Vrms Vmp & Vavg.

$$V_{rms} : V_{avg} : V_{mp} = \sqrt{\frac{3KT}{m}} : \sqrt{\frac{8KT}{\pi m}} : \sqrt{\frac{2KT}{m}}$$

$$= 1.73\sqrt{\frac{KT}{m}} : 1.59\sqrt{\frac{KT}{m}} : 1.414\sqrt{\frac{KT}{m}}$$

$$= 1 : 0.92 : 0.817$$

$$V_{rms} > V_{avg} > V_{mp}$$

Applications of Fermi Dirac Statistics:-

Free Electron Theory:-

It is of 2 type

I) Classical (Lorentz-Drude Theory)

II) Quantum (Sommerfeld Theory).

Classical Free Electron theory:

According to Classical free Electron theory Electrons are assumed completely free. A single free Electron is surrounded by large Number of free Electron and positive ion core.

Assumptions:

* In this theory it is assumed that when a free electron moves in a solid its potential Energy is zero. i.e Electron can move Freely throughout the crystal

* Electron can move Freely inside the solid. But it can't leave the surface. (outside No force on Electron but inside a constant force on Electron)

This is an infinite barrier so No electron can cross the barrier

Features:- Free electron gas obey Maxwell boltzmann statistics.

II) It successfully defines ohm's law.

III) These free Electron can move Freely so Metals have high Electrical & thermal conductivity.

Failure of Classical free electron theory.

I) It can't explain temperature dependence of Electrical Resistivity.

II) It fails to Explain Electronic heat capacity and Paramagnetic susceptibility of free electron.

Quantum Free Electron theory:

Classical theory assumed that electron in Free Electron gas follow M-B Statistics. but in Quantum free Electron theory electron follow Fermi Dirac Statistics as Pauli Exclusion principle applicable on Electron.

→ All Assumption of Quantum free Electron theory are same as classical Free Electron theory except now Electron follow Fermi Dirac Statistics. (Pauli Exclusion Principle).

<u>Note</u>:- (Pauli Exclusion principle:- No two Electron can have same Quantum State).

Assumptions -

I) Energy of free electron are quantized

II) Free e⁻ obey Pauli Exclusion Principle

III) Distribution of free e⁻ obey Fermi- Dirac quantum Statistics.

IV) Free e⁻ have same Potential Energy everywhere within metal

V) Electrons are treated free.

Energy Distribution among free electron!

We have to find Distribution of Electron Energy in a Metal

Number of Electron with Energy E_i is given by-

$$n(E)\,d(E) = \frac{g(E)\,d(E)}{e^{\alpha}e^{E/KT}+1} \quad -①$$

Electron Energy State is given by -

$$g(E)\,d(E) = \frac{8\sqrt{2}\,\pi V m^{3/2}}{h^3}\;\frac{E^{1/2}dE}{\text{[illegible]}}$$

Substituting $g(E)d(E)$ in ①

$$n(E)\,d(E) = \frac{8\sqrt{2}\,\pi V m^{3/2}}{h^3}\;\frac{E^{1/2}dE}{e^{\alpha}e^{E/KT}+1}$$

$\alpha = \frac{E_F}{KT}$

$$\boxed{n(E)\,d(E) = \frac{8\sqrt{2}\,\pi V m^{3/2}}{h^3}\;\frac{E^{1/2}dE}{e^{(E-E_F)/KT}+1}}$$

Fermi Energy: Fermi Energy is the Energy difference between highest & lowest occupied state.

Suppose a metal contains N free Electrons

Total Number of Free Electrons is equal to the total Number of quantum States upto Energy E_F.

$$N = \int_0^{E_F} g(E)\,dE$$

$$N = \frac{8\sqrt{2}\pi V m^{3/2}}{h^3} \int_0^{E_F} E^{1/2}\,dE$$

$$= \frac{16\sqrt{2}\pi V m^{3/2}}{3h^3} E_F^{3/2}$$

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

$$\boxed{E_F = \frac{h^2}{2m}\left(\frac{3N}{8\pi V}\right)^{2/3}}$$ — Fermi Energy

OR

Using $\left(\hbar = \frac{h}{2\pi}\right)$

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

Electronic Specific heat:-

Electronic Specific Heat of Electron is defined as the Ratio of Portion of Heat Used by Electron to Rise the temperature of the System.

we have

Internal Energy Per mole of Metal is.

$$E_e = \frac{3}{2} NKT = \frac{3}{2} RT \qquad \left(K = \frac{R}{N}\right)$$

R - Gas Constant. ~~N = Free Electron.~~

N - Avogadro Number

Then Molar Specific Heat of Electron Should be.

$$C_{ve} = \left(\frac{dE_e}{dT}\right)_V = \frac{3}{2} R$$

Total Specific Heat of Metal Should be

$$C_V = 3R + \frac{3}{2}R = \frac{9}{2}R$$

$$\boxed{C_V = \frac{9}{2}R}$$ — Electronic Specific Heat.

Fermi Distribution Function:

$$f(E) = \frac{1}{e^{\left(\frac{E-E_F}{KT}\right)}+1}$$

This describe the Probablity of occupancy of N e^-.

OR

At temperature T the Probablity of occupation of an Electron State of Energy E is given by Fermi Distribution Function.

Behaviour at Different temperature:

i) $T=0K, \; E<E_F$

$$f(E) = \frac{1}{e^{-ve/0}+1} = \frac{1}{e^{-\infty}+1} = 1$$

$$\Rightarrow \boxed{f(E)=1}$$

Probablity of State to be filled is 1 ie State is 100% filled.

ii) $T=0K, \; E>E_F$

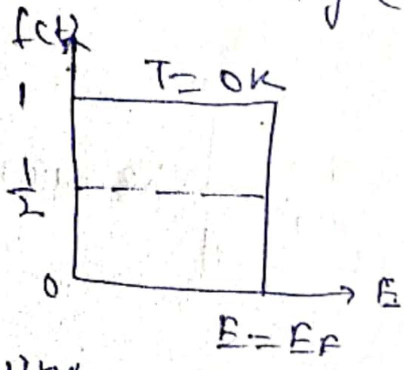
$$f(E) = \frac{1}{e^{+ve/0}+1} = \frac{1}{e^{\infty}+1} = 0$$

$$\Rightarrow \boxed{f(E)=0}$$

It means No State is filled ie complety empty

iii) $T=0, \; E=E_f$

$$\boxed{f(E) = \frac{1}{2}}$$



Fermi level is the level of 50% occupancy. Fermi level lying between complelty filled and completly empty level.

Q. Use Fermi distribution function to obtain value F(E) for $(E-E_F) = 0.01eV$ at 200K.

Sol. Difference between Energy level $(E-E_F) = 0.01eV$

$$= 0.01 \times 1.6 \times 10^{-19} J = 1.6 \times 10^{-21} J$$

We have Fermi Distribution function -

$$F(E) = \frac{1}{1 + e^{(E-E_F)/KT}}$$

$$= \frac{1}{1 + e^{(1.6 \times 10^{-21}) / 1.38 \times 10^{-23} \times 200}}$$

$$= \frac{1}{1 + e^{0.5797}} = 0.3589$$

Q. Calculate Fermi Energy & Fermi temperature in a Metal. Fermi velocity of Electron in Metal is $0.86 \times 10^6 ms^{-1}$

Sol. Given

velocity of electron $v = 0.86 \times 10^6 ms^{-1}$

Mass of Electron $m = 9.1 \times 10^{-31} kg$

Electronic charge $e = 1.6 \times 10^{-19} C$

Boltzmann's constant $k = 1.38 \times 10^{-23} JK^{-1}$

Now Fermi Energy $E_F = \frac{1}{2} mv^2$

$$= \frac{1}{2} \times 9.11 \times 10^{-31} \times 0.86 \times 10^6$$

$$= 3.368 \times 10^{-19} J$$

Fermi Temperature $T_F = \frac{E_F}{k}$

$$= \frac{3.368 \times 10^{-19}}{1.38 \times 10^{-23}} = 2.43 \times 10^4 K$$

Fermi Temperature T_F is $2.43 \times 10^4 K$

Numericals!—

Q Calculate the different number of ways of arranging 6 fermions in 10 Elementary phase cells.

Sol. According to Fermi-Dirac statistics different ways of arranging ni fermions in gi phase cell of i^{th} energy level is given by -

$$(W)_{F.D} = \frac{g_i!}{(g_i-n_i)!\,n_i!}$$

Hence $n_i=6$ & $g_i=10$

$$= \frac{10!}{(10-6)!\,6!}$$

$$= \frac{10\times9\times8\times7\times\cancel{6!}}{4\times3\times2\times1\times\cancel{6!}} = 210$$

Q Calculate the number of Different arrangement of 8 Indistinguishable Particles among seven cells, there being no restriction on number of particles in obeying B-E statistics.

Sol. According to B.E Statistics No. of Different arrangement of ni indistinguishable particle in gi cell is given by -

$$(W)_{BE} = \frac{(n_i+g_i-1)!}{n_i!\,(g_i-1)!}$$

$n_i=8$, $g_i=7$

Hence $$(W)_{BE} = \frac{(8+7-1)!}{8!\times(7-1)!} = \frac{14!}{8!\,6!}$$

$$= \frac{14\times13\times12\times11\times10\times9\times\cancel{8!}}{\cancel{8!}\times(6\times5\times4\times3\times2\times1)}$$

$$= 3003$$

Example 3.1 *An electron gas obeys the Maxwell-Boltzman statistics. Calculate average thermal energy (in eV) of an electron in the system at 300 K.* **[GGSIPU, March 2015 (2 marks)]**

Solution. $$E=\frac{3}{2}k_BT=\frac{3}{2}\times1.38\times10^{-23}\times300\text{ J}=\frac{3\times(1.38\times10^{-23})\times300}{2\pi(1.6\times10^{-19})}\text{ eV}=0.039\text{ eV}$$

Example 3.2 *At what temperature would one in a thousand of atom in a gas of atom hydrogen be in $n=2$ energy level ?*

Solution. For hydrogen $$n(E)=-\frac{13.6}{n^2}\text{ eV}$$

$$n(E_1)=n_1=-13.6\text{ eV}$$

$$n(E_2)=n_2=-3.4\text{ eV}$$

$g(E)=$ no. of states formed $=2n^2$

$$g(E_1)=g_1=2 \text{ and } g(E_2)=g_2=8$$

For Maxwell-Boltzmann distribution is

$$\frac{n_2}{n_1}=\frac{g_2}{g_2}\frac{e^{-E_2/k_BT}}{e^{-E_1/k_BT}}=\frac{8}{2}e^{-(E_2-E_1)/k_BT}$$

or $$\frac{1}{10^3}=4e^{-(E_2-E_1)/k_BT} \quad\text{or}\quad e^{(E_2-E_1)/k_BT}=\frac{10^4}{2.5}=4000$$

Taking logarithms both the sides

$$\frac{E_2-E_1}{k_BT}=\ln 4000$$

$$k_BT=\frac{(E_2-E_1)}{\ln 4000}=\frac{10.2\text{ eV}}{8.29}$$

$$T=\frac{10.2\times1.6\times10^{-19}}{8.29\times1.38\times10^{-23}}\text{ K}=1.43\times10^4\text{ K}$$

$$T=14300\text{ K}=14300-273=14027°\text{C}$$

Dying Stars:-

1) White / Black Dwarfs.

A Star like our Sun will become a white dwarf when it will exhaust its Nuclear Fuel; which then settle down to become a white Dwarfs.

White dwarfs have no way to keep themselves hot, Eventually such stars cool completly & become black dwarfs

Typical Data of white Dwarfs -

Content - Mostly Helium
Density - 10^7 g/cc
Mass - 10^{33} g = Mass of Sun
Central Temperature = 10^7 K = Sun's Temperature.

At its central temperature Helium atoms are expected to be completly ionised, we regard the gas of electron as ideal Fermi gas.

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3N}{8\pi V}\right)^{3/2} = 20\,\text{MeV}$$

$$T_F = 10^{11}\,\text{K}$$

Also No White ~~dwar~~ dwarf Star can have Mass larger than.

$$M_o = 10^{23}\,g \simeq \text{Mass of Sun}$$

If, $M_o = 1.4 \times$ Mass of Sun

This Mass is known as Chandrasekhar limit.

II) Neutron Stars:-

Neutron stars are typically about 10 Miles in diameter have about 1.4 time the mass of ain, sun and spin very Rapidly. Neutrons stars are fascinating because they are densest object known. Due to small size and high density, a neutron star posses a surface gravitational field of about 300,000 times that of Earth.

Magnetic field about 1,000,000,000,000 times stronger than Earth.

III) Black holes!-

Black holes are object so dense that not even light can escape their gravity and nothing can escape from inside a black hole.

Two Existance of two types of black holes.

I) Mass with 4-15 times of Mass of Sun.

II) with mass of a typical Galaxy.

This evidence comes not from seeing the black holes directly, but by obesrving the behaviour of stars & other material near them.

Formulae at a Glance

3.1 Volume of each phase cell

$$\delta V = \delta x\,\delta y\,\delta z\,\delta p_x\,\delta p_y\,\delta p_z$$

$$\delta x\,\delta p_x \geq \hbar,\ \ \delta y\,\delta p_z \geq \hbar \text{ and } \delta z\,\delta p_z \geq \hbar$$

$$\delta V = \hbar^3 \qquad \left[\because\ \hbar = \frac{h}{2\pi}\right]$$

3.2 Maxwell-Boltzmann Statistics

(*i*) The distribution law $n_i = \dfrac{g_i}{e^{(\alpha + E_i/k_BT)}}$

(*ii*) Molecular energy in an ideal gas

$$E = \frac{2\pi N}{(\pi k_BT)^{3/2}}\frac{3}{4}(k_BT)^2\sqrt{\pi k_BT} = \frac{3}{2}Nk_BT$$

and $\overline{E} = \dfrac{3}{2}k_BT$

(*iii*) Maxwell-Boltzmann velocity distribution law

$$n(v)dv = \frac{\sqrt{2}Nm^{3/2}}{(\pi k_BT)^{3/2}}v^2 e^{-\frac{mv^2}{2k_BT}}dv$$

(*a*) RMS velocity $v_{rms} = \sqrt{\dfrac{3k_BT}{m}}$

(*b*) Average velocity $= \overline{v} = \sqrt{\dfrac{8k_BT}{\pi m}}$

(*c*) Most probable velocity $(v_p) = \sqrt{\dfrac{2k_BT}{m}}$

3.3 (*i*) Symmetric wave function $\psi_s(1,2) = +\psi(2,1)$

(*ii*) Antisymmetric wave function

$$\psi_A(1,2) = -\psi(2,1)$$

3.4 Bose-Einstein statistics

(*i*) Distribution law $n_i = \dfrac{g_i}{(e^{\alpha + E_i + k_BT} - 1)}$

(*ii*) Planck's radiation law

$$dE = E(\nu)d\nu = \frac{8\pi h\nu^3}{c^3}\frac{1}{(e^{h\nu/k_BT} - 1)}d\nu$$

(*iii*) Rayleigh-Jeans law $E(\nu)d\nu = \dfrac{8\pi\nu^2 k_BT}{c^3}d\nu$

(*iv*) Wein's displacement law

$$\lambda_{\max}T = \text{Constant}$$

(*v*) **Bose-Einstein Condensation**

(*a*) Critical temperature

$$T_C = \frac{h^3}{2\pi mk_BT}\left(\frac{1}{2.612}\frac{n}{V}\right)^{2/3}$$

(*b*) Rest of particles

$$n_0 = n\left[1 - \Sigma\left(\frac{T}{T_C}\right)^{3/2}\right] \text{ for } T < T_C$$

3.5 Fermi Dirac Statistics

(*i*) Distribution law $n_i = \dfrac{g_i}{(e^{\alpha + E_i/k_BT} + 1)}$

(*ii*) Fermi momentum $p_F = \left(\dfrac{3N}{8\pi V}\right)^{1/3}h$

(*iii*) Fermi Energy $E_F = \dfrac{p_F^2}{2m} = \dfrac{h^2}{2m}\left(\dfrac{3N}{8\pi V}\right)^{2/3}$

(*iv*) Ground state energy

$$E_0 = \frac{8\pi V}{h^3}\frac{p_F^5}{10m} = \frac{3}{5}NE_F$$

(*v*) Mean energy of Fermion $\overline{E} = \dfrac{E_0}{N} = \dfrac{3}{5}E_F$

(*vi*) Electronic heat capacity

$$(C_v)_{El} = \frac{\pi^2}{2}Nk_B\left(\frac{T}{T_F}\right) = aT$$

(*vii*) Sommerfield constant $a = \dfrac{Nk_B{}^2\pi^2}{2E_F}$

Miscellaneous Solved Numerical Problems

Problem 3.1 *A gas has only two particles A and B Show that with the help of diagrams, how these two particles can be arranged in three series 1, 2, 3 using (i) Maxwell-Boltzmann, (ii) Bose-Einstein and (iii) Fermi-Dirac statistics.*

Solution. (*i*) **Maxwell-Boltzmann statistics :**

The two particles are distinguishable.

There is no limit to the number of particles in any one state.

The total number of ways $= 3^2 = 9$.

States	Possible distribution in various states								
1	A	B	–	–	A	B	AB	–	–
2	B	A	A	B	–	–	–	AB	–
3	–	–	B	A	B	A	–	–	AB

(*ii*) **Bose-Einstein statistics :**

If A and B are quantum particles, they are indistinguishable. Thus they have to be given the same name, say A.

There is no limit to the number of particles in any one state.

The total number of ways $= 6$

States	Possible distribution in various states					
1	A	A	–	AA	–	–
2	A	–	A	–	AA	–
3	–	A	A	–	–	AA

(*iii*) **Fermi-Dirac statistics :**

The particles are indistinguishable and not more than one particle can be in any one state.

The total number of ways $= 3$

States	Possible distribution in various states		
1	A	A	–
2	A	–	A
3	–	A	A

Problem 3.2 *Show that on increasing temperature, the number of atoms in excited state increases.*

Solution. $n(E) = g(E) . f(E)$

For Maxwell-Boltzmann distribution

$$n(E_i) = \frac{g(E_i)}{e^{(\alpha + E_i/k_BT)}} = g(E_i) A e^{-E_i/k_BT}$$

Then $n(E_1) = g(E_1) A e^{-E_1/k_BT}$

and

$n(E_2) = g(E_2) A e^{-E_2/k_BT}$

$$\Rightarrow \quad \frac{n(E_2)}{n(E_1)} = \frac{g(E_2)}{g(E_1)} e^{-(E_2 - E_1)/k_BT}$$

On increasing temperature $\Rightarrow n(E_2) > n(E_1)$

Problem 3.3 *(a) Show that at* $E = E_F$ *and* $T \neq 0\,K$*. The occupancy is equal to 0.5. (b) Show that at* $E < E_F$ *and* $T = 0\,K$*. The occupancy of state is perpendicular and at* $E > E_F$ *and* $T = 0\,K$*, the occupancy of state is zero.*

Solution. From Fermi-Dirac statistics

$$n_i = \frac{g_i}{e^{\alpha + E_i/k_B T} + 1}$$

This is written as $$n(E) = \frac{g(E)}{e^{(E-E_F)/k_B T} + 1} = g(E)\, f(E)$$

Then occupancy $$f(E) = \frac{1}{(e^{(E-E_F)/k_B T} + 1)}$$

(a) When $T \neq 0$ and $E = E_F$ then $$f(E) = \frac{1}{e^{0} + 1} = \frac{1}{1+1} = \frac{1}{2} = 0.5$$

(b) When $T = 0$ and $E < E_F$ then $$f(E) = \frac{1}{e^{-\infty} + 1} = \frac{1}{0+1} = 1$$

Problem 3.7 *At what temperature can we expect a 10% probability that electrons in a metal will have an energy which is 1% above* E_F *? The Fermi energy of the metal is 5.5 eV.* **[GGSIPU, May 2014 (4.5 marks)]**

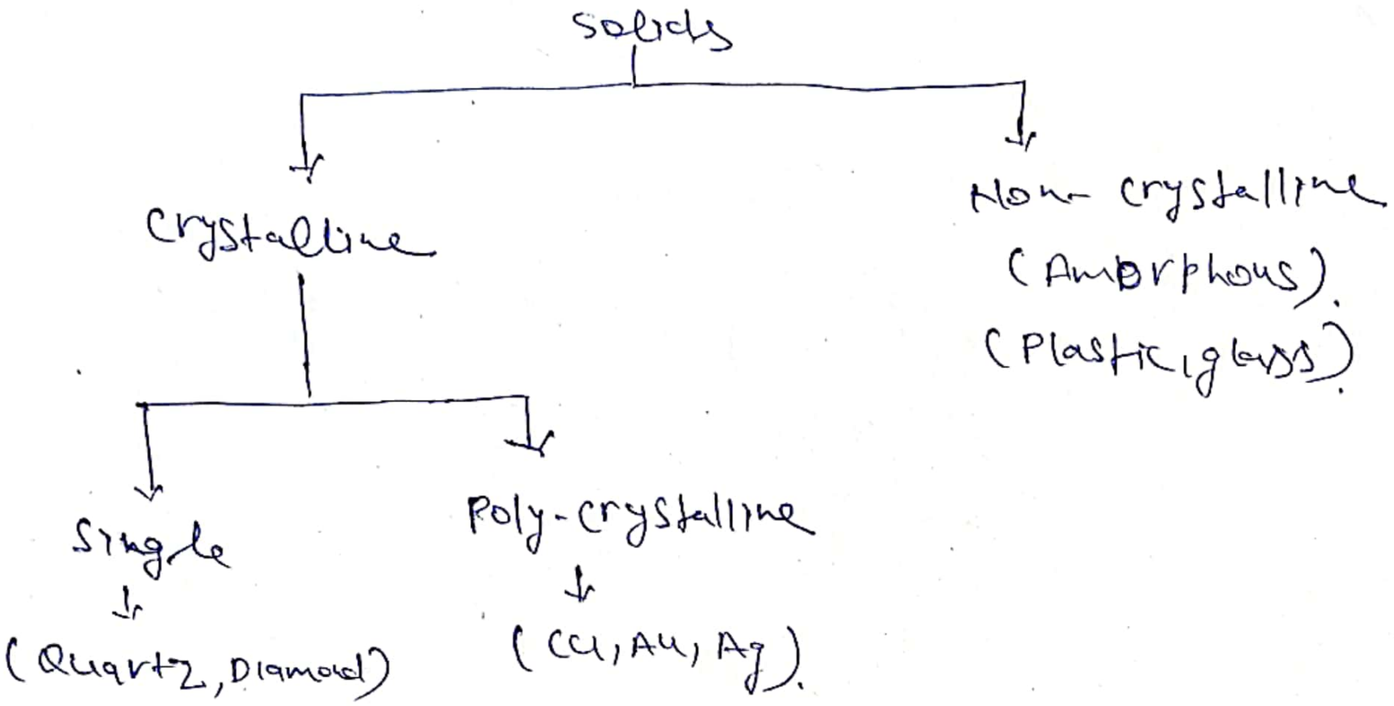
Solution. Given : $f(E) = 10\%$, $E = E_F + 1\%$ of E_F, $E_F = 5.5\,\text{eV}$, $T = ?$

$$f(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1}$$

$$E = 5.5 + \frac{5.5}{100} = 5.5 + 0.555\,;\ \ E - E_F = 0.555.$$

$$0.1 = \frac{1}{\left(\exp.\dfrac{0.555 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23}\,T}\right) + 1} = \frac{1}{\exp.\left(\dfrac{637.7}{T}\right) + 1} \quad \text{or} \quad T = 290.2\ \text{K}$$

UNIT-3 CRYSTAL STRUCTURE



Crystalline solids:- crystalline solids are characterize by regular or Periodic Arrangement of Atom or Molecules

* Every solid is made up of Atom or Molecule.

* Atoms are repeating themselves after certain distance.

Non crystalline Solids:- (Amorphous)

→ are characterize by random arrangement of Atoms or Molecules.

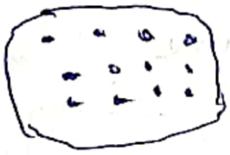
→ Arrangement of Atoms will describe their properties.

→ Plastic is Non-crystalline.

→ copper is crystalline

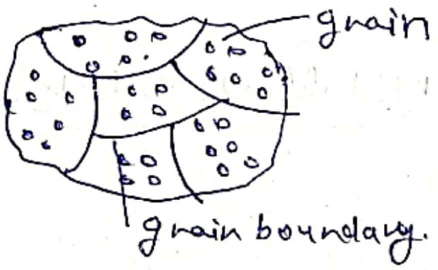
→ Diamond & copper both are crystalline, but Diamond is a single crystal & copper is a poly crystalline.

Single crystal:- Any solid object in which an order three Dimensional arrangement of atom ion or Molecule is repeated throughout the entire volume.



Polycrystalline crystals:- Polycrystalline is the aggrigate of large Number of single crystals.

Small single crystals are known as Grain. & boundries repeating these crystals are grain boundary.

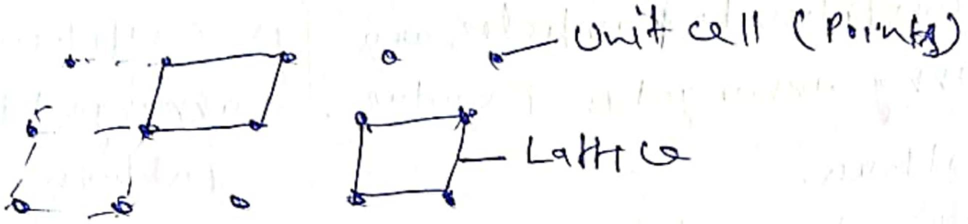


Note:- In Nature Most of the solids are in the form of crystalline solids because crystalline solid is more stable as compare to Amorphous solids.

Difference between Crystalline Solids & Amorphous Solids

Crystalline Solids	Amorphous Solids.
1) Constituents particles are ~~array~~ arranged in Regular Pattern.	1) Constituent Particles are arranged in irregular pattern.
II) They have definite Shape	II) They have indefinite shape
III) They have sharp melting point.	III) They melt over a range of temperature (i-j)
IV) They have definite Enthalpy of Fusion	IV) Don't have definite Enthalpy of Fusion
V) They have long order arrangement	V) Have Short order arrangement.
VI) They are more hard	VI) They are less hard
VII) They are true solids (Cu, Fe Salt etc	VII) Supercooled liquid. Glass, Rubber, Plastics.
VIII) They are Anisotropic	VIII) There are isotropical

Space lattice:- Geometrical Regular arrangements of ~~Points~~ Repeated Points in space.



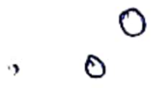
Bravais Lattice:- Three dimensional array of points such that each points is surrounded by Neighbouring points in an identical way.

Note:- lattice will be a Bravais lattice or space lattice if each lattice point has identical surroundings.

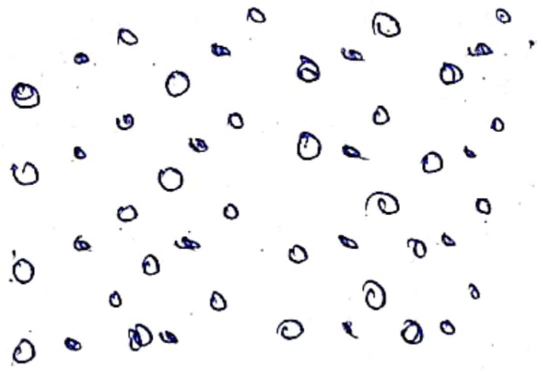
Basis:- Basis is an atom or group of Atoms. By Attaching the basis to each lattice Point we get crystal structure

Lattice + Basis = crystal

Space lattice



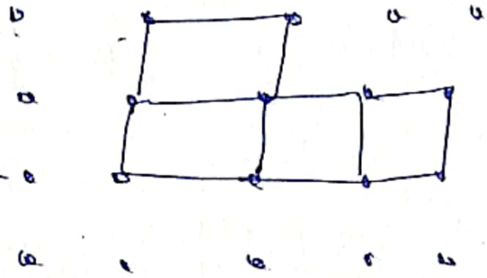
Basis



crystal structure

Unit cell:- "Smallest Repeating Unit of the crystal or lattice"

Note:- Unit cell on continuous Repetation can generate whole lattice or crystal.



~~Unit cell~~ If we want to construct a crystal structure. we have to arrange unit cell side by side.

Unit cells are of two type:-

I) Primitve

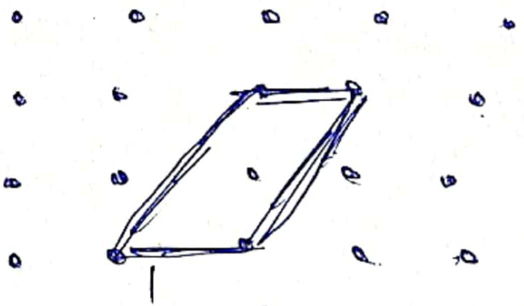
II) Non-Primitive.

Primitive:- Lattice Points belonging only to the corner of unit cells.

Non-Primitive:- Lattice Points are belonging to the corner as well as other position of unit cell.

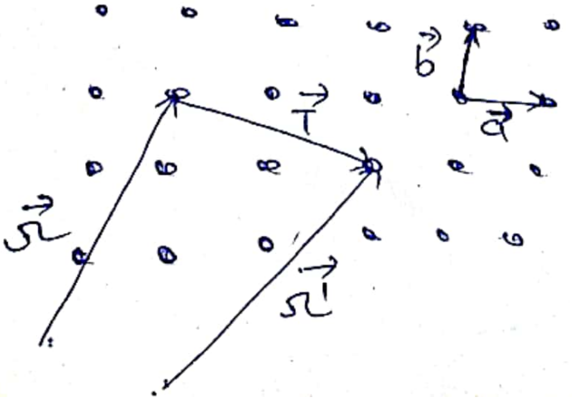
Note:- Effective Number of Lattice Point for Primitive cell per unit cell is 1

→ For Non-Primitive unit cell Effective Number of lattice points are more than one.



Non-Primitive unit cell.

Translation vector:- Mathematically a lattice is defined by three fundamental vector $\vec{a}\,\vec{b}\,\vec{c}$ such that atomic Arrangement look exactly identical when viewed from any two points $\vec{r}$ & $\vec{r}\,'$



$$\boxed{\vec{r}\,' = \vec{r} + u\vec{a} + v\vec{b} + w\vec{c}}$$

u,v,w are integers

Types of Unit cell:- 3 types mainly.

a) **Simple Cubic cell (S.C.C):-** one atom is present at each corner of cube and 1/8 part is contributed by each atom inside the cube (unit cell). So total number of atom per unit cell in SCC is $\frac{1}{8}\times 8 = 1$

b) **Body centered Cubic (BCC):**

- One atom ~~is~~ present at each corner of the cube contribute 1/8
- So one atom is contributed by 8 atoms at 8 corner $1/8 \times 8 = 1$.
- One single (complete) atom is present at the center of cube contribute completly to cube.

So total number of atom $= \frac{1}{8}\times 8 + 1 = 1 + 1 = 2$

(C) **Face centered Cubic (FCC):-**

Particles or atoms are arranged at each corner as well as each faces

So contribution.

Corner	Faces
$1/8 \times 8$	$\frac{1}{2}\times 6$

Total Number of atom $= 3 + 1 = 4$

Co-ordination Number:- Number of nearest touching particles in a closed packing structure.

Types of Closed Packing:-

- 2-Dimensional
  - Square closed Packing (SCP)
  - Hexagonal Closed Packing (HCP)
- 3-Dimensional
  - Cubic Closed Packing (ABC-ABC type)
  - Hexagonal Closed Packing AB-AB type

I) Square Closed Packing:-

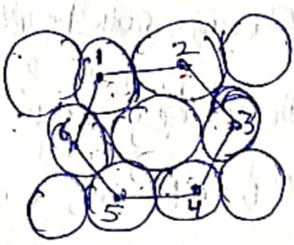
The central Atom is touched by four Neighbouring atom.

% occupied by atom in crystal = 52.4 %

Cordination Number = 4.

II) Hexagonal Closed Packing (2-D)

When one layer is normal and atom of Second ~~lg~~ layer are put in the depression of 1st layer then it give rise to HCP in 2-Dimesion.



% of space occupied = 62.4 %

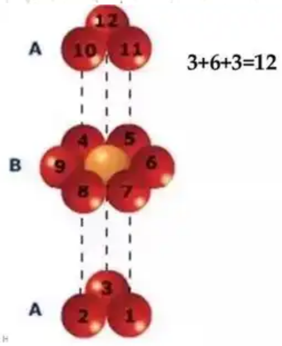
Coordination Number = 6.

III) ~~Cubic~~ Hexagonal Closed Packing (HCP) in 3D:-

When atom of third layer are put in the depression of tetrahedral voids then it give rise to HCP.

% of Space occupied -74 %

Coordination Number -12

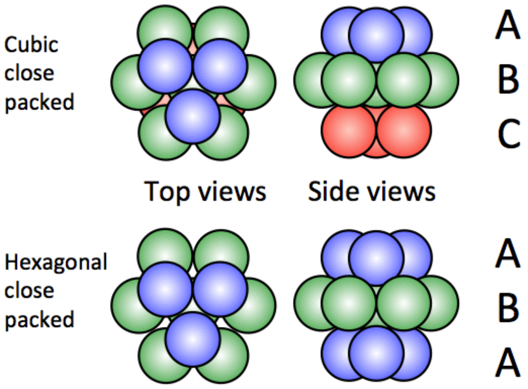


Scanned

Cubic Closed Packing (CCP) in 3D:-

when the second layer arranged on the first layer to give rise to octahedral and tetrahedral voids in the second layer.

When atom of third layer are put in the depression of these voids then give rise to CCP type packing



% Space occupied - 74%.

Coordination Number - 12

Voids or holes in crystals! These are unoccupied or blank space are left between atom when they are closely packed.

They are generally two types.

1) Tetrahedral void!- The void or hole which is created by four sphere in contact.

2) Octahedral void!- The void or hole created by six sphere in contact

Void or hole also called Interstics.

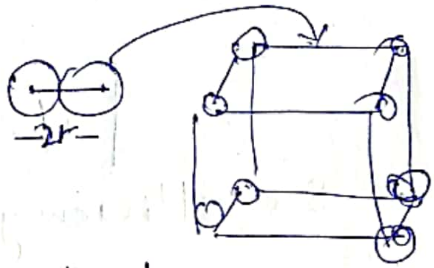
Packing Fraction or Efficiency of Packing:-

It is defined as the % of space occupied by the atom in a unit cell. It is different for different arrangement.

⇒

$$\% \text{ efficiency} = \frac{\text{Vol. of Sphere} \times \text{No. of Sphere}}{\text{Total Vol. of Cube}} \times 100$$

I) SCC:- Relation between edge length (a) and radius of atom in SCC is.



$a = 2r$

$\Rightarrow \boxed{r = a/2}$

In SCC there ~~are~~ is only 1 atom which contribute inside cube

$\text{Vol} = \frac{4}{3}\pi r^3$

$$\Rightarrow \% \text{ efficiency} = \frac{\frac{4}{3}\pi r^3 \times 1}{(2r)^3} \times 100$$

$$\boxed{\% \text{ efficiency} = 54\%}$$

II) FCC:- Relation bet edge length a and radius of atom r in FCC is

$r = \frac{\sqrt{2}a}{4}$ or $\boxed{a = \frac{4r}{\sqrt{2}}}$

No. of sphere is = 4

$$\% \text{ Efficiency} = \frac{\frac{4}{3}\pi r^3 \times 4}{(2\sqrt{2}r)^3} \times 100$$

$$\boxed{\% \text{ Efficiency} = 74\%}$$

iii) BCC:- Relation between edge length and radius of atom (r) is $4r = \sqrt{3}a$

$$\boxed{a = \frac{4r}{\sqrt{3}}}$$

No. of Sphere contributing in cube in case of BCC is 2

So % efficiency $= \dfrac{\frac{4}{3}\pi r^3 \times 2}{\left(\frac{4r}{\sqrt{3}}\right)^3} \times 100$

$$\boxed{\% \text{ efficiency} = 68\%}$$

So efficiency of Packing is 68% in BCC.

Note

In BCC

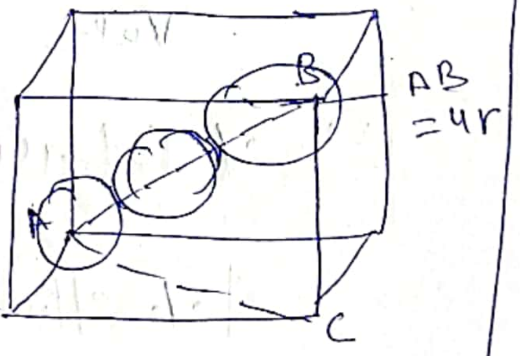
$AC = \sqrt{2}a$

$AB^2 = AC^2 + BC^2$

$= (\sqrt{2}a)^2 + a^2$

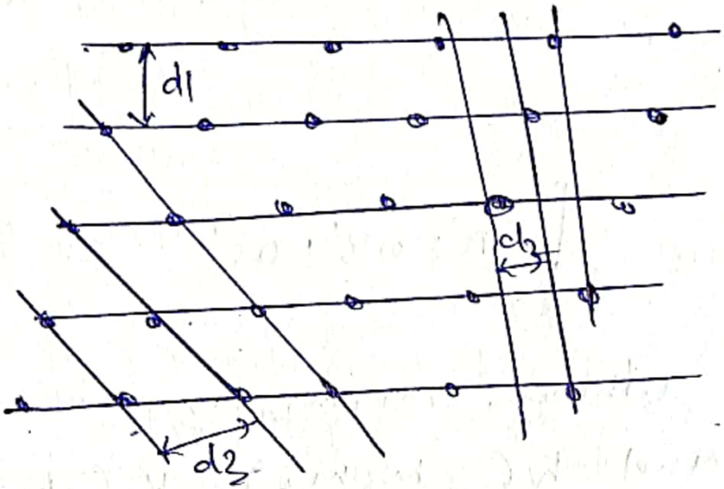
$$\boxed{AB = \sqrt{3}a}$$

or $\boxed{4r = \sqrt{3}a}$



Lattice Plane of a crystal :- A lattice plane may be considered as an aggregate of set of parallel equally spaced plane passing through the lattice points.

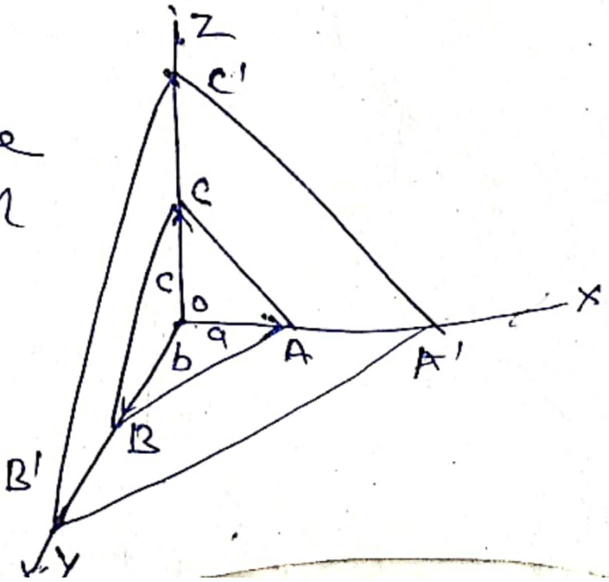
The equally spaced planes are called lattice planes and perpendicular distance between adjacent plane is called interplaner spacing (d).
(d_1, d_2, d_3 are interplanar spacing)



Miller indices :- The position & orientation of lattice plane in a crystal are determined by three whole numbers, which have same ratio with one another as the reciporocal of the intercepts of the plane on the three crystal axes. These number are denoted as h,k,l known as Miller indices.

Let OX, OY, OZ be the three axes parallel to the crystal axes the plane XOY, XOZ, ZOY are parallel to the face of crystal

Let ABC be a standard plane cutting all three axes at point A, B, C with
$OA = a$, $OB = b$, $OC = c$
be the three intercept.



This law State that " the face which is Parallel to the Plane whose intercept on the three Axes are $m_1 a$; $m_2 b$ & $m_3 c$ is a possible face of crystal. (Affected orientation)

Thus $OA' : OB' : OC' = m_1 a : m_2 b : m_3 c$

$$= \frac{a}{m_2 m_3} : \frac{b}{m_1 m_3} : \frac{c}{m_1 m_2}$$

$$\boxed{OA' : OB' : OC' = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}}$$

Where m_1, m_2, m_3 are Small whole Number and $h (= m_2 m_3)$, $k (= m_1 m_3)$, $l (= m_1 m_2)$ Hence (h, k, l) are the Miller indices of the Plane A', B', C' with respect to Standard Plane.

* **Note** Miller indices of Standard Plane are always $(1, 1, 1)$.

Q: In a crystal lattice plane cut the intercept of a, 2b, 3C along three axes where a, b, C are primitive vector of unit cell. Determine Miller indices of given plane.

Sol:

$$a : 2b : 3c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

$$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 1 : 2 : 3$$

$$h : k : l = 1 : \frac{1}{2} : \frac{1}{3}$$

$$= 6 : 3 : 2$$

$$h = 6, \; k = 3, \; l = 2$$

Q Deduce the Miller indices of a plane which cut off intercept in the ratio 1a : 3b : -2c, along three axes, where a, b, c are primitive.

Sol.

$$1a : 3b : -2c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

$$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 1 : 3 : -2$$

$$h : k : l = 1 : \frac{1}{3} : -\frac{1}{2} = 6 : 2 : -3$$

$$h = 6, \; k = 2, \; l = -3$$

Q An orthorhombic crystal has axial vector in ratio a : b : c :: 0.424 : 1 : 0.367. Find the Miller indices of those crystal plane whose Miller indices are in the ratio

i) 0.212 : 1 : 0.183

ii) 0.848 : 1 : 0.732

Sol. i)

$$p : q : r = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

$$0.212 : 1 : 0.183 = \frac{0.424}{h} : \frac{1}{k} : \frac{0.367}{l}$$

M.I = $h : k : l = 2 : 1 : 2$

11) $0.848 : 1 : 0.732 = \frac{0.424}{h} : \frac{1}{k} : \frac{0.367}{l}$

$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 2 : 1 : 2$

Q Find the Miller indices of an orthorombic crystal which cut intercept of 3a, 4b along x & y Axes.

Sol.

$3a : 4b : \infty = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$

$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 3 : 4 : \infty$

$h : k : l = \frac{1}{3} : \frac{1}{4} : \frac{1}{\infty}$

$h : k : l = 4 : 3 : 0$

Q Find the Ratio of intercept of three Axes by ~~(1 $\bar{3}$~~ $(1\,\bar{3}\,2)$ plane in a simple cubic lattice

Sol. P, q, r be the intercept along x, y, z axis Resp.

$P : q : r = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$

(given $h = 1$, $k = -3$, $l = 2$)

$P : q : r = \frac{a}{1} : \frac{a}{-3} : \frac{a}{2}$ (for simple cubic)

$P : q : r = 6 : -2 : 3$

Q Lattice constant for a cubic lattice is a. Deduce the spacing between (011) (101) & (112) plane.

Sol.

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d(011) = \frac{a}{\sqrt{0^2 + (1)^2 + (1)^2}} = \left(\frac{a}{\sqrt{2}}\right)$$

Braggs X-Ray Diffraction:-

It is the relation between spacing of Atomic planes in crystal and agle of incidence at which these planes Produce the Most intense reflection.

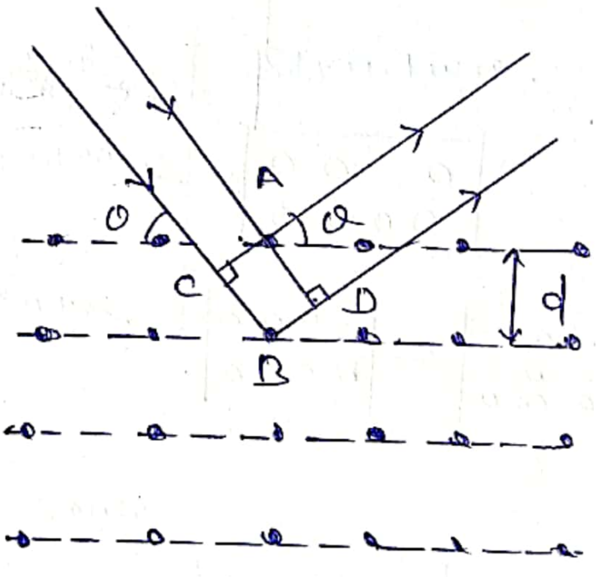
OR

When an X-Ray incident into a crystal, its angle of incidence, θ will reflect with same angle of Scattering θ. Then the path difference d is equal to whole Number n of wavelength λ.

OR

Diffracted beams are found when the Reflection from various plane of Atom interfere constructively

Figure shows a Particular set of Atomic planes in a crystal, d being the interplanar spacing. Suppose a Monochromatic X-Ray beam is incident at an angle θ. It is Scattered by the Atom. line A & B.



The path difference for the waves reflected from adjacent planes is,

$$CB+BD = d\sin\theta + d\sin\theta$$

$$\boxed{2d\sin\theta = n\lambda}$$

↓

Bragg's law.

Q In Bragg's spectrometer using set of Atomic plane of a crystal of interplanar spacing 2.8 A°. The glacing angle for 1st order maxima was 10°. Find the wave length of x-rays employed. At what angle would the second order maxima occur.

Sol From Braggs Eqn

$$2d\sin\theta = n\lambda$$

$$\lambda = \frac{2d\sin\theta}{n} \quad (n=1)$$

$d = 2.8$ A° $\sin\theta = \sin 10° = 0.1736$

$n = 1$

$$\lambda = \frac{2 \times 2.8 \times 0.1736}{1} = 0.97 \text{A}°$$

For second order maxima $n=2$. Then

$$\sin\theta = \frac{n\lambda}{2d} = \frac{2 \times 0.97 \text{A}°}{2d}$$

$$= \frac{2 \times 0.97 \text{A}°}{2 \times 2.8 \text{A}°} = 0.346$$

$$\theta = \sin^{-1}(0.346) = 20.3$$

Interplanar spacing:- The Separation between Successive lattice plane known as Interplanar Spacing.

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

Q Lattice constant for a cubic lattice is a for a cubic lattice. Deduce the spacing between (011) (101) & (112) planes.

Sol:

$$d_{011} = \frac{a}{\sqrt{0^2+1^2+1^2}} = \frac{a}{\sqrt{2}}$$

$$d_{101} = \frac{a}{\sqrt{1^2+0^2+1^2}} = \frac{a}{\sqrt{2}}$$

$$d_{112} = \frac{a}{\sqrt{1^2+2^2+1^2}} = \frac{a}{\sqrt{6}}$$

Q Calculate the Interplanar Spacing for (321) planes in a simple cubic lattice whos lattice Constant is 4.2×10^{-8} cm.

Sol.

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$d = \frac{4.2 \times 10^{-8}}{\sqrt{3^2+2^2+1^2}}$$

$$= \frac{4.2 \times 10^{-8}}{\sqrt{14}} = \frac{4.2 \times 10^{-8}}{3.74}$$

$$= 1.12 \times 10^{-8}$$

$$d = 1.12\,A^\circ$$

Q2 An x-ray Analysis of Cubic Crystal is carried, using x-rays of wavelength 0.58 A°. Bragg's reflections are observed at glacing angle 6.45°, 9.15° and 11.1°. find interplanar spacing of crystals.

Sol. Bragg's Equ^n for 1st order is

$$2d \sin\theta = \lambda$$

d_1, d_2, d_3 be the int planar spacing at glacing angle 6.45°, 9.15°, 11.1° resp. Then

$$d_1 = \frac{\lambda}{2\sin 6.45^\circ} = \frac{0.58}{2\times 0.1123} = 2.58\,A^\circ$$

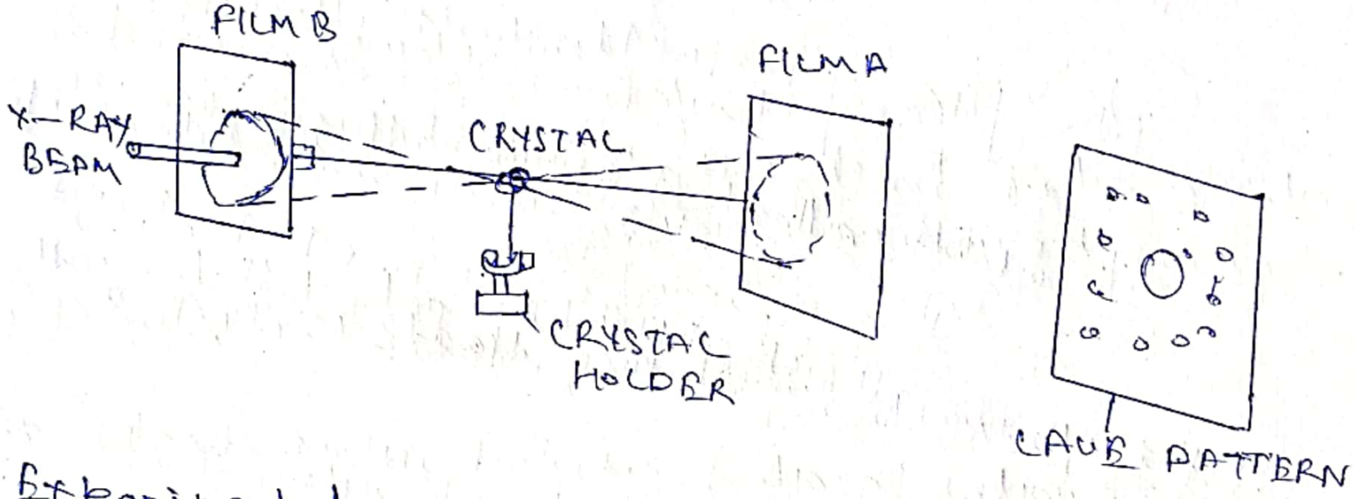
$$d_2 = \frac{\lambda}{2\sin 9.15^\circ} = \frac{0.58}{2\times \underset{0.1590}{\cancel{0.11523}}} = 1.82\,A^\circ$$

$$d_3 = \frac{\lambda}{2\sin 11.1^\circ} = \frac{0.58}{2\times 0.1590} = 1.51\,A^\circ$$

$$d_1 : d_2 : d_3 = 2.58\,A^\circ : 1.82\,A^\circ : 1.51\,A^\circ$$

$$= 1 : 0.705 : 0.585 = 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}}$$

Laue Method!- In Laue's method, a single crystal is held stationary in a continuous x-ray beam. The crystal diffracts the discrete value of λ for which the crystal planes of spacing d and the incidence angle θ satisfy the Bragg's equation.



Experimental arrangement is shown in figure. A Continuous (0.2 A° to 2A°) x-ray beam, well collimated by Pinhole arrangement, is allowed to fall on a crystal. A flat film A is placed to recive the transmitted diffracted beam

- * Each spot in laue Pattern correspond to an interference Maximum for a set of crystal plane satisfying the bragg's Equation $2d\sin\theta = n\lambda$ for a wavelength selected from continuous beam.
- * The distribution of spot depends on the symmetry of crystal and its orientation wrt X-Ray beam.

Applications:- Used for rapid determination of crystal orientation and symmetry.

II) Used to study crystalline imperfection

Seven crystal system:-

When a unit cell has lattice Points only at corner called simple or Primitive unit cell. In all there are seven type of simple or Primitive unit cell.

		Axial Distance	Axial Angle
I)	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
II)	Tetrahedral	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
III)	orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
IV)	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ ; \beta \neq 90^\circ$
V)	Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
VI)	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
VII)	Hexagonal	$a = b \neq c$	$\alpha \neq \beta = 90^\circ, \gamma = 120^\circ$

Crystal Structure of Nacl :- (FCC)

The crystal of Nacl contains same Na^+ & Cl^- ions both have coordination Number of 6. Radius Ratio of Nacl is $\frac{Na^+}{Cl^-} = .524$ which suggest that ~~Nacl~~ Cl^- forms cubic closed Packed structure in which Na^+ ions occupy octahedral void in the lattice hence both have coordination Number of 6:6.

$6:6 :: Na^+ : Cl^-$

Crystal Structure of Diamond! (FCC)

The space lattice of Diamond is face-centered cubic (FCC). with a basis of two carbon atom associated with each lattice Point.

In diamond each carbon atom forms covalent bond with four other carbon atoms, that occupy four corner of cube in tetrahedral structure.

length of each bond is 1.54 A°

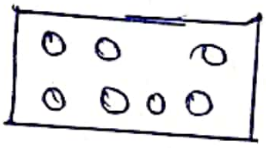
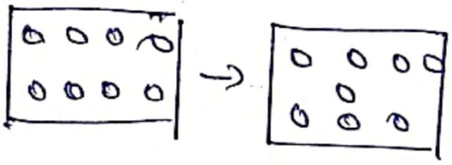
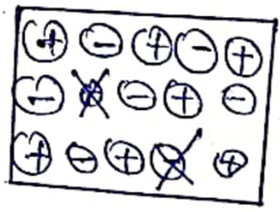
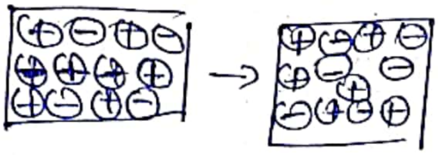
Angle between bond is 109.5 A°

Coordination Number of crystal = 4

Number of Atom Per unit cell = 8

Defects.

- Point Defects (Atomic Defects).
  - Stoichiometric
    - Non Ionic
      - Vacancy Defects
      - Interstial Defects
    - Ionic
      - Schottky Defects
      - Frenkel Defects.
  - Non Stoichiometric
    - Metal Excess
    - Metal Deficiency
  - Impurity Defects.
- Electronic Defects

Defects	Definition	Solids	Density	Structure.
① Vacancy	Some of lattice sites are vacant	Non-Ionic	Decrease	
ii) Interstial	Some of the Constituent atom occupy Interstial site	Non Ionic	Same	
iii) Schotky	Equal No. of Cation & Anion Removed	Ionic	Decrease	
iv) Frenkel	one of the Cation & Anion occupy Interstial site	Ionic	Same	

S No.	Condition.	Schotky Defect	Frenkel Defect
I)	Size of Cation & Anion.	Size of Cation = Size of Anion. (Small Difference)	Anion (Size) > Cation (Size).
II)	Coordination Number	High	Low.
III)	Example	NaCl, KCl KBr	AgCl, Zn

Defects

Imperfection in solids! At Absolute zero (0°K), there is no Molecular motion and therefore disorder is zero. As the temperature increase the random motion of Particle takes place, due to which atom leave their correct Position & cause defects.

Point Defects!- Mainly two types.

I) Stoichiometric Defects!- In this defect Ratio of cation and Anion ~~change~~. Doesn't change.

Eg. Frenkel and Schottky Defects.

II) Non-Stoichiometric Defects!- Ratio of Cation & Anion changes.

Eg. Metal Excess & Metal Deficiency Defects.

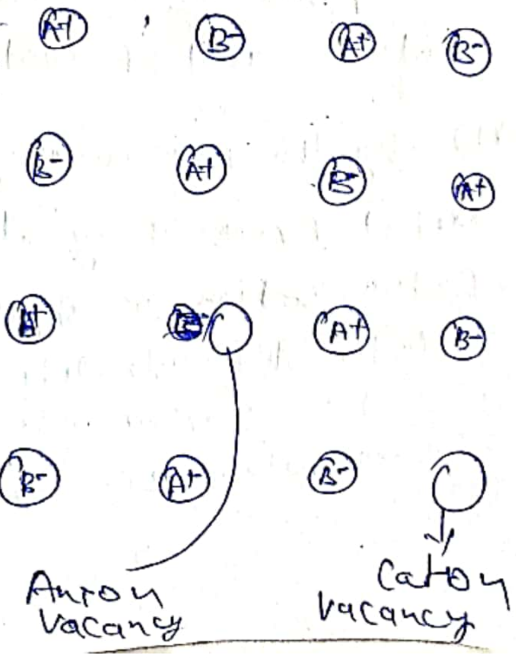
I) Schottky Defect!- When Equal Number of cation & Anion Missed from lattice site

* occur in those Solids which has High co-ordination Number.

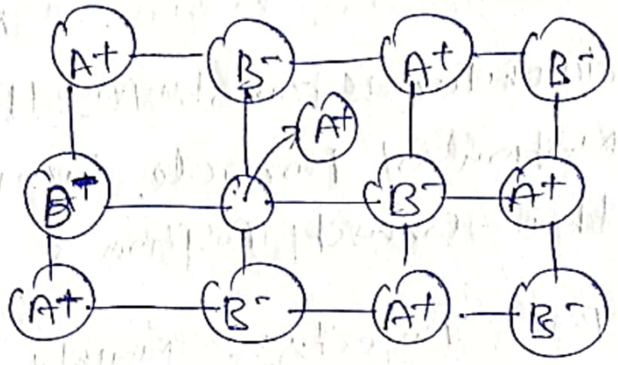
* occur in those Solids which has Nearly Similar Size of Cation & Anion.

Imp * Density of crystal decrease during this defect.

Eg NaCl, CsCl, KCl, KBr etc.



Frenkel Defect:- This defect arises when an ion leave its correct lattice position and occupies interestial site.



→ Ionic compound remains electrically Neutral & Stoichiometry of compound also remains same.

→ Occur in the crystal of low Co-ordination Number and large difference in size of ion.

Eg. AgCl, AgBr, AgI, ZnS.

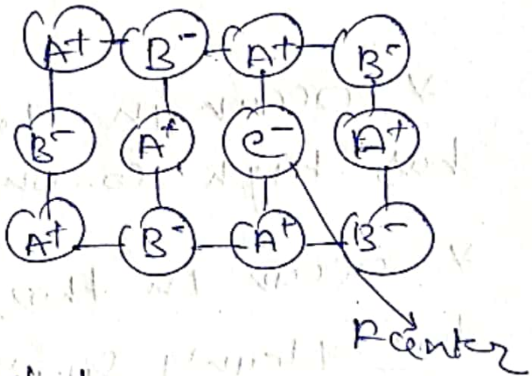
→ This defect don't change the density of crystal.

* AgBr shows both Schottky & Frenkel Defect

Non-Stoichiometric Defects:-

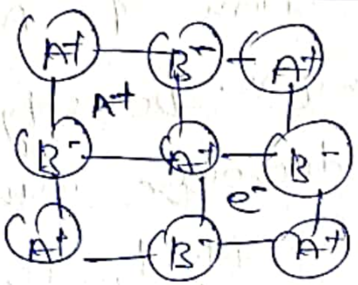
I) Metal Excess Defect (due to Anion vacancy)

In this defect the -ve ion is missed from lattice site. The hole caused by -ve ion. is occupied by e⁻ to maintain the electrical neutrality. The Hole occupied by e⁻ are called color centres and F centres. Eg. NaCl, KCl.



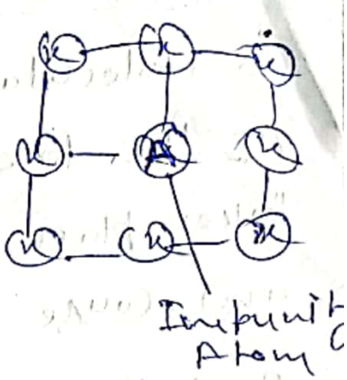
II) By the presence of Extra cation and electron in interstitial site

Metal Excess may also be caused by an Extra cation occupying the interstitial site. Electrical Neutrality is maintained by an e⁻ present in another interstitial site. This defect occur when ZnO is heated in crystal.

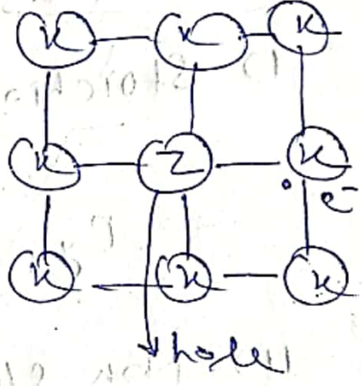


$$ZnO \longrightarrow Zn^{++} + \frac{1}{2}O_2 + 2e^-$$

Impurity defect:- In covalent crystal when a crystal of 14 group is doped with impurity of 15 group then an extra e^- is present. This type of doping (impurity adding) give rise to a semiconductor of n-type.



ii) When a crystal of 14 group is doped with the impurity of 13 group then there is a deficiency of one e^- which break a hole in the crystal lattice due to which current flow. This type of doping give rise to a p-type semiconductor.



Note (n type – Negative or e^- excess,
P type – Positive or e^- deficiency)

UNIT-4

Band Theory of Solids:-

Band theory of solids:- This is the theory of valence electron which are Nearly free.

Free electron theory was successful in Explaining the various Electronic + thermal properties of Metal like-

I) Specific Heat

II) Temperature Suspectability

III) Temperature dependence of Electrical Resistivity.

But it can't Explain the Distinction between Conductor insulator + Semiconductor.

Band theory Explain that Each atom has a discrete set of Energy levels

1S, 2S, 2p, 3S, 3p ------- .

The splitted Energy levels are (becomes so Numerous) so close together forming Energy bands.

Na- $1S^2 2S^2 2p^6 3S^1$

3S - 3S level is the first occupied level to be splitted into band.

2p - 2p level doesn't split until the interatomic distance becomes smaller.

OR Energy bands in solid correspond to Energy level in Atom.

* Electrical properties in solid depend upon its Energy band Structure.

Depending on the Nature of band occupation by electron and on the width of forbidden band, all the solids can be classified as conductors, insulator & semiconductor.

Valence band:- Filled level form a band known as valence band.

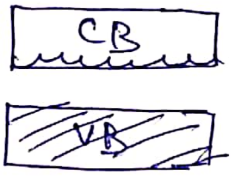
Conduction band:- Unfilled level form an another band known as conduction band.

Energy gap:- V.B & C.B seprated by some energy gap known as forbidden Energy gap.

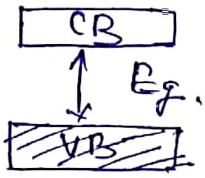
Classification of Solids:-

Solids can be classified into three types:-

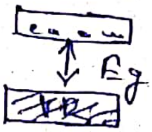
I) Metal or Conductor:- C.B either partially filled or V.B & C.B partially overlap each other.



II) Insulator:- VB is completly filled and CB is completely empty & forbidden Energy gap is quite large.



III) Semiconductor:- At 0K in semiconductor VB is completely & CB is completely Empty. Energy gap is smaller than insulator.



Semi conductors:-

A solid substance whose conductivity lies between an insulator and that of most metals.
(Either due to addition of Impurity or because of temperature effect).

Types of Semi conductors:-

I) Interinsic semiconductor II) Extrinsic Semiconductor

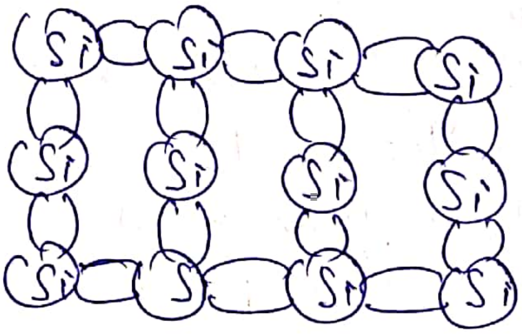
I) Intrinsic Semiconductor:- A pure semiconductor is known as intrinsic semiconductor.

1) On the basis of Band theory:-

At 0K Semiconductors are insulators but at room temp. Some electron gain Energy due to thermal and moving from VB to CB.

* Vacancy is created in VB called Hole.
* Motion of hole in VB and electron in CB is Responsible for Electronic conduction.

II) On the basis of crystal structure:- Atoms are strongly bound by covalent bond.



→ On receiving Additional Energy some electron break their bond and Produce free electron & equal No. of Holes.

Thus effective current in Semiconductor is the sum of Electronic current & Holic current.

Extrinsic Semiconductor:-

Process of Addition of impurity to a Pure Semiconductor. Doped Semiconductor called Extrinsic semiconductor.

Types of Extrinsic Semiconductor:-

I) N- type Semiconductor II) P- type Semiconductor.

I) N- type Semiconductor:-) Internsic Semiconductor doped with. Petavalent Impurity atom.

1) on the basis of crystal structure:-

* The impurity atom when Mixed with Si or Ge atom, form covalent bond with Neighbouring Si or Ge atom.

* At room temperature some covalent bond break and Produce equal Number of Holes and free electrons.

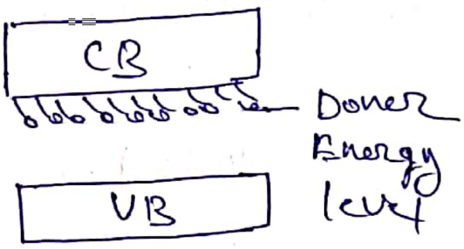
* The Number of electrons are large compare to holes.

* Electrons are Majority charge carrier and Holes are Minority charge carriers.

→ Conduction is Mainly due to Electron + Holes.

2) on the basis of Band theory:-

→ ~~Where~~. Impurity atom generate a New Energy level just below the CB known as doner energy level.



→ Now it is easy for them to jump from. VB to CB.

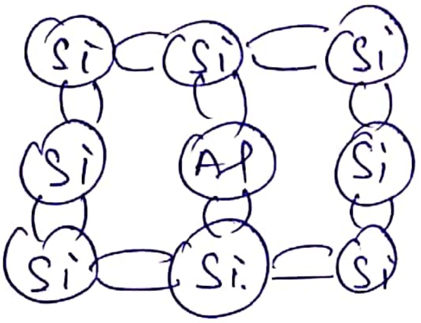
→ All electron of doner energy level jumps to CB at room temperature.

→ Some electron of VB also jumps to CB.

Hence the Number of electron in CB is large as compare to VB.

P-type Semiconductor:-

on the basis of crystal structure:-



- When trivalent impurity atom is Mixed with Si or Ge, they replace Si or Ge atom and form covalent bond with. Neighbouring Si or Ge.

→ Number of holes are very large as compare to Electrons. (due to trivalent impurity)

→ At room temperature covalent bond break and Produe equal Number of Holes and electrons.

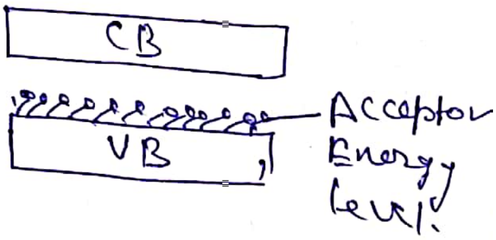
→ Holes are Majority and electron are Minority charge carrier.

⇒ conduction is Mainly due to Holes, there fore such semi-conductor known as P-type semiconductor.

on the basis of band theory:-

Impurity atom generate an energy level just above the top of valence band, this Energy level known as acceptor level.

→ Thus electron from VB easily shift to acceptor level and generate holes in VB.



⇒ Electron from VB also goes to CB generating equal Number of Holes in VB.

→ Hence holes are Majority charge carrier electrons are Minority charge carrier in P-type Semi conductor.

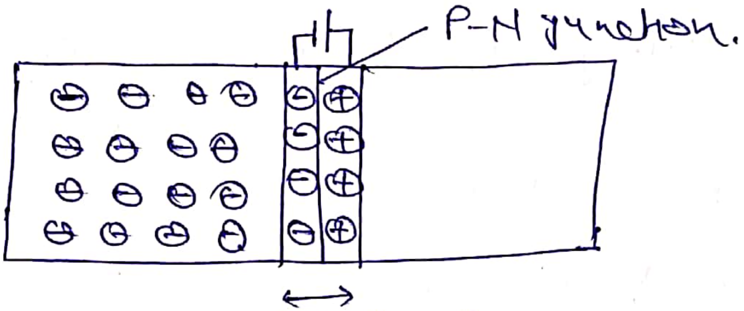
Differene between..-

I) Intrinsic Semi conductor	Extrinsic Semi Conductor.
i) Pure Semi Conductor	1) Impure Semi conductor
ii) $n_h = n_e$	2) $n_h \neq n_e$
iii) Conductivity is low	III) conductivity is High.
iv) Conductivity depand only on temperature	IV) Conductivity depand on temperature and concentration of Doping..

n-type Semi Conductor	P-type Semi Conductor.
I) Impurity atom is Pentavalent	I) Impurity Atom is Trivalent
II) Electrons are Majority & Holes are Minority charge carriers. $n_e > n_h$	II) Electrons are Minority and holes are Majority Charge carriers $n_h > n_e$
III) Impurity atom is known as Donor atom	III) Impurity atom is known as acceptor Atom.
IV) Donor level is formed just below the conduction band	IV) Acceptor level is formed just above the valence band
V) Conduction is Mainly due to electrons	V) Conduction is Mainly due to holes.

P-N junction diode:- when P-type crystal is placed in contact with n-type crystal then common surface of contact of P & n type semiconductor is known as P-N junction. diode.

Depletion region & Potential barrier:-



when a P-N junction is formed, holes move from p to n region and electrons move from n to P region through the junction (due to difference in concentration of charge carrier in two region).

* The holes and electrons diffusing towards each other combine near the junction. Thus a layer is formed near the junction (with junction in the middle), which doesn't have any type of free charge carrier and is called depletion Region.

* Depletion Region prevent the further movement of electron & holes through the junction.

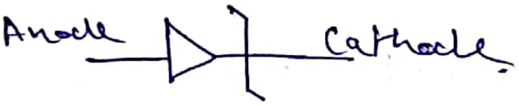
* Thus a barrier is setup in P-N junction against the movement of charge carrier.

Note:- I) For Ge it is 0.3 V II) For Si it is 0.7 V.

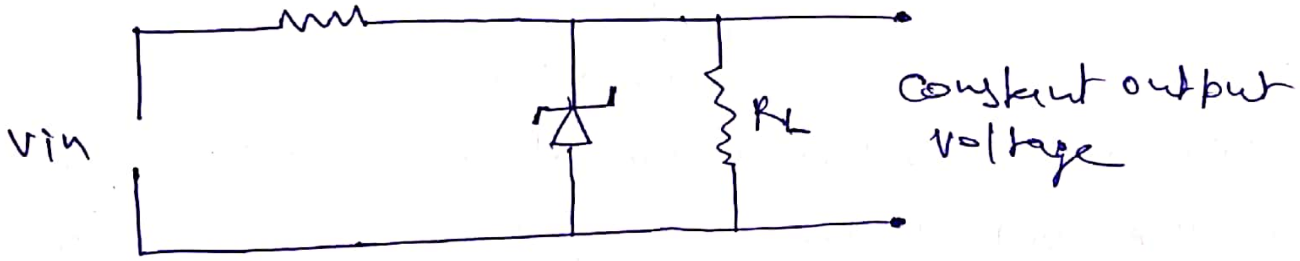
III) Magnitude of potential barrier depend on nature of semiconductor & doping concentration.

~~(IV) [illegible] depletion [illegible] about [illegible]. barrier for Si~~

Zener Diode:- This diode consist of special heavily doped P-n junction, designed to conduct in reverse direction when a certain specified voltage is reached.



Zener diode as voltage Regulator:- The circuit diagram using zener diode as voltage Regulator is shown in fig.



→ ~~Ex~~. When input voltage increase, resistance of zener diode decrease (due to breakdown of zener Diode) and hence current through zener diode increase.

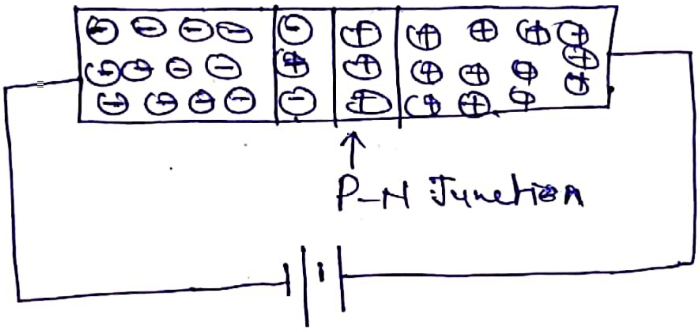
→ AS a Result of this large voltage drop occurs across dropping resistance R. Hence output voltage across RL remains constant.

→ when input voltage decrease:- resistance of zener diode increase and hence current through zener diode decrease. So small voltage drop takes place across R. Hence output voltage RL maintained constant.

Biasing :- Applying an External Potential Difference on the faces of junction is called Biasing.

It is of two type -

1) **Forward Biasing** :- In this biasing Negative terminal of the battery is connected to 'n' region and Positive terminal is connected to p- region.



Characteristics :-

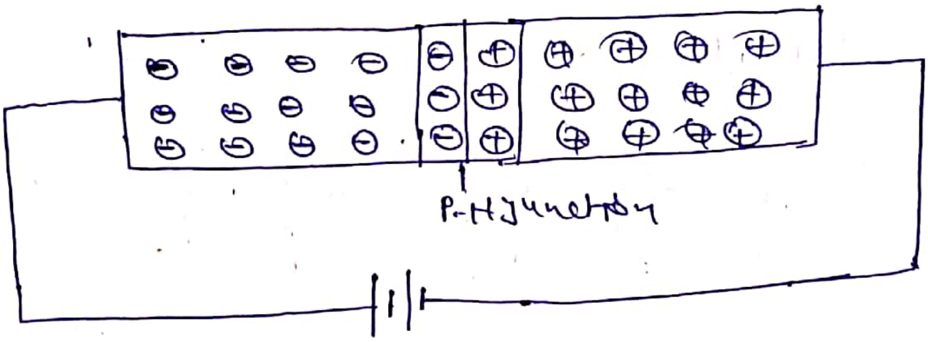
I) A current of mA order flows through the junction.

II) In Semiconductor current is due to both type of Majority charge carrier.

III) In forward biasing diode offer low resistance and width of depletion region decrease.

IV) Resistance of P-N Junction Diode is Non-ohmic

ii) **Reverse Biasing:-** In this biasing +ve terminal of the battery is connected to n-type Semiconductor and -ve terminal is connected to p-type Semiconductor.



Characteristics:- i) A small current of μA order flows through the junction due to the movement of charge carrier.

ii) In external circuit current is due to free electrons.

iii) In reverse biasing P-N junction offers high resistance and width of depletion region increase.

iv) In reverse biasing current increase suddenly at a particular reverse biased voltage known as breakdown voltage. This Phenomenon is known as avlenche breakdown. At this voltage diode may damage.

P-N Junction (Energy band diagram with Fermi Energy)

I) P-N Junction (No bias).

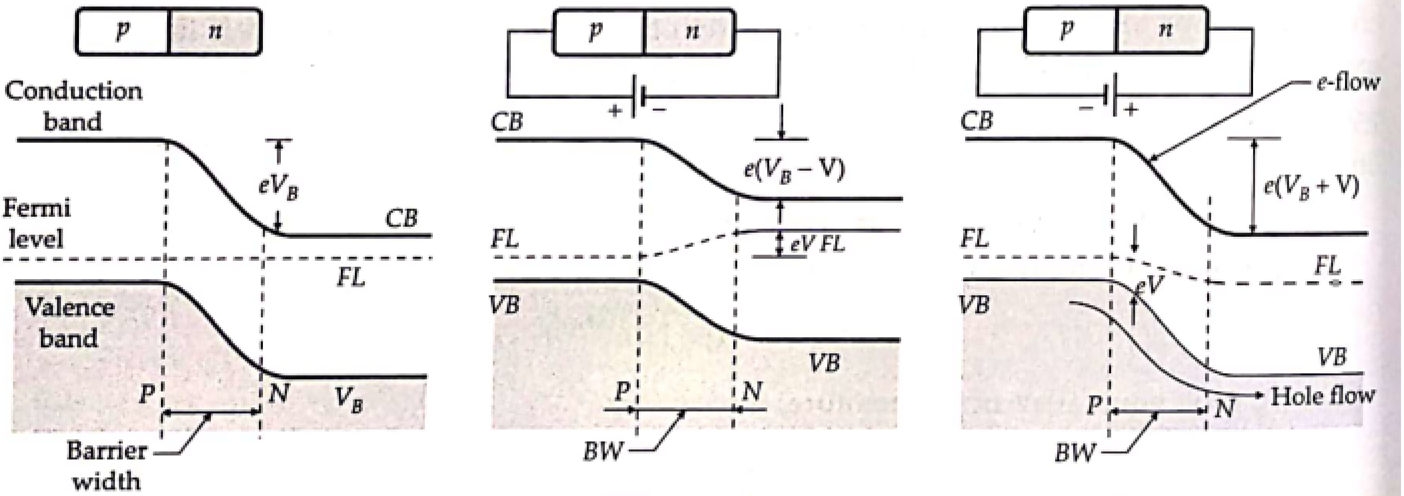
When P-N junction is in Equilibrium, number of carrier diffusing from P side to N-side is Equal to Number of carrier diffusing from N to P side. consequently there is no current across junction.

II) P-N-Junction (Forward bias)

Fermi level rise by eV and their Energy band adjust their position so as to suit the elevation of Fermi level. Due to increase in Energy on N-side potential barrier is reduced to $e(V_B - V)$

III) P-N-Junction: (Reverse Bias)

It lower the Fermi level on N-side by an amount of eV raising the barrier height $e(V_B + V)$ and increasing the depletion width too. consequently current is very much Reduced in Reverse biasing of P-N junction



(a) No bias (b) Forward bias (c) Reverse bias

Important

Kronig Penny Model:-

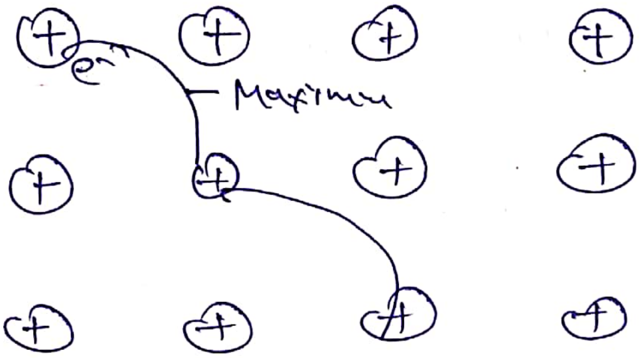
In order to find the allowed energy of electrons in Solids, we Must Solve the Schrodinger Equation for an electron in ~~Solids~~ a crystal lattice.

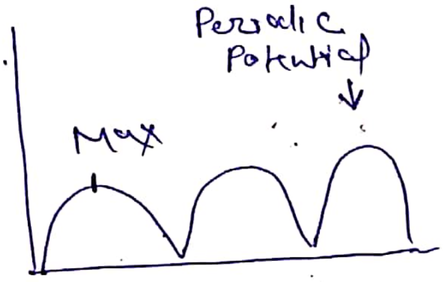
"Kronig & Penney Suggested a Simplified Model Consisting of an infinite row of rectangular Potential well. Each well represent an approximation to the Potential Produce by one ion."

OR

Kronig Penny Model is a Simplified Model for electron in one Dimensional Periodic Potential.

Let us consider a crystal lattice, let us discuss the variation of Potential Energy in a crystal lattice.



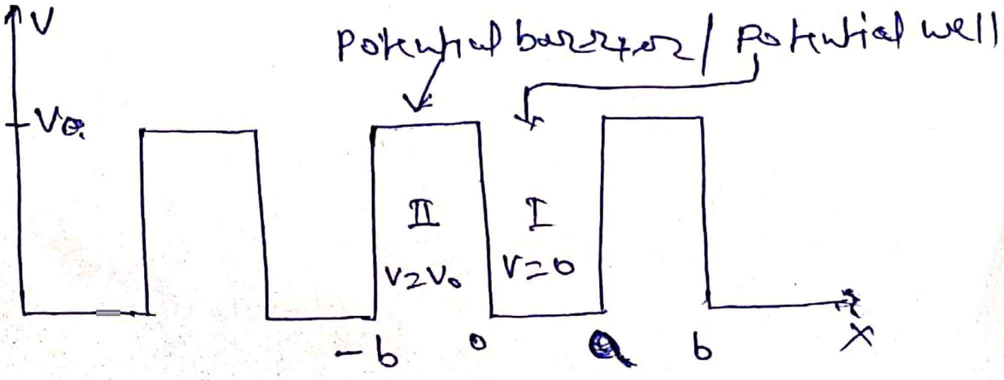


The Highest Potential is Halfway between the Atoms.

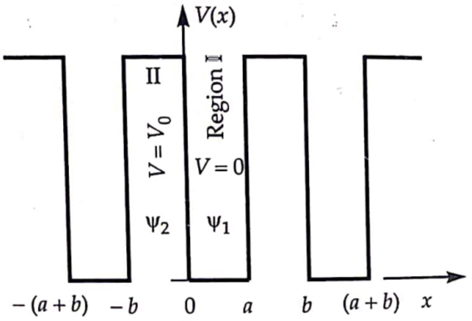
Kronig Penny Consider these Periodic Potential as Rectangular Step.

Potential barrier Potential = Maximum

Potential well Potential = 0



$$\begin{cases} V=0\ , & 0<x<a & \text{Region-I} \\ V=V_0\ , & -b<x<0 & \text{Region-II} \end{cases}$$



For region I Schrodinger wave Equ^n is

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

$V=0 \Rightarrow$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m E\psi}{h^2} = 0 \quad -①$$

For Region-II Schrodinger wave Equ^n is-

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m(E-V_0)}{h^2}\psi = 0 \quad -②$$

Let $\alpha^2 = \frac{8\pi^2 m E}{h^2}$ $-③$ $\qquad -\frac{8\pi^2 m(E-V_0)}{h^2} = \beta^2$ $-④$

Using ③, ④ in ① & ②

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad -⑤$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad -⑥$$

Also let $\psi = e^{ikx}u_k(x)$ $-⑦$

being a periodic function.

Now General solution of Equation ⑤ & ⑥ will be-

$$u_1(x) = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+kx)x} \quad — ⑧$$

$$u_2(x) = Ce^{(\beta-ikx)} + De^{-(\beta+ik)x} \quad — ⑨$$

Solving the above Equation we get

$$\boxed{\frac{P}{\alpha a}\sin\alpha a + \cos\alpha a = \cos ka} \quad — ⑩$$

↓

Kronig - Penny Model Equation.

where $P \rightarrow$ Strength with which electrons in a crystal are attracted to the ions on the crystal lattice site

a - Interatomic Distance.

Now CASE-I

when $P = 0$

From ⑩ $\cos\alpha a = \cos ka$.

$\Rightarrow \alpha a = ka$

$\alpha = \cancel{k}\, K$

$\alpha^2 = \cancel{k^2}\, k^2$

$$\frac{8\pi^2 mE}{h^2} = \left(\frac{2\pi}{\lambda}\right)^2$$

$$\frac{8\pi^2 mE}{h^2} = \left(\frac{2\pi}{h/p}\right)^2$$

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

- * value of E indicate that Energy of Electron is kinetic Energy.
- * Hence Electron can move freely
- * It indicate Nature of Conductor

CASE-II $P = \infty$

From ⑩

$$\frac{\sin\alpha a}{\alpha a} + \frac{\cos\alpha a}{P} = \frac{\cos ka}{P}$$

$\Rightarrow \sin\alpha a = 0$

$\sin\alpha a = \sin n\pi$

$\alpha a = n\pi$

$\alpha^2 = \frac{n^2\pi^2}{a^2}$

$$\left(\frac{8\pi^2 mE}{h^2}\right) = \frac{n^2\pi^2}{a^2}$$

$$\boxed{E = \frac{n^2h^2}{8ma^2}}$$

- * n - order, m - Mass of e^-
- * This Eqnⁿ of Energy is similar to potential well Equation
- * Value of E indicate potential well.
- * Potential well indicate bound electron
- * It indicate Nature of Insulator.

Important

Brillouin zones!- 1) In one Dimensional lattice

Volume around the origin covered by Bragg's Plane called Brillouin zones.

(Note:- Bragg's Plane is Perpendicular drawn between two lattice points).

OR

The Electron moving in a Perfect Periodic ~~lattice~~ Potential lattice can have Energy only in the allowed region called zones.

OR

In the k-space (k is Propagation constant), the graph between Energy (E) & k is discontinuous, The volume between these discontinuties is known as Brillouin zones.

These discontinuities in one dimensional lattice occurs when $k = \frac{n\pi}{a}$, where k is Negative or positive integer.

$$k = \pm\frac{\pi}{a}, \pm\frac{2\pi}{a}, \pm\frac{3\pi}{a}, \pm\frac{4\pi}{a} ---$$

The first reflection and the first Energy gap occurs at $k = \pm\frac{\pi}{a}$ because the wave reflected from one atom in a linear lattice interfer constructively with the Nearest Neighbouring atom,

Then the segment $-\frac{\pi}{a} \leq k < +\frac{\pi}{a}$ calle first Brillouin zone.

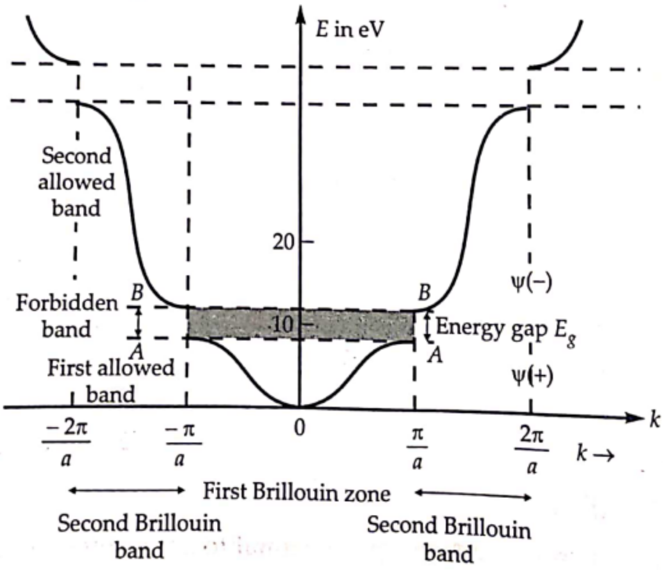
The Second Reflection and second Energy gap occur at $k = \pm\frac{2\pi}{a}$

∴ k space between $-\frac{2\pi}{a}$ to $-\frac{\pi}{a}$ and $+\frac{\pi}{a}$ to $+\frac{2\pi}{a}$

OR $-\frac{2\pi}{a} \leq k - \frac{\pi}{a}$ and $+\frac{\pi}{a} \leq k \leq +\frac{2\pi}{a}$

Called Second Brillouin zone. —— etc

The first and second Brillouin zone and Energy gap are shown by plotting value of E & K as shown below.



The first and second BZ and energy gap.

II) Two Dimensional lattice.

Consider X–Y plane be the square ABCD. The boundries of square is given by -

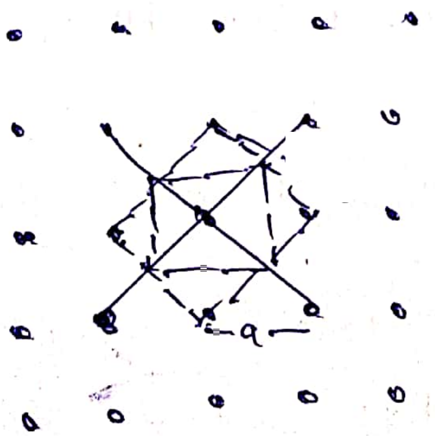
$$k_x = \pm\frac{\pi}{a}, \quad k_y = \pm\frac{\pi}{a}$$

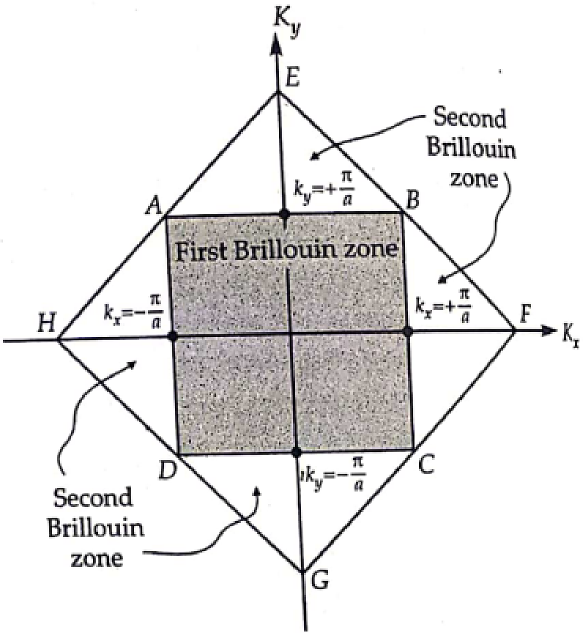
is first Brillouin zone.

Now the boundries of second square EFGH is given by -

$$k_x = \pm\frac{2\pi}{a}, \quad k_y = \pm\frac{2\pi}{a}.$$

is second Brillouin zone.





First and second BZ in 2D lattice.

Effective Mass!- * Important

Mass exhibited by an electron when inside the Semi Conductor is called Effective Mass.

OR

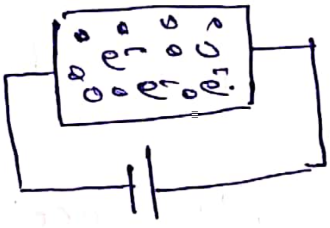
Deviation of electron behaviour in the crystal lattice from free electron behaviour can be taken into account by considering the Electron to have Effective Mass M^*.

$$\boxed{\frac{1}{M^*} = \frac{4\pi^2}{h^2}\frac{d^2E}{dk^2}}$$

$M^* \rightarrow$ Effective Mass.

Electron moving inside the Semi Conductor is moving under the influence of atom and other electrons.

Due to this Electrostatic field act on electron known as crystal field. This is called internal Electric field. This result effective mass of e^- (M^*).



Derivation:- Accounding to quantum theory e^- moving with velocity v is equivalent to wave packet (group of wave) moving with v_g (group velocity). i.e.

$$\Rightarrow v = v_g = \frac{d\omega}{dk} \quad -①$$

Also $E = h\nu = \frac{h}{2\pi} \times 2\pi\nu \Rightarrow \boxed{E = \hbar\omega}$ $-②$

Diff ② wrt k we get.

$$\frac{dE}{dk} = \hbar\frac{d\omega}{dk} \Rightarrow \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} \quad -③$$

Comparing ① & ③ we get $v = \frac{1}{\hbar}\frac{dE}{dk}$ $-④$

Now According to de broglie hypothesis.

$$\lambda = \frac{h}{p}$$

$$p = \frac{h}{\lambda} \Rightarrow \frac{h}{\lambda} \times \frac{2\pi}{2\pi}$$

$$\Rightarrow p = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k$$

$$p = \hbar k$$

Diff wrt t

$$\frac{dp}{dt} = \hbar \frac{dk}{dt} \Rightarrow F = \hbar \frac{dk}{dt}$$ (By Newton Second Law $F = \frac{dp}{dt}$).

$$\Rightarrow \hbar \frac{dk}{dt} = F = eE \quad -⑤$$

Now Diff ④ wrt t we get.

By ④

$$v = \frac{1}{\hbar} \frac{dE}{dk} \Rightarrow \frac{dv}{dt} = \frac{1}{\hbar} \frac{d^2E}{dk^2} \frac{dk}{dt} \quad -⑥$$

from ⑤ $$\frac{dk}{dt} = \frac{F}{\hbar}$$

Also Acceleration $a = \frac{dv}{dt}$

from ⑥ $$a = \frac{1}{\hbar} \frac{d^2E}{dk^2} \frac{dk}{dt}$$

$$a = \frac{1}{\hbar} \frac{d^2E}{dk^2} \frac{F}{\hbar}$$

$$\frac{a}{F} = \frac{1}{\hbar} \frac{d^2E}{dk^2}$$

Taking $a/F = m^*$ we get

$$\boxed{m^* = \frac{1}{\hbar} \frac{d^2E}{dk^2}}$$ - Effective Mass.

If $m^* = m$ then electron in crystal behaves a free electron.

Example 6.3 *The energy near the valence band edge of a crystal is given by* $E = -10^{-39}k^2\ Jm^2$. *An electron with wave vector* $10^{10}\ \hat{k}_x\ m^{-1}$ *is removed from an orbital in the completely filled valence band. Determine effective mass and momentum.*

Solution. Given : $E = -10^{-39}k^2$. Hence $\frac{d^2E}{dk^2} = -2\times10^{-39}$

Effective mass of the electron

$$m^* = \hbar^2 / \frac{\partial^2 E}{\partial k^2} = -\frac{(1.05\times10^{-34})^2}{2\times10^{-39}} = -5.5\times10^{-30}\,\text{kg}$$

Momentum of electron $= \hbar k = 1.05\times10^{-34}\times10^{10}\hat{k}_x \quad = 1.05\times10^{-24}\hat{k}_x\ \text{Js m}^{-1}$.

Comparison between Ordinary Diode and Zener Diode

S.No.	*Ordinary Diode*	*Zener Diode*
1.	Ordinary diode is operated in forward biased condition.	Zener diode is always operated in reverse biased condition.
2.	It utilizes the forward characteristics.	It utilizes, the reverse characteristics. In forward bias it acts like a *PN* junction diode.
3.	It does not have any sharp breakdown voltage.	If property doped, it has a sharp breakdown V_Z.

Fermi level :-

The Maximum Energy that electron may posses at 0K is the Fermi Energy (E_F).

" Fermi level is the surface of the sea of electron at Absolute zero, where no electron will have enough energy to rise above the surface."

Now in order to know how many of Electronic Energy State in the valence band and conduction band will be occupied at different temperature Fermi-factor $f(E)$ is introduce as -

$$f(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1}$$

where k_B - Boltzmann constant

T - Temperature in K

E_F - fermi level of Energy in eV.

E - given Energy occupied by Electron under condition of thermal Equilibrium.

Now I) $E > E_F$ & $T = 0$ $\quad f(E) = \frac{1}{1 + \exp(\infty)} = 0$

II) $E < E_F$ & $T = 0$ $\quad f(E) = \frac{1}{1 + \exp(-\infty)} = 1$

III) $T = TK$ and $E = E_F$

$$f(E) = \frac{1}{e^0 + 1} = \frac{1}{2}$$

which means when temperature is not

which means when temperature is not ~~0~~ 0K but some higher value say T=1000K then some ~~electrons~~ covalent bond will break and some electron will transfer to conduction band.

Example 6.7 *Fermi energy of an intrinsic semiconductor is 0.6 eV. The low lying energy level in the conduction band is 0.2 eV above the Fermi level. Calculate the probability of occupation of this level by an electron at room temperature.*

Solution. Given $E_F = 0.6$ eV, then $E = (0.6 + 0.2)$ eV $= 0.8$ eV

The probability of occupation of an energy level by an electron is given by the F-D distribution law

$$f(E) = \frac{1}{1 + \exp\frac{E - E_F}{k_B T}} = \frac{1}{1 + \exp\frac{(0.8 - 0.6)\,\text{eV} \times 1.6 \times 10^{-19}\,\text{J}}{1.38 \times 10^{-23}\,\text{JK}^{-1} \times 300\,\text{K}}}$$

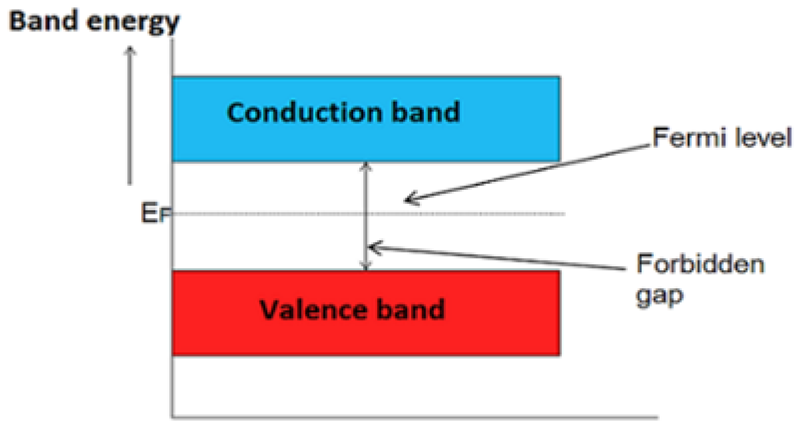
$$= \frac{1}{1 + \exp 7.7} = 0.0004 = 0.04\ \%$$

Fermi level in Intrinsic Semiconductor:-

* In Intrinsic or pure semiconductor, the number of holes in valence band is equal to number of electrons in conduction band.

* The probability of occupation of energy levels in conduction band and valence band are equal.

* Fermi level for intrinsic semiconductor lies in the middle of forbidden band.



Fermi level for intrinsic semiconductor is given as-

$$E_F = \frac{E_C + E_V}{2}$$

where E_F — Fermi level

E_C - Conduction band.

E_V - valence band.

Fermi level in extrinsic semiconductor:-

* In. extrinsic semiconductor, the number of electron in conduction band and number of holes in valence band are not equal.

* Hence, the probability of occupation of energy in conduction. band and. valence band are not equal.

* Fermi level for extrinsic semiconductor lies close to the conduction or valence band.

1) Fermi level in n-type semiconductor:-

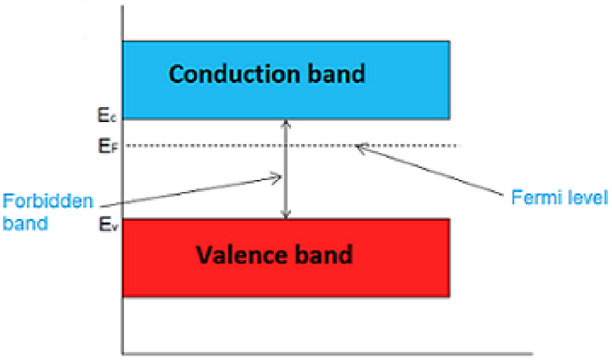
* At room temperature, the number of electrons in conduction band is greater than number of holes in valence band.

* Probability of occupation of energy levels by electron in the conduction band is greater than the Probability of occupation of energy levels by holes in valence band.

* Therefore the Fermi level in n-type semiconductor lies close to conduction band.

Fermi level for n-type Semiconductor is given as -

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



EF - Fermi level

EC - Conduction band

k_B - Boltzmann Constant

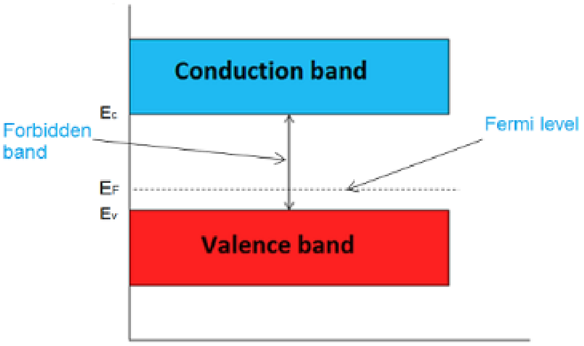
T - Absolute Temperature

Nc - Effective density of State in CB

ND - Concentration of Doner atom.

Fermi level in P-type Semiconductor:-

- * Number of holes in valence band is greater than the number of electron in conduction band.
- * Probability of occupation of Energy levels by the holes in the valence band is greater than the probability of occupation of Energy level in the Conduction band.
- * Therefore the Fermi level in P-type Semiconductor lies close to valence band.



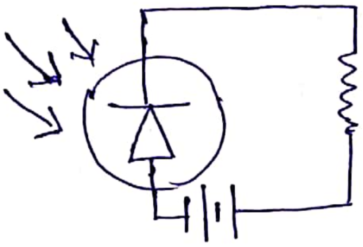
The Fermi level for P-type Semiconductor is given as -

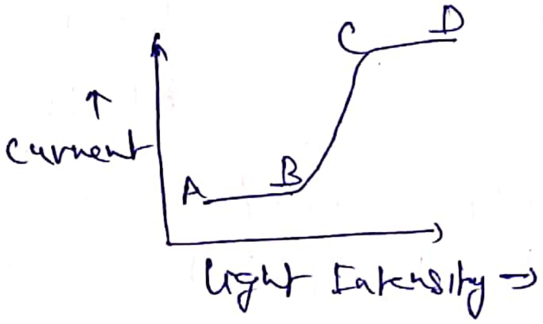
$$E_F = E_V + k_BT \log \frac{N_V}{N_A}$$

Nv - effective density of State in VB

NA - Concentration of Acceptor ion.

- **Photo diode:→** A photodiode is a p-n junction diode, Made from photosensitive semi conducting material, whose conductivity is controlled by light falling on it.





In can work in two form Photodetector as well as solar cell.

Basically Photodiode is a P-n junction diode designed to respond under Photon absorption.

There will be Absorption only if $\boxed{h\nu > E_g}$

LED:→ (Light Emitting Diode)

LED is forward bias P-n junction diode.

If we apply forward bias then. Electron Hole Pair recombine near the junction, hence recombination energy emitted in the form of Photon of Energy $\boxed{h\nu = E_g}$

→ Here we use direct band gap semi conductor such that most of light must be emitted in the form of Photon Energy of photon depends on the bandgap of semi conduct

$$E_g = h\nu$$

$$\boxed{E_g = \frac{hc}{\lambda} = \frac{1240}{\lambda\,(nm)}\ eV}$$

* LED emit incoherent Light.

Parameters of LED:-

I) **Quantum Efficiency of LED:-** It is defined as

$$Q.E = \frac{\text{Optical Power out}}{\text{Electrical Power in}} \leq 1$$

Q.E (η) = 80% means 80% of electrical power convert into optical power.

Here Power is Energy per second

E.g. Energy (per sec) = $nh\nu$

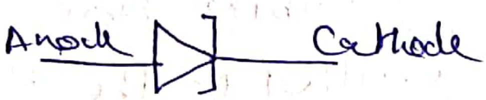
$n \Rightarrow$ no. of photons per sec.

By this formula we can calculate no. of photons/sec

II) **Slope Efficiency:-** It is defined as optical power out divided by input current.

$$\text{Slope efficiency} = \frac{\text{Optical Power out}}{\text{Input Current}} \left(\frac{W}{A}\right)$$

Tunnel Diode:- A tunnel Diode is a heavily doped PN junction Diode



→ Tunnel Diode shows negative resistance, so it can be used as amplifier, oscillators and in any switching circuits.

→ When votage value increase, current flow decrease

→ Tunnel Diode is based on tunnel Effect

→ Heavily doped P-type + n-type semiconductor in tunnel diode results in a narrow depletion region.