Module - 1 - Wave Mechanics

De-broglie waves :- According to De-broglie a moving particle is associated with a wave whose wavelength depends upon mass and velocity of the moving particle. Such waves are called De-broglie waves or matter waves.

Acc. to Debroglie

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

where h is Planck's constant

$$= 6.63 \times 10^{-34} \text{ Js}$$

m = mass of moving particle.
v = velocity of moving particle.
p = momentum of moving particle.

By Planck's theory

$$E = h\nu$$

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

$$\lambda = \frac{hc}{E} = \frac{hc}{mc^2} = \frac{h}{mc}$$

here mc = momentum of photons

Hence whatever is true for a moving particle, the same theory is applied for photons.

Numerical :- Calculate wavelength ~~momentum~~ of electrons and photons moving with velocity

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$v = 2 \times 10^8$ m/s

8d

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{9.11 \times 10^{-31} \times 2 \times 10^8}$$

$$\lambda = \frac{h}{mc} = \frac{6.63 \times 10^{-34}}{6.022 \times 10^{-23} \times 3 \times 10^8}$$

~~###~~

Kinetic Energy

$$E_k = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$$

$$p = \sqrt{2mE_k}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE_k}}$$

for a particle having charge q & accelerated through Potential difference V,

$$E_k = qV$$

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

for a particle in thermal equilibrium

$$E_k = \frac{3}{2}K_B T$$

where k_B = Boltzmann Constant
$= 1.38 \times 10^{-23}$ J/K

$$d = \frac{h}{\sqrt{3mk_BT}}$$

Wave velocity or Phase velocity :-

The velocity with which planes of constant phase propagate through the medium is known as wave velocity or phase velocity.
or the velocity of advancement of monochromatic wave is known as wave velocity or phase velocity.

Eqn of plane progressive wave is,

$$y = a\sin(\omega t - kx)$$

where, ω = angular frequency
$= 2\pi\nu = \frac{2\pi}{T}$

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

Here phase of wave is
$(\omega t - kx)$ = constant

Differentiating w.r.t time

$$\omega - k\frac{dx}{dt} = 0$$

$$\text{or, } \frac{dx}{dt} = \frac{\omega}{k} = u \text{ (phase vel.)} \text{ or } v_p$$

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Hence phase velocity is the ratio of angular frequency ω to the propagation constant K.

$$u = \frac{\omega}{K} = \frac{2\pi\nu}{2\pi/\lambda}$$

$$\boxed{u = \nu\lambda}$$

Also, $E = h\nu$

$$= \frac{hc}{\lambda} = \frac{huc}{h} \quad \boxed{\lambda = \frac{h}{mv}}$$

or, $\nu = \frac{Ec}{E}$

$$\bar{E} = \frac{hu}{\lambda}$$

$$= \frac{hu}{h} mv \quad \boxed{\lambda = \frac{h}{mv}}$$

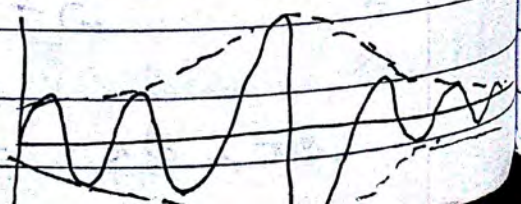
$$\bar{E} = umv$$

or, $u = \frac{\bar{E}}{mv} = \frac{mc^2}{mv} = \frac{c^2}{v}$

from above expression we find that

$$\therefore c > v,$$

phase velocity is greater than the velocity of light which is not possible. Hence to overcome this problem group velocity was calculated in which large no. of waves were assumed to travel as single group.



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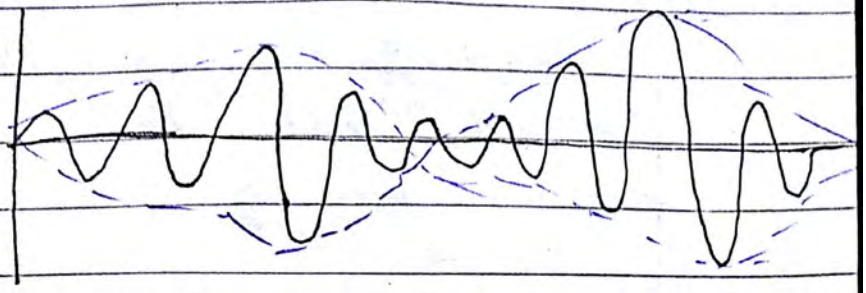
Group velocity



It is the velocity with which slowly varying envelope of modulated pattern due to group of waves travel in the medium.

Consider a group of waves consisting of two components given by

$$y_1 = a \sin(\omega_1 t - k_1 x) \quad \text{---(i)}$$

$$y_2 = a \sin(\omega_2 t - k_2 x) \quad \text{---(ii)}$$

Resultant wave,

$$y = y_1 + y_2$$

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

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

put, $\omega_1 - \omega_2 = \Delta\omega$, $k_1 - k_2 = \Delta k$

$\omega_1 + \omega_2 \simeq \omega$, $\frac{k_1 + k_2}{2} = k$

$$y = 2a \sin(\omega t - kx) \cos\left(\frac{\Delta\omega}{2} t - \frac{\Delta k x}{2}\right) \quad \text{— (3)}$$

comparing eqn (iii) with eq. (i) and (ii) we find that the amplitude of the resultant wave is

$$A = 2a \cos\left(\frac{\Delta\omega}{2} t - \frac{\Delta k x}{2}\right)$$

~~Eqn (iii)~~

Resultant wave is superposition of two components

(i) $\sin(\omega t - kx)$ which gives the expression for phase velocity

$$v = v_p = \frac{\omega}{k}$$

(ii) $\cos\left(\frac{\Delta\omega}{2} t - \frac{\Delta k}{2} x\right)$

which will give the expression for group velocity given by.

$$v_g = \frac{\Delta\omega/2}{\frac{\Delta k}{2}}$$

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

$$v_g = \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{d(2\pi/\lambda)}$$

$$= \frac{d\nu}{d(1/\lambda)} = -\frac{1}{\lambda^2} \frac{d\nu}{d\lambda}$$

(3) $$\boxed{v_g = \frac{-\lambda}{\lambda^2}\frac{dv}{d\lambda}}$$

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

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

$$\therefore \frac{\omega}{k} = \frac{E}{p}$$

$$\therefore \boxed{v_g = \frac{d\omega}{dk} = \frac{dE}{dp}}$$

Relation b/w group vel. and phase vel.

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

$$= u + k\frac{du}{dk} \quad \text{---} (1)$$

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

$$dk = -\frac{2\pi}{\lambda^2} d\lambda$$

$$\therefore \frac{dk}{dk} = -\frac{\lambda}{d\lambda} \quad \text{---} (2)$$

put (2) in eq (1)

$$\boxed{v_g = u - \lambda\frac{du}{d\lambda}}$$ for dispersive medium.

or

$$\boxed{v_g = v_p - d\lambda\frac{v_p}{d\lambda}}$$

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for non-dispersive medium, medium in which waves of all wavelength travel with same speed.

$$\frac{dv}{d\lambda} = 0$$

$$\boxed{G = \frac{dv}{d\lambda}}$$

$$\boxed{v_g = v_p}$$

X Que Prove that product of X

Relationship between phase velocity and particle velocity.

(for non-rel. case) & for free particle.

$\because u = \omega/k$. Also $\omega = 2\pi\nu$, $k = \frac{2\pi}{\lambda}$

$u = \nu\lambda$

$$= \frac{E}{h} \cdot \frac{h}{mv}$$

$$= \frac{\frac{1}{2}mv^2}{mv} \quad = \boxed{\frac{v}{2} = u}$$

$$\boxed{v_p = \frac{v}{2}}$$

Relation b/w Group vel. and particle velocity. (Non rel. case)

$$G = \frac{d\omega}{dk} = \frac{dE}{dp}$$

Here, $E = \frac{1}{2} m v^2$

$$dE = m v\, dv$$

$$p = mv$$

$$dp = m\, dv$$

$$G = \frac{dE}{dp} = \frac{m v\, dv}{m\, dv} = v$$

$$\boxed{G = v} \quad \text{or} \quad \boxed{v_g = v}$$

Rel^n between Group velocity and particle vel. (Rel. case)

$$G = \frac{d\omega}{dk} = \frac{dE}{dp}$$

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

$$2E\,dE = 2pc^2\,dp$$

$$\therefore \frac{dE}{dp} = \frac{pc^2}{E} = \frac{mvc^2}{mc^2} = v$$

$$\therefore G = \frac{dE}{dp} = v$$

or, $$\boxed{v_g = v}$$

Ques Prove that the product of phase velocity and the group velocity is equal to Square of the speed of light?

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Sol) $u = c^2$

v

$\therefore u \times v = c^2$

$\therefore \boxed{u \times G = c^2}$

Ques Calculate de-Broglie wavelength of electron and photon each of energy. 2 electron volt.

Sol) for photons $\lambda = \frac{hc}{E}$

Ques A particle of rest mass m_0 has kinetic energy K. Show that its debroglie wavelength is given by

$$\lambda = \frac{hc}{\sqrt{K(K + 2m_0c^2)}}$$

Sol)

$$\lambda = \frac{h}{mv} \quad \text{— (1)}$$

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

now Squaring both sides

$$m^2 = \frac{m_0^2}{1 - \frac{v^2}{c^2}}$$

$$m^2 \left(1 - \frac{v^2}{c^2}\right) = m_0^2$$

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$$1 - \frac{v^2}{c^2} = \frac{m_0^2}{m^2}$$

$$\frac{v^2}{c^2} = 1 - \frac{m_0^2}{m^2}$$

$$\frac{v^2}{c^2} = \frac{m^2 - m_0^2}{m^2}$$

or, $m^2 v^2 = c^2 (m^2 - m_0)$

$\therefore$ eqn (1) becomes,

$$\lambda = \frac{h}{\sqrt{c^2 (m^2 - m_0^2)}}$$

Multiplying and dividing by c.

$$\lambda = \frac{hc}{\sqrt{c^4 (m^2 - m_0^2)}}$$

$E_k = c^2 (m - m_0)$

$$\lambda = \frac{hc}{\sqrt{c^2 (m - m_0) c^2 (m + m_0)}}$$

$$\therefore \lambda = \frac{hc}{\sqrt{k \{ c^2 (m - m_0 + 2m_0) \}}}$$

$$= \frac{hc}{\sqrt{k \{ k + 2m_0 c^2 \}}}$$ Hence proved..

Hmf

Ques Show that when e^- are accelerated through potential difference, V, these wavelengths taking relativistic character into account

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$$\lambda = \frac{h}{\sqrt{2eVm_0}}\left(\frac{1-eV}{m_0c^2}\right)$$

Sol Relative character.

$$E_K = c^2(m - m_0)$$

$$= c^2\left[\frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} - m_0\right]$$

$$= m_0c^2\left[\frac{1}{\sqrt{1-\frac{v^2}{c^2}}} - 1\right]$$

$$= m_0c^2\left[\left(1-\frac{v^2}{c^2}\right)^{-1/2} - 1\right]$$

$$= m_0c^2\left[1 + \frac{v^2}{2c^2} - 1\right]$$

$$\boxed{E_k = \frac{1}{2}m_0v^2}$$ directly with this

then

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

$$= \frac{h}{m_0v}$$

$$\frac{}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$= \frac{h}{m_0v}\left[1-\frac{v^2}{c^2}\right]^{1/2}$$

$$= \frac{h}{m_0v}\left[1-\frac{v^2}{2c^2}\right] - (1)$$

$E_K = eV = \frac{1}{2}m_0v^2$

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$$\Rightarrow v = \sqrt{\frac{2eV}{m_0}}$$

putting this value in eqn (1)

$$= \frac{h}{\sqrt{2eVm_0}}\left(1 - \frac{eV}{m_0c^2}\right)$$ Hence proved

Ques Show that phase velocity of de-broglie waves associated with a moving particle having rest mass m_0 is given by

$$v_p = c\sqrt{1 + \left(\frac{m_0c\lambda}{h}\right)^2}$$

Ans $$\lambda = \frac{h}{mv} = \frac{h}{\frac{m_0v}{\sqrt{1 - \frac{v^2}{c^2}}}}$$

$$= \frac{h}{m_0v}\sqrt{1 - \frac{v^2}{c^2}}$$

$$= \frac{h}{m_0}\sqrt{\left[\frac{1}{v^2} - \frac{1}{c^2}\right]} \quad \text{---(1)}$$

$$\because v_p = \frac{c^2}{v}$$

$$\text{or, } \frac{1}{v} = \frac{v_p}{c^2}$$

$$\Rightarrow \frac{1}{v^2} = \frac{v_p^2}{c^4} \quad \text{---(2)}$$

putting value of v^2 in eqn (1)

$$\lambda = \frac{h}{m_0}\sqrt{\left[\frac{c^4}{v_p^2} - \frac{1}{c^2}\right]} \Rightarrow \frac{h}{m_0}\sqrt{\frac{c^4}{v_p^2 c^2}}$$

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$$\lambda = \frac{h}{m_0 c}\sqrt{\frac{v_p^2}{c^2} - 1}$$

$$\frac{m_0 c\lambda}{h} = \sqrt{\frac{v_p^2}{c^2} - 1}$$

$$\text{or, } \frac{v_p^2}{c^2} - 1 = \left(\frac{m_0 c\lambda}{h}\right)^2$$

$$\text{or } v_p = c\sqrt{1 + \left(\frac{m_0 c\lambda}{h}\right)^2}$$

Que Two particles A and B are in motion if the wavelength associated with particle A is 5×10^{-8} m/s. Calculate wavelength of the particle B if its momentum is $\frac{1}{2}$ that of A.

Sol

$$\lambda_A = \frac{h}{p_A}$$

$$\lambda_B = \frac{h}{p_B} = \frac{h}{\frac{p_A}{2}} = \frac{2h}{p_A}$$

$$= 2\lambda_A$$

$$= 10^{-7} \text{ m}$$

Que Show that wavelength of 150 gm rubber ball moving with velocity 30 m/s is short enough to be determined?

Sol

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{0.15 \times 30}$$

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Q.) Energy of particle at absolute temperature T is of order of $k_B T$. Calculate wavelength of thermal neutrons at 27°C.

Given mass of deuteron = $m_p = 1.67 \times 10^{-27}$ kg

$k_B = 1.38 \times 10^{-23}$ J/K

Sol.

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mk_B T}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 1.38 \times 10^{-23} \times 302}}$$

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Heisenberg Uncertainity principle.

The simultaneous determination of exact position and momentum of small moving particles is impossible.

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

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

or, $\Delta x \cdot \Delta p \geq \frac{h}{2}$

or, $\Delta x \cdot \Delta p \approx h$

$\Delta x \equiv$ incertainity in position of particle
$\Delta p \equiv$ " " momentum.

$$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

$$\geq \frac{h}{2}$$

$$\approx h$$

$\Delta E \equiv$ uncertainity in energy of particle
$\Delta t \equiv$ " " time " "

Application of Uncertainity principle.

1) Electrons do not exist inside the nucleus

Proof: Let us assume e⁻ exist inside the nucleus.

Nuclear radius $\approx 10^{-15}$ m or 1 fm

$\therefore \Delta x \approx$ diameter of nucleus

$= 2 \times 10^{-15}$ m

$$\Delta p = \frac{h}{\Delta x}$$

$$= \frac{6.63 \times 10^{-34}}{2 \times 10^{-15}}$$

$$= 3.31 \times 10^{-19} \text{ Kg m/s}$$

$$E = \sqrt{p^2c^2 + m_0^2c^4}$$

$$E = \sqrt{(3.31 \times 10^{-19})^2 (3 \times 10^8)^2 + (9.11 \times 10^{-31})^2 (3 \times 10^8)^4}$$

$$E = 62 \text{ MeV}$$

Hence for the e^- to reside inside the nucleus 62 MeV energy is needed. However during β^- decay process it was proved that for the e^- to reside inside the nucleus 8 eV energy is needed which varies widely from our calculated result. Hence our initial assumption is wrong. Therefore e^- can not exist inside the nucleus.

2) Spectral lines have finite width.

⇒ Schroedinger Time independent Eq^n.

General differential equation of wave is

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} \quad -(1)$$

where u = phase velo.

$\psi \equiv$ wave function

Soln of eqn (1) is of form.

$$\psi = \psi_0 e^{-i\omega t}$$

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

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

putting in eqn (1)

Eqn (1) may be written as

$$\nabla^2\psi + \frac{\omega^2}{u^2}\psi = 0$$

$$\therefore \nabla^2\psi + k^2\psi = 0 \quad -(3)$$

$$\therefore k^2 = \frac{4\pi^2}{\lambda^2} = \frac{4\pi^2}{h^2}p^2$$

$$= \frac{p^2}{\hbar^2} \quad \left(\because \hbar = \frac{h}{2\pi}\right)$$

putting in eqn (3)

$$\nabla^2\psi + \frac{p^2}{\hbar^2}\psi = 0 \quad -(4)$$

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-(1) $E = K + V$

$K = E - V$

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

or, $p^2 = 2m(E - V)$

putting in eqn (4)

$$\therefore \boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0}$$

↓

Time independent SWE

-(2)

For free particle

$V = 0$

$$\therefore \boxed{\nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0}$$

↓

SWE for free particle.

Time dependent SWE

$\psi = \psi_0 e^{-i\omega t}$

$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-\omega t}$

$= -i\omega\psi$

$= -i(2\pi\nu)\psi$

$= -i\frac{2\pi E}{\hbar}\psi$

$= i\frac{E}{\hbar}\psi$

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or, $E\psi = \frac{-\hbar}{i}\frac{\partial \psi}{\partial t}$

multiply and divide by i

$= i\hbar \frac{\partial \psi}{\partial t}$ — (1)

putting value of $E\psi$

Since SWE is

$$\nabla^2 \psi + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

$$\therefore \nabla^2 \psi + \frac{2m}{\hbar^2}\left(i\hbar \frac{\partial \psi}{\partial t} - V\psi\right) = 0$$

multiply whole eqn by $\frac{\hbar^2}{2m}$.

$$\therefore \frac{\hbar^2}{2m}\nabla^2 \psi + i\hbar \frac{\partial \psi}{\partial t} - V\psi = 0$$

or, $$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi + V\psi}$$

Time dependent SWE

or, $$\boxed{E\psi = H\psi}$$

where $H = \frac{-\hbar^2}{2m}\nabla^2 + V$

$H \equiv$ Hamiltonian opesator

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~~Ortho~~ orthogonality and normalization of wave fn of ψ.

If $\int \psi^* \psi \, d\tau = 1$ (normalized)

If $\int \psi^* \psi \, d\tau = 0$ (orthogonal)

If $\psi = \sin \pi x$, $d\tau = dx$

$\psi^* = \sin \pi x$

$\psi = e^{i\theta}$

$\psi^* = e^{-i\theta}$ $d\tau = d\theta$

$\psi = \cos y + i \sin y$

$\psi^* = \cos y - i \sin y$ $d\tau = dy$

Que find out $\psi = e^{ikz}$ is an acceptable ideal function where k is some finite constant. range $-a \leq z \leq a$

Also normalize it given wave.

Physical interpretation of wave function.

wave function ψ gives the behaviour of particle at a particular position 'x', and for given instant of time 't'.

Its magnitude is large where the probability of finding the particle is high. However it has a small magnitude where the probability of finding the particle is low. In other words

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we can regard ψ as the probability of finding the particle at a given position.

Properties of wave function / Born postulate of ψ.

1. It must be finite everywhere
2. It must be single valued.
3. ψ and its first derivative must be continuous.

ques → $\psi = \sin t$ is $0 < \frac{1}{2} < \frac{\pi}{2}$

$\frac{d\psi}{dt} = \cos t$

Soln.

$\psi = e^{ikz}$

$\frac{d\psi}{dz} = ike^{ikz}$

$= ik\psi$

Que Normalise the wave fn e^{ikx} for $-a < x < a$

Sol Let $\psi = Ae^{ikx}$

$\psi^* = A^* e^{-ikx}$

$\int_{-a}^{a} \psi^* \psi \, dx = 1$

or, $\int_{-a}^{a} A^* e^{-ikx} A e^{ikx} \, dx = 1$

or, $|A|^2 \int_{-a}^{a} dx = 1$

$|A|^2 [x]_{-a}^{a} = 1$

or, $|A|^2 [2a] = 1$

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cor. $A = \frac{1}{\sqrt{2a}}$

Q. Normalise the wave function $\psi = \frac{\sin \pi x}{L}$ $0 < x < L$.

Sol. Let $\psi = A \frac{\sin \pi x}{L}$

$\psi^* = A^* \sin \frac{\pi x}{L}$

$\int_{-a}^{a} \psi^* \psi \, dx = 1$

or, $\int_{-a}^{a} A^* \sin \frac{\pi x}{L} \, A \sin \frac{\pi x}{L} \, dx = 1$

$|A|^2 \int_0^L \sin^2 \frac{\pi x}{L} \, dx = 1$

$|A|^2 \int_0^L \left[\frac{1 - \cos 2\pi x/L}{2}\right] dx = 1$

or, $\frac{|A|^2}{2} \left[x - \frac{\sin 2\pi x/L}{2\pi/L}\right]_0^L = 1$

or, $\frac{|A|^2}{2} \left[L\right] = 1$

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

$A = \frac{\sqrt{2}}{L}$ $\therefore \psi = \sqrt{\frac{2}{L}} \frac{\sin \pi x}{L}$

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Operators

1) Position operator $\hat{x}, \hat{y}, \hat{z}$
2) Energy operator,
$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

3) Hamiltonian operator
$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

4) Momentum operator

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

$$\omega = 2\pi\nu = \frac{2\pi E}{h} = \frac{E}{\hbar}$$

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

$$\psi = \psi_0 e^{-\frac{i}{\hbar}(Et - px)}$$

$$\frac{\partial \psi}{\partial x} = \frac{-i}{\hbar} p \psi_0 e^{\frac{i}{\hbar}(Et - px)}$$

or, $$\frac{\partial \psi}{\partial x} = \frac{ip\psi}{\hbar}$$

$$\therefore p\psi = \frac{\hbar}{i}\frac{\partial \psi}{\partial x}$$

multiplying and dividing by i

$$\therefore p\psi = -i\hbar \frac{\partial \psi}{\partial x}$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

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$$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$

$$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

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

Ques write down position / energy / hamiltonian and momentum operator

Ans Don't Desire operators.

Expectation values of operators

$$\langle x \rangle = \int \psi^* \hat{x} \psi \, d\tau$$

$$\langle y \rangle = \int \psi^* \hat{y} \psi \, d\tau$$

$$\langle E \rangle = \int \psi^* \hat{E} \psi \, d\tau \qquad \hat{E} = i\hbar \frac{\partial}{\partial t}$$

$$= \int \psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \psi \, d\tau$$

$$= i\hbar \int \psi^* \frac{\partial \psi}{\partial t} \, d\tau$$

$$\langle \hat{p}_x \rangle = \int \psi^* \hat{p}_x \psi \, d\tau$$

$$= \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \, d\tau$$

$$= -i\hbar \int \psi^* \frac{\partial \psi}{\partial z} \, d\tau$$

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Que find the expectation value of p and p^2 for the wave function $\psi = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$ for $0 < x < L$

Sol $\langle p \rangle = \int \psi^* \hat{p} \psi \, dx$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \left(-i\hbar \frac{\partial}{\partial x}\right)\left(\sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\right) dx$$

$$= -i\hbar \frac{2}{L} \int_0^L \sin\frac{\pi x}{L} \frac{\partial}{\partial x} \sin\frac{\pi x}{L} \, dx$$

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

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

$$= \frac{-i\hbar\pi}{L^2} \cdot \int_0^L \sin\frac{2\pi x}{L} \, dx$$

$$= \frac{-i\hbar\pi}{L^2} \left[-\cos\frac{2\pi x}{L} \Big/ (2\pi/L) \right]_0^L$$

$$= \frac{-i\hbar\pi}{L^2} \left[\frac{\cos 2\pi L}{2\pi/L} - \cos 0 \right]$$

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$$\langle p^2 \rangle = \int \psi^* (\hat{p})^2 \psi \, dx$$

$$= \int_0^L \sqrt{\frac{2}{L}} \frac{\sin \pi x}{L} \left(-i\hbar \frac{d}{dx}\right)^2 \left(\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}\right) dx$$

$$= \frac{-2\hbar^2}{L} \int_0^L \sin \frac{\pi x}{L} \frac{d^2}{dx^2} \sin \frac{\pi x}{L} \, dx$$

$$= +\frac{2\hbar^2 \pi^2}{L^2 L} \int_0^L \sin^2 \frac{\pi x}{L} \, dx$$

$$\langle p^2 \rangle = \frac{\hbar^2 \pi^2}{L^3} \int_0^L \left(1 - \cos 2\pi x/L\right) dx$$

$$= \frac{\pi^2 \hbar^2}{L^3} \left[x - \frac{L}{2\pi} \sin 2\pi x/L \right]_0^L$$

$$= \frac{\pi^2 \hbar^2}{L^2}$$

Imp Q. Find the expectation value of energy for the wave function

$$\psi = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \quad \text{for } 0 < x < L$$

Sol $\langle E \rangle = \frac{\langle p^2 \rangle}{2m}$

$$\therefore \langle p^2 \rangle = \frac{\pi^2 \hbar^2}{L^2}$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{\pi^2 \hbar^2}{2mL^2}$$

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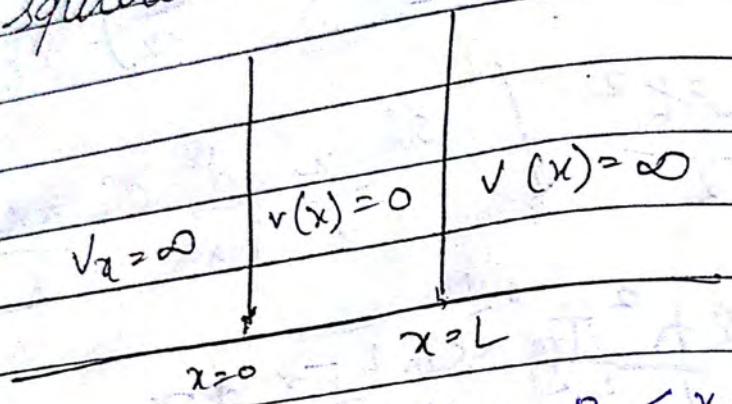
Particle in one dimensional box or square well potential.



$V(x) = 0$ for $0 < x < L$

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

So region I, is inside well, SWE is

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

or, $$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad \text{—(1)}$$

where $\alpha^2 = \frac{2mE}{\hbar^2}$ —(2)

Let soln of eqn (1) is

$$\psi = Ae^{i\alpha x} + Be^{-i\alpha x} \quad \text{—(3)}$$

Boundary conditions,

At $x = 0$, $\psi = 0$ —(4)

At $x = L$, $\psi = 0$ —(5)

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Applying (4) in (3)

$A + B = 0$

$B = -A$

∴ eq (3) may be written as,

$\psi = Ae^{-i\alpha x} - Ae^{-i\alpha x}$

$= A\left[e^{i\alpha x} - e^{-i\alpha x}\right]$

or, $\psi = A\left[\cos\alpha x + i\sin\alpha x - \cos\alpha x + i\sin\alpha x\right]$

$= 2iA\sin\alpha x$

$\boxed{\psi = A'\sin\alpha x}$ — (6) where $A' = 2iA$

Apply a boundary eqn in eqn (6)

$0 = A'\sin\alpha L$

or $\sin\alpha L = 0$

$\alpha L = n\pi \quad (n = 0, 1, 2, \ldots)$

or, $\alpha = \frac{n\pi}{L}$ — (7)

∴ eqn (8) will become,

$\boxed{\psi = A'\sin\frac{n\pi}{L}x}$ — (8)

Energy Eigen value,

From (2) and (7)

$\sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{L}$

or, $\boxed{E = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ — (9) $(n = 1, 2, 3 \ldots)$

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$$\therefore E = \frac{n^2 h^2}{8mL^2} \quad \text{--- (10)} \qquad \because \hbar = \frac{h}{2\pi}$$

$(n = 1, 2, 3 \ldots$

Significance of zero point energy

Here $n \neq 0$ because at $n = 0$ the wave function of the particle becomes zero (eqn 8) which means the particle is not present at all. This contradicts our initial assumption that atleast one particle is present inside the box.

$n \neq 0$ also means that the particle cannot have zero energy. Hence the lowest possible energy (ground state energy) which the particle can have will be when $n = 1$.

At $n = 1$

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

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

$$\left.\begin{aligned} E_2 - E_1 &= \frac{3h^2}{8mL^2} \\ E_3 - E_2 &= \frac{5h^2}{8mL^2} \end{aligned}\right\}$$

At $n = 3$, $E_3 = \frac{9h^2}{8mL^2}$

$\therefore$ energy levels are not equally distributed

Normalised wave function

$$\int_0^L \psi^* \psi \, dx = 1$$

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$$\text{or} \int_0^L A^* \sin\frac{n\pi x}{L} \; A \sin\frac{n\pi x}{L} dx = 1$$

$$\text{or,} \quad |A|^2 \int_0^L \sin^2\frac{n\pi x}{L} dx = 1$$

$$\text{or,} \quad \frac{|A|^2}{2} \int_0^L (1 - \cos 2n\pi x/L) dx = 1$$

$$\text{or,} \quad \frac{|A|^2}{2} \left[x - \frac{L \sin\frac{2n\pi x}{L}}{2n\pi} \right]_0^L = L.$$

$$\text{or,} \quad |A|^2 = \frac{2}{L}$$

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

Hence normalized wave fn is

$$\psi = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \quad \text{——— (IV)}$$

Eqn (IV) represents the normalised wave function of the particle trapped in one dimensional box of length L.

At, $n = 1$, $\psi = 0$ at $x = 0$ and $x = L$

At, $n = 2$, $\psi = 0$ at $x = 0$, $x = \frac{L}{2}$ and $x = L$

At, $n = 3$, $\psi = 0$ at $x = 0$, $x = \frac{L}{3}$, and $x = \frac{2L}{3}$ and $x = L$

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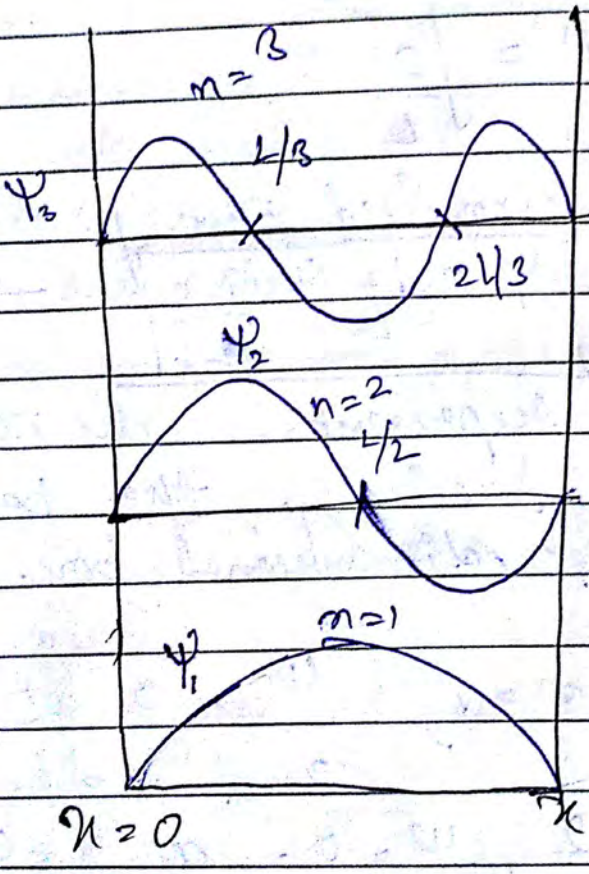
At $n=1$, two nodes are present at $x=0$ and $x=L$.

At $n=2$, 3 nodes are present at $x=0$, $x=\frac{L}{2}$ and $x=L$

At $n=3$, 4 nodes are present at $x=0$, $x=\frac{L}{3}$, $x=\frac{2L}{3}$ and $x=L$.

Hence we concluded that there are $(n+1)$ nodes for each value of n.



Probability $P = |\psi|^2$

$$= \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

Probability max when

$$\frac{n\pi x}{L} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2} \ldots$$

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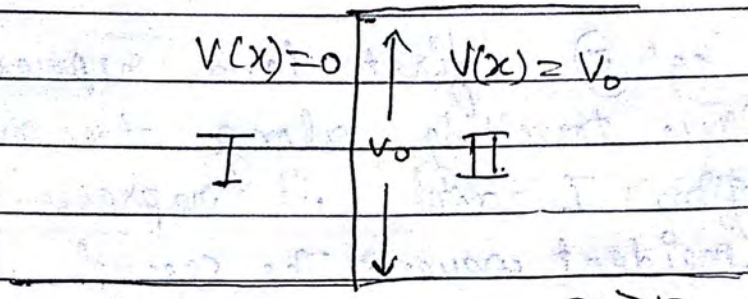
or, $x = \frac{L}{2\pi}, \frac{3L}{2\pi}, \frac{5L}{2\pi}$ ---

Step potential
or
Finite square well
or
Potential Barrier.



$V(x) = 0$ for $x < 0$
$V(x) = V_0$ for $x > 0$

Schrodinger wave eqn in region I,

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2} E\psi_1 = 0$$

or, $$\frac{d^2\psi_1}{dx^2} + \frac{p_1^2}{\hbar^2}\psi_1 = 0 \quad \text{---(1)}$$

where $p_1^2 = 2mE$ --- (2)

SwE in region II $(E - V_0)\psi_2$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2} = 0$$

or, $$\frac{d^2\psi_2}{dx^2} + \frac{p_1^2}{\hbar^2}\psi_2 = 0 \quad \text{--- (3)}$$

where $p_2^2 = 2m(E - V_0)$ — (4)

Soln of eqn (1) and (3) is,

$$\psi_1 = Ae^{ip_1 x/\hbar} + Be^{-ip_1 x/\hbar} \quad \text{— (5)}$$

$$\psi_2 = Ce^{ip_2 x/\hbar} + De^{-ip_2 x/\hbar} \quad \text{— (6)}$$

In eqn (5) first term represents the wave travelling along +ve axis in region I and it represents the incident wave. The second term represents the wave travelling along -ve x-axis in region I and it represent the reflected wave.

In eqn (6) first term represents the wave travelling along +ve x-axis in region II and it represents the transmitted wave. Since region II is a continuous region. Hence nothing is reflected back in the region II. Hence the second term of region II should not exist. Hence the wave function of the particle in region II will be given by

$$\psi_2 = Ce^{ip_2 x/\hbar} \quad \text{— (7)}$$

Here A, B & C are constants which are determined by the boundary condition

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Boundary condition,

$$\psi_1 = \psi_2 \quad \text{at } x = 0. \quad \text{—(8)}$$

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad \text{at } x = 0 \quad \text{—(9)}$$

—(5)

—(6) Applying boundary condition 8 in eqn (5) and (7)

$$A + B = C \quad \text{—(10)}$$

$$\frac{d\psi_1}{dx} = \frac{ip_1}{\hbar}\left[Ae^{ip_1x/\hbar} - Be^{-ip_1x/\hbar}\right] \quad \text{—(11)}$$

$$\frac{d\psi_2}{dx} = \frac{ip_2}{\hbar} Ce^{ip_2x/\hbar} \quad \text{—(12)}$$

Applying (9) in eq (11) and (12),

$$\frac{ip_1}{\hbar}[A - B] = \frac{ip_2}{\hbar} C.$$

$$\text{or } A - B = \frac{p_2}{p_1} C \quad \text{—(13)}$$

adding eqn (10) and (13)

$$2A = \left(1 + \frac{p_2}{p_1}\right) C$$

$$\text{or, } 2A = \left(\frac{p_1 + p_2}{p_1}\right) C$$

$$\text{or, } \boxed{\frac{C}{A} = \frac{2p_1}{p_1 + p_2}} \quad \text{—(14)}$$

$$\frac{B}{A} = \frac{p_1 - p_2}{p_1 + p_2}$$

Reflectance = R = $\frac{\text{Magnitude of reflected}}{\text{"}\quad\text{"}\quad\text{incident wave}}$

Transmittance T = $\frac{\text{magnitude of transmitted}}{\text{"}\quad\text{"}\quad\text{incident wave}}$

Case I when $E > V_0$

$p_2 \equiv$ real

$$R = \left|\frac{B}{A}\right|^2 = \left(\frac{p_1 - p_2}{p_1 + p_2}\right)^2$$

$$T = \left|\frac{C}{A}\right|^2 = \left(\frac{2p_1}{p_1 + p_2}\right)^2$$

$R + T = 1$

When $E = V_0$,

$p_2 = 0$

$R = 1$

$T = 0$

- B

Probability current density

$$(S_x)_I = \frac{\hbar}{2im}\left[\psi_1^* \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx}\right]_{A_1}$$

After this we can directly work result

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$$\psi_1 = Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar}$$

$$\psi_1^* = A^*e^{-ip_1x/\hbar} + B^*e^{ip_1x/\hbar}$$

wave

$$\frac{d\psi_1}{dx} = \frac{ip_1}{\hbar}\left[Ae^{ip_1x/\hbar} - Be^{-ip_1x/\hbar}\right.$$

wave

$$\frac{d\psi_1^*}{dx} = -\frac{ip_1}{\hbar}\left[A^*e^{-ip_1x/\hbar} - B^*e^{ip_1x/\hbar}\right]$$

$$= \frac{\hbar}{2im}\left[(A^*e^{-ip_1x/\hbar} + B^*e^{ip_1x/\hbar})\frac{ip_1}{\hbar}\right.$$

$$\left.(Ae^{ip_1x/\hbar} - Be^{-ip_1x/\hbar})\right.$$

$$- \left\{(Ae^{-ip_1x/\hbar} + Be^{-ip_1x/\hbar})\left(\frac{-ip_1}{\hbar}\right)(A^*e^{-ip_1x/\hbar} - B^*e^{ip_1x/\hbar})\right.$$

$$(S_x)_I = \frac{\hbar}{2im} \times \frac{ip_1}{\hbar}\left[A^*A + BA^*e^{2ip_1x/\hbar} - A^*Be^{-2ip_1x/\hbar}\right.$$

$$\left. - B^*B + AA^* + BA^*e^{-2ip_1x/\hbar} - AB^*e^{2ip_1x/\hbar} - BB^*\right]$$

$$= \frac{p_1}{2m}\left[2|A|^2 - 2|B|^2\right]$$

$$= \frac{p_1}{m}\left[|A|^2 - |B|^2\right]$$

$$(S_x)_{II} = \frac{\hbar}{2im}\left[\psi_2^*\frac{d\psi_2}{dx} - \psi_2\frac{d\psi_2^*}{dx}\right]$$

Ans

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$$\psi_2 = Ce^{ip_2x/\hbar}$$

$$\psi_2^* = C^* e^{-ip_2x/\hbar}$$

$$\frac{d\psi_2}{dx} = \frac{ip_2}{\hbar} Ce^{ip_2x/\hbar}$$

$$\frac{d\psi_2^*}{dx} = \frac{-ip_2}{\hbar} C^* e^{-ip_2x/\hbar}$$

$$(S_x)_{II} = \frac{\hbar}{2im}\left[\left(C^* e^{-ip_2x/\hbar}\right)\left(\frac{ip_2}{\hbar} Ce^{ip_2x/\hbar}\right) - CC^* e^{-ip_2x/\hbar}\left(\frac{-ip_2}{\hbar} C^* e^{-ip_2x/\hbar}\right)\right]$$

$$(S_x)_{II} = \frac{p_2}{2m}\left[2|C|^2\right]$$

$$(S_x)_{II} = \frac{p_2}{m}|C|^2$$

$$R = \frac{p_1/m\ |B|^2}{(p_1/m)|A|^2} = \frac{|B|^2}{|A|^2} = \left(\frac{p_1-p_2}{p_1+p_2}\right)^2$$

$$T = \frac{(p_2/m)|C|^2}{(p_1/m)|A|^2} = \frac{p_2}{p_1}\left(\frac{C}{A}\right)^2$$

$$= \frac{p_2}{p_1} \times \frac{4p_1^2}{(p_1+p_2)^2} = \frac{4p_1p_2}{(p_1+p_2)^2}$$

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$$R + T = 1$$

Case II when $E = V_0$

$$p_2 = \sqrt{2m(E - V_0)} = 0$$

$\therefore T = 0$

$R = 1$

Case III when $E < V_0$

$p_2 \equiv$ imaginary

$$p_2 = \sqrt{2m(E - V_0)}$$

$$= \sqrt{(-1)\,2m(V_0 - E)}$$

$$= i\sqrt{2m(V_0 - E)}$$

$$p_2^* = -i\sqrt{2m(V_0 - E)} = -p_2$$

$$(S_x)_{II} = \frac{\hbar}{2im}\left(\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}\right)$$

$$\psi_2 = C e^{i p_2 x/\hbar}$$

$$\psi_2^* = C^* e^{-i p_2^* x/\hbar} = C^* e^{i p_2 x/\hbar}$$

$$\frac{d\psi_2}{dx} = \frac{i p_2}{\hbar} C e^{i p_2 x/\hbar}$$

$$\frac{d\psi_2^*}{dx} = \frac{i p_2}{\hbar} C^* e^{i p_2 x/\hbar}$$

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$$(S_x)_{II} = \frac{\hbar}{2im}\left[(C^* e^{ip_2 x/\hbar})\left(\frac{ip_2}{\hbar} C e^{ip_2 x/\hbar}\right) - (C e^{ip_2 x/\hbar})\left(\frac{ip_2}{\hbar} C^* e^{ip_2 x/\hbar}\right)\right]$$

$$(S_x)_{II} = 0$$

$$T = 0$$

$$R = 1$$

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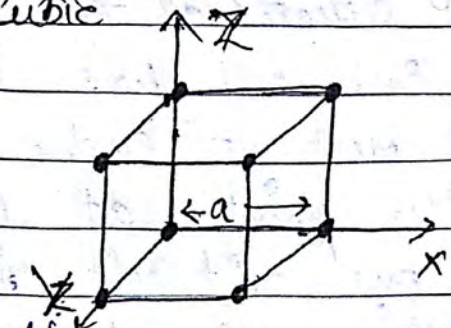
Cubic crystals

(i) Simple cubic



In this there are one lattice point per unit cell. Lattice point is situated at the corners of the cube. A unit cell containing only one lattice point is called primitive cell. Therefore simple cubic lattice is also called primitive P-lattice.

coordination no.

$$\pm a\hat{i},\ \pm a\hat{j},\ \pm a\hat{k}$$

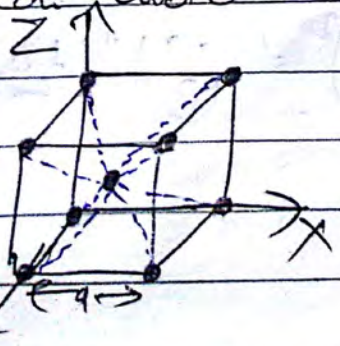
$(\pm a, 0, 0)$, $(0, \pm a, 0)$, $(0, 0, \pm a)$

$(a, 0, 0)$ $(-a, 0, 0)$
$(0, a, 0)$ $(0, -a, 0)$
$(0, 0, a)$ $(0, 0, -a)$

Distance b/w nearest neighbours

$\sqrt{a^2 + 0^2 + 0^2} = a$ (lattice constant)

(ii) Body centered cubic



there is one lattice point at each corner of the cube and one lattice point is situated at the center of the body. Each cell has 8 corners and 8 cells meet at each corner. Therefore 1 lattice point at corner belongs to one unit cell. Also there is one lattice point at centre of the body therefore total no of lattice point in any one cell.

$(1 \times 8) + 1 = 2$

Hence Bcc has 2 lattice points per unit cell.

Coordination no.

$\left(\pm \frac{a}{2}\hat{i}, \pm \frac{a}{2}\hat{j}, \pm \frac{a}{2}\hat{k}\right)$

$\left(+\frac{a}{2}, \pm\frac{a}{2}, +\frac{a}{2}\right)\left(-\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)\left(\frac{-a}{2}, \frac{-a}{2}, \frac{a}{2}\right)$

$\left(-\frac{a}{2}, \frac{-a}{2}, -\frac{a}{2}\right)\left(\frac{-a}{2}, \frac{a}{2}, \frac{-a}{2}\right)\left(\frac{a}{2}, \frac{-a}{2}, \frac{-a}{2}\right)$

$\left(\frac{a}{2}, \frac{-a}{2}, \frac{a}{2}\right)\left(\frac{a}{2}, \frac{a}{2}, \frac{-a}{2}\right)$

Distance b/w nearest neighbours

$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} \Rightarrow \sqrt{\frac{3a^2}{4}} = \frac{\sqrt{3}a}{2}$

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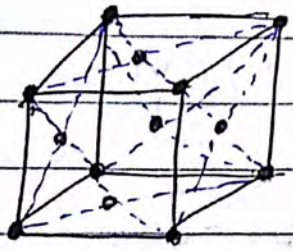
(iii) Face centered cubic lattice



In this there is one lattice point at each corner of cube and one lattice point at center of each face of the cube. Each unit cell has 8 corners and 8 cells meet at each corner. Therefore $\frac{1}{8}$ th of lattice point at corners belong to any one cell. Also there is one lattice point at center of face of the cell and it is shared by two cells. Therefore only 1 lattice point belongs to any one cell. Since a cell has 8 corners and 6 faces therefore total no of lattice point is $\left(\frac{1}{8}\times 8\right) + \left(\frac{1}{2}\times 6\right) = 4$

Coordination no: 12

$\left(\pm\frac{a}{2}\hat{i}, \pm\frac{a}{2}\hat{j}, 0\right)$ $\left(\pm\frac{a}{2}\hat{i}, \pm\frac{a}{2}\hat{k}\right)$ $\left(0, \pm\frac{a}{2}\hat{j}, \pm\frac{a}{2}\hat{k}\right)$

$\left(\frac{a}{2}, \frac{a}{2}, 0\right)$ $\left(\frac{-a}{2}, \frac{-a}{2}, 0\right)$ $\left(\frac{a}{2}, \frac{-a}{2}, 0\right)$ $\left(\frac{-a}{2}, \frac{a}{2}, 0\right)$

$\left(\frac{a}{2}, 0, \frac{a}{2}\right)$ $\left(\frac{-a}{2}, 0, \frac{-a}{2}\right)$ $\left(\frac{a}{2}, 0, \frac{-a}{2}\right)$ $\left(\frac{-a}{2}, 0, \frac{a}{2}\right)$

$\left(0, \frac{a}{2}, \frac{a}{2}\right)\left(0, -\frac{a}{2}, -\frac{a}{2}\right)\left(0, \frac{a}{2}, \frac{a}{2}\right)\left(0, -\frac{a}{2}, \frac{a}{2}\right)$

Distance b/w nearest neighbours.

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + 0} = \frac{a}{\sqrt{2}}$$

Ans Prove that for a cubic lattice constant 'a' is given by

$$a = \left(\frac{nM}{Nf}\right)^{1/3}$$

n = no. of mol per unit volume.
M = mol. wt.
N = avogadro no.
f = density.

a = lattice constant.

$\text{Vol.} = a^3$

$$f = \frac{m}{a^3}$$

$$m = \frac{nM}{N}$$

$$f = \frac{nM}{Na^3}$$

$$a^3 = \left(\frac{nM}{Nf}\right)^{1/3}$$

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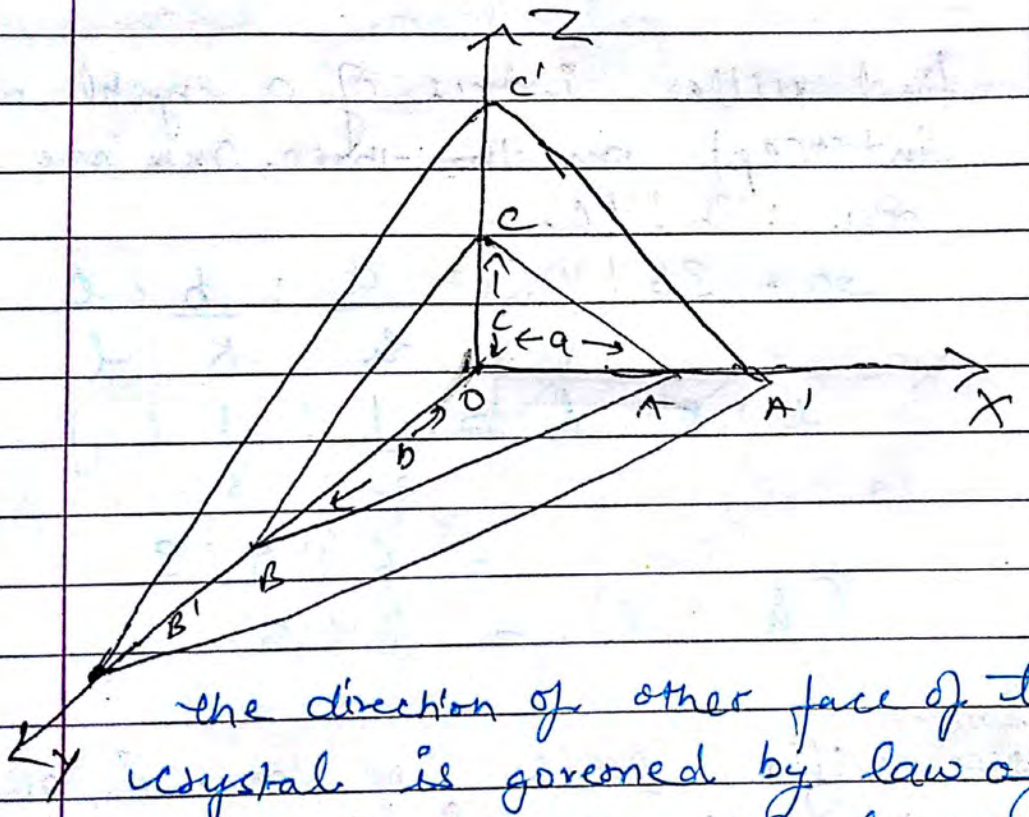
Miller Indices

Position and orientation of a lattice plane in a crystal is determined by smallest whole number. Same ratios with one another as reciprocal of intercept of the plane on three crystal axis. These are denoted by h, k, l and are called as miller indices.



The direction of other face of the crystal is governed by law of rational indices. This law states that a phase which is parallel to a plane whose intercepts on the three axis are $m_1 a$, $m_2 b$, $m_3 c$ where m_1, m_2 and m_3 are smallest whole no. is the possible face of the crystal.

If A', B', C' is the possible face of a crystal then OA : OB : OC = $m_1 a : m_2 b : m_3 c$

$$= \frac{a}{m_2 m_3} : \frac{b}{m_1 m_3} : \frac{c}{m_1 m_2}$$

$$= \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

where $h = m_2 m_3$

$k = m_1 m_3$

$l = m_1 m_2$

Qw Find miller indices of a crystal which intercept on the three axis are $2a : 3b : 4c$.

Sol $2a : 3b : 4c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$

$$h : k : l = \frac{1}{2} : \frac{1}{3} : \frac{1}{4}$$

$$= 6 : 4 : 3$$

$$(h\ k\ l) = (6\ 4\ 3)$$

Qw Deduce miller indices of plane in an orthorhombic crystal which cuts intercepts $3a, -2b, \frac{3c}{2}$.

$$3a : -2b : \frac{3c}{2} = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

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Que: An orthorhombic crystal has axial ratios in the ratio a : b : c is 0.424 : 1 : 0.367 find miller indices whose intercept are in the ratio ..

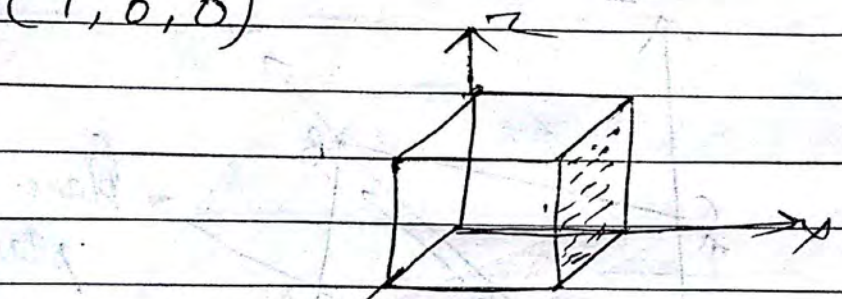
0.212 : 1 : 0.183.

Sol:

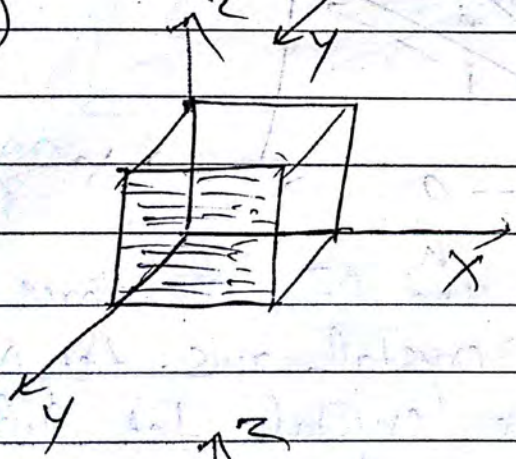
$$0.212 : 1 : 0.183 = \frac{0.424}{h} : \frac{1}{k} : \frac{0.367}{l}$$

Sketching of lattice plane

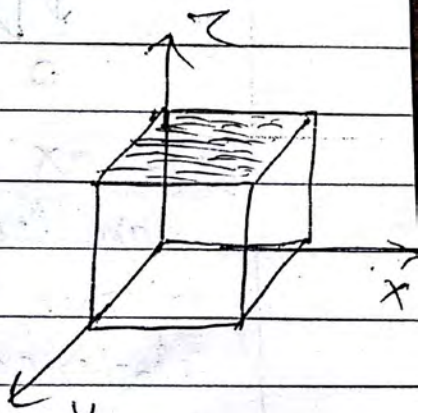
(1, 0, 0)



(0, 1, 0)



(0, 0, 1)



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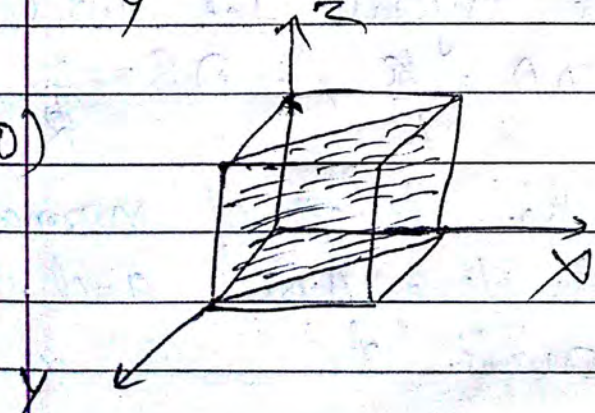

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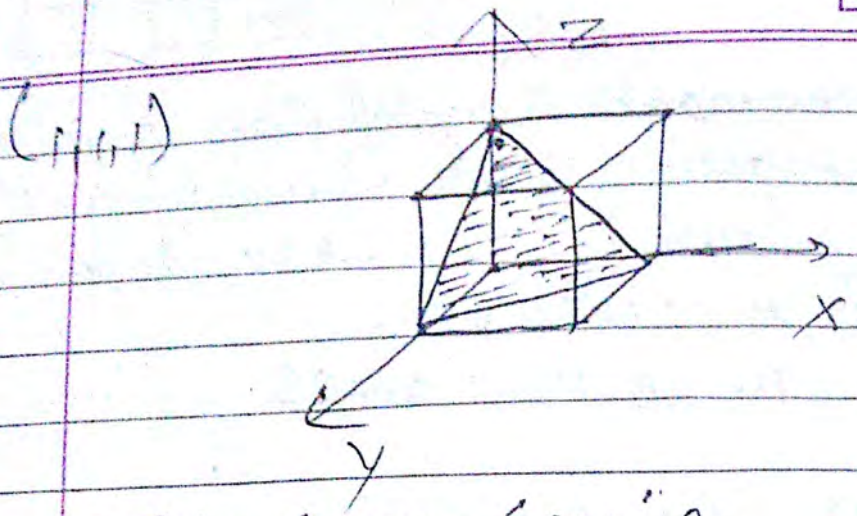
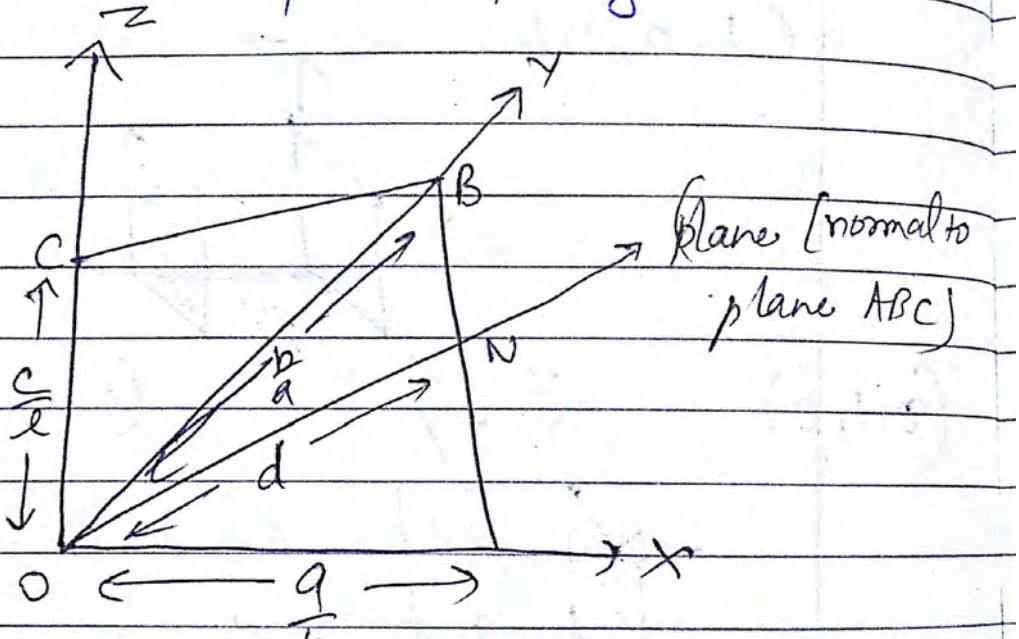


Interplanar Spacing

The separation between successive lattice planes of cubic, tetragonal and ~~orthogonal~~ orthorhombic crystal for which $\alpha = \beta = \gamma = 90°$ is called interplanar spacing.



Let OX, OY and OZ are three axis parallel to crystal axis. Let A, B, C are plane of the crystal. Let A, B, C have intercept. $OA = \frac{a}{h}$, $OB = \frac{b}{k}$, $OC = \frac{c}{l}$

Let ON is the length of normal from origin to the plane ABC and is equal to small 'd' which is called

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Interplanar spacing. Let $\theta_a, \theta_b, \theta_c$ are the angles which ON makes with the three axis

Direction cosines of ON are,

$\cos\theta_a = \frac{ON}{OA}$, $\cos\theta_b = \frac{ON}{OB}$, $\cos\theta_c = \frac{ON}{OC}$

Also,

$\cos\theta_a^2 + \cos\theta_b^2 + \cos\theta_c^2 = 1$

or, $\left(\frac{ON}{OA}\right)^2 + \left(\frac{ON}{OB}\right)^2 + \left(\frac{ON}{OC}\right)^2 = 1$

or, $\frac{d^2}{(a/h)^2} + \frac{d^2}{(b/k)^2} + \frac{d^2}{(c/l)^2} = 1$

or, $d^2\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right] = 1$

or, $\boxed{d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}}$

for cubic crystals, $a = b = c$.

$$\boxed{d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}}$$

Simple cube

$d_{100} = a$

$d_{110} = \frac{a}{\sqrt{2}}$

$d_{111} = \frac{a}{\sqrt{3}}$

$d_{100} > d_{110} > d_{111}$

$$= 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}}$$

Body centred

In BCC crystal there exist an additional plane half-way between 100 and 111 crystal

$$d_{100} = \frac{a}{2}$$

$$d_{110} = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{a}{2\sqrt{3}}$$

$$d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{\sqrt{2}} : \frac{1}{2\sqrt{3}}$$

multiplying min. by 2 $= 1 : \sqrt{2} : \frac{1}{\sqrt{3}}$

Face centred

In fcc crystals there exist an additional plane halfway between 100 and 110 plane

$$d_{100} = \frac{a}{2}$$

$$d_{110} = \frac{a}{2\sqrt{2}} \qquad d_{111} = \frac{a}{\sqrt{3}}$$

$$d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{2\sqrt{2}} : \frac{1}{\sqrt{3}}$$

multi. by 2 in min. $= 1 : \frac{1}{\sqrt{2}} : \frac{2}{\sqrt{3}}$

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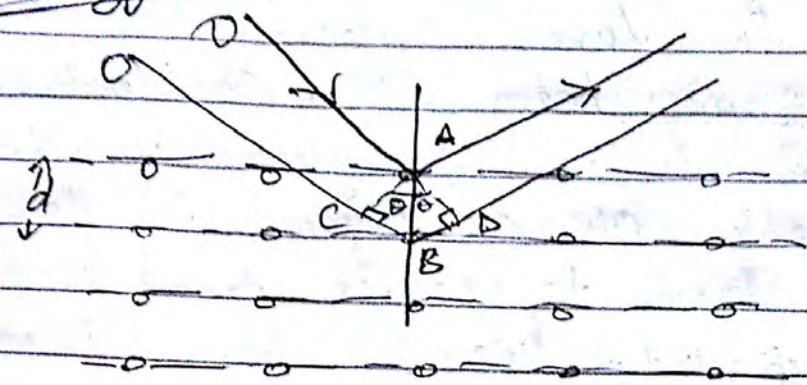
Bragg's Law



Diffraction of X-rays in crystal is called Bragg's Law

Let an X-ray beam is incident on on a crystal at point A it scattered in random directions. 'd' is the smallest separation b/w the crystals - BC and BD are perpendicular on the reflected ray.

path difference =

$$BC + BD$$
$$= d\sin\theta + d\sin\theta$$
$$= 2d\sin\theta$$

for maxima.

$$\boxed{2d\sin\theta = n\lambda}$$ Bragg's law

Laue's Experiment.

In Laue's method, a single crystal is held stationery in a continuous X-ray beam. The crystal diffracts the wavelength for w/h. the crystal plane or spacing & the incidence

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angle and satisfies the Bragg's law
in Laue's experiment, a continuous
expose beam wave coalinated by a
pin hole arrangement is allowed to
fall on a crystal. A flat film is
placed to receive transmitted and
reflected beams. The diffraction pattern
consists of a series of known as
Laue's pattern
The distribution of spots in Laue's pattern
depend upon the symmetry of crystal
and its orientation with respect to
X-ray beam.

Application:- This method is convinient for rapid
determination of crystal orientation &
symmetry. It is succeeded in Solid
State exp. It is also ~~known as~~ used to
study crystalline imperfection. Under
mechanical and thermal treatment.

In a crystal lattice there exits many sets
of planes with different orientation &
spacing with. can cause. If we draw
from a common origin, normal to all
set of planes, the length of each
normal being proportional to
the reciprocal of the interplanar
spacing, the end point of normal
form lattice. is called reciprocal lattice

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Module III Semiconductors and Super-conductors

Semiconductors - ~~[illegible]~~ free e^-, metals

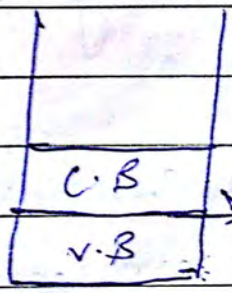
Insulators - NO free e^-, wood, plastic

Semiconductors - Si, Ge

- Intrinsic (pure Semiconductors)
- Extrinsic
  - P type (donor impurities) (B, Al)
  - N type (acceptor impurities) (As, Antimony)

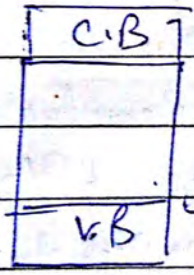
Classification of solids on bases of Band-diagram.

Conductors



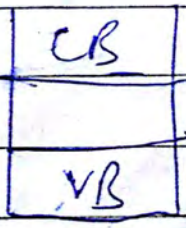
→ overlapping of C.B & V.B

Insulators

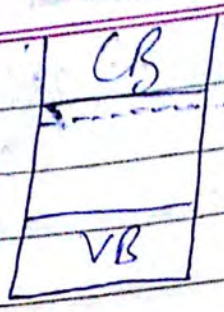


E_g = 3ev

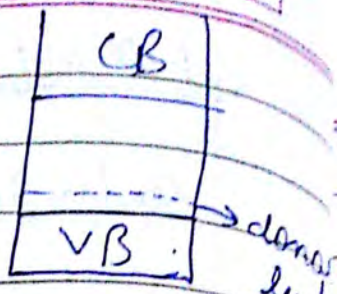
Intrinsic Semiconductor



E_g = 1ev

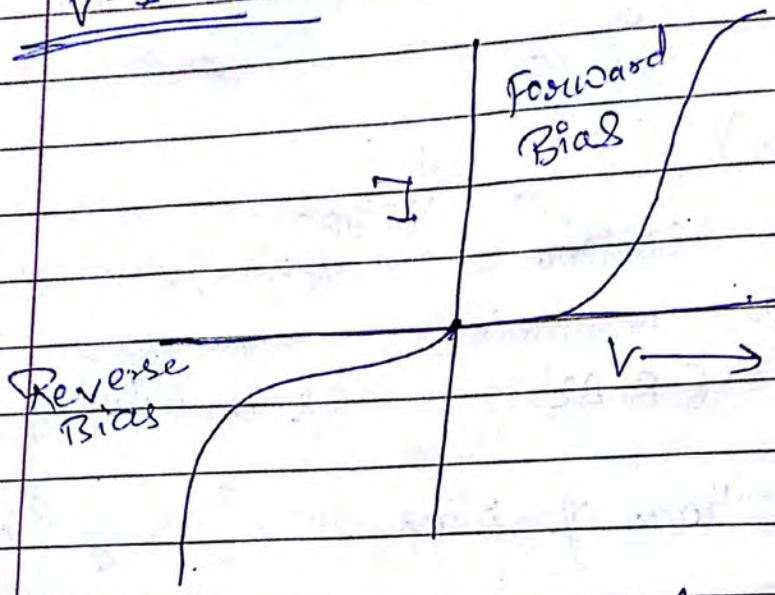


p-type semiconductor



n-type semi

V-I curve



* ~~Formation~~ position of fermi level in semiconductors

In intrinsic semiconductors fermi level lie exactly lie between conduction Band and valence Band.

In p-type semiconductor the fermi level is just below the bottom of CB

In n-type semiconductor the fermi-level lie just above the top of V.B.

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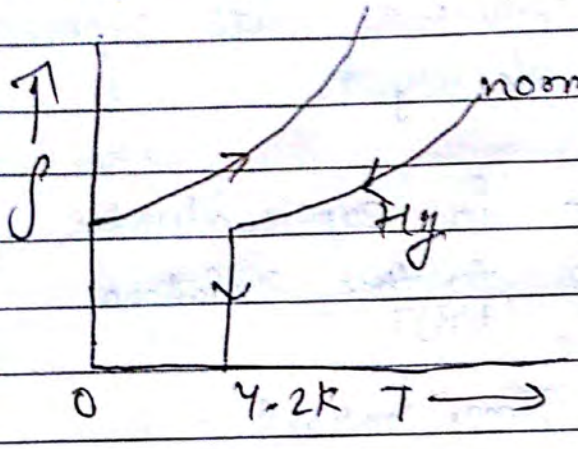
Superconductors

In 1911, Kammerling onnes of at very low temperature the resistivity of Mercury firstly decreases with the decrease in temp. but at 4.2 Kelvin the resistance suddenly drops to zero.



the temp. at which this phase ~~transist~~ transition occurs is known as critical temperature or transition temperature.

Similar observations were made for alluminium, lead, tin, In, Zn. This phenomenon of electrical resistivity at a particular transition temperature is known as superconductivity and the materials which follow this phenomenon is known as superconductors.

Properties of superconductors

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1) At room temp. superconductors have higher resistivity than normal metals.

2) Transition temp. is different for different isotopes. It decreases with the increase in atomic weight, this is known as isotopic effect in superconductors.

3) When large magnetic field is applied in the superconductors. its superconducting property is destroyed.

4) The current in superconductors flows according to the relation

$$i = i_0 e^{(L/R)T}$$

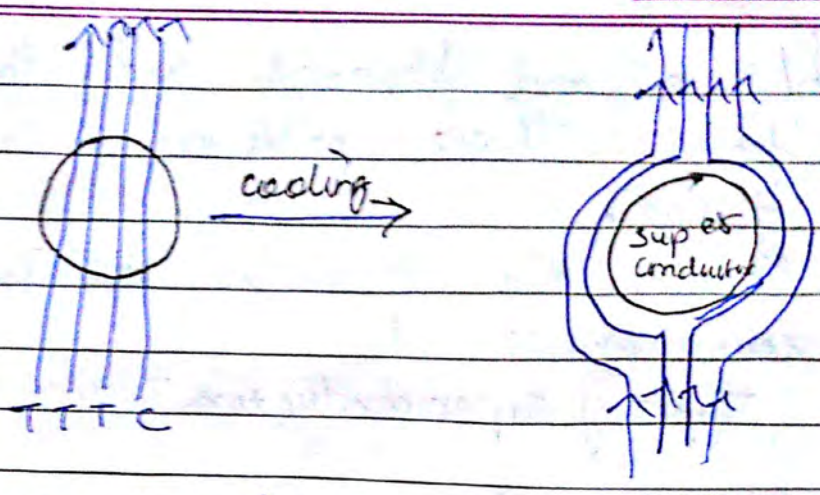
$\frac{L}{R}$ = Time constant

$$R \to 0 \quad , \frac{L}{R} \to \infty$$

the current in superconductors flows for infinite period of time till the temp. remains constant. this current is called persistent current.

Meissner effect:-

When a long superconductor is cooled it magnetic fields below critical temperature, the magnetic lines of force are pushed out of the specimens of superconductor. This phenomenon is called as meissner effect



(Normal state) $T < T_c$

$$\vec{B}_{int} = \mu_0 (\vec{H} + \vec{M})$$

where μ_0 = permeability of free space.

$\vec{H}$ = Magnetic field intensity

$\vec{M}$ = Magnetic moment per unit volume.

Here $B_{int} = 0$

$\mu_0 (\vec{H} + \vec{M}) = 0$

or, $\vec{H} = -\vec{M}$

$$\chi = \frac{M}{H}$$

$$\boxed{\chi = -1}$$

Meissner effect is a kind of diamagnetism

BCS Theory (Bardeen, Cooper and Schrieffer)

explained that just like electrons with opposite spins form pairs, there is attractive interaction

b/w e⁻ and phonons and they form pairs. These pairs are called cooper pairs.
Phonons are quanta of longitudinal sound waves.

Types of superconductors

Type I and Type II superconductors

1) In Type I superconductors, superconducting is abruptly destroyed when the strength of applied magnetic field rises above a critical value. In Type II superconductors when the magnetic field is increased above a critical value it leads to a mixed state in which an increasing amount of magnetic flux penetrates in the material but there is no electric current inside the material.

2) Type I superconductors are also called soft superconductors. Type II are called hard superconductors.

3) In Type I superconductors the diamagnetic moment drops to zero and resistivity rises to its normal value. In Type II materials the diamagnetic moment start to decrease but the resistance does not return this is called mixed state of Type II superconductors

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Density of states for free e⁻ (Derivation of exp. for fermi energy)

SWE,

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

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

for 3-Dimension

$$E_{n_x, n_y, n_z} = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$

or,

$$\frac{p^2}{2m} = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$

or,

$$n_x^2 + n_y^2 + n_z^2 = \frac{4L^2p^2}{h^2}$$

$$= \left(\frac{2L}{h}\right)^2 p^2 = R^2 \quad \text{(say)}$$

— (1)

where $\vec{R}$ = any vector from origin to any lattice point.

Allowed no° of integers in the range R & R+dR is,

$$dN = \frac{1}{8} 4\pi R^2 dR \quad \text{— (2)}$$

Since, $R^2 = \left(\frac{2L}{h}\right)^2 p^2$

$$2RdR = \left(\frac{2L}{h}\right)^2 2p\,dp.$$

or, $$dR = \left(\frac{2L}{h}\right)^2 \frac{p}{R} dp$$

$$= \left(\frac{2L}{h}\right)^2 \frac{1}{(2L/h)}\, dp$$

$$= \left(\frac{2L}{h}\right) dp$$

eqn (2) becomes,

$$dN = \frac{1}{2} 4\pi \left(\frac{2L}{h}\right)^2 \cdot p^2 \cdot \left(\frac{2L}{h}\right) dp$$

$$= \frac{4\pi L^3}{h^3} p^2 dp$$

Since e^- have two spins hence allowed no. of wavefunctions in the momentum range p and p+dp will be,

$$Z(p)dp = 2\pi p^2 dp \frac{V}{h^3} \quad \text{——(3)}$$

$\because p^2 = 2mE$

$$2p\,dp = 2m\,dE$$

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

or, $$dp = \frac{m}{\sqrt{2mE}} dE$$

eqn (3) may be written as,

$$Z(E)dE = 2\pi (2mE) \frac{m}{\sqrt{2mE}} \frac{dE\,V}{h^3}$$

$$= 4\pi (2m)^{3/2} E^{1/2} dE \frac{V}{h^3}$$

$$= \frac{4\pi V}{h^3} (2m)^{3/2} E^{1/2} dE$$

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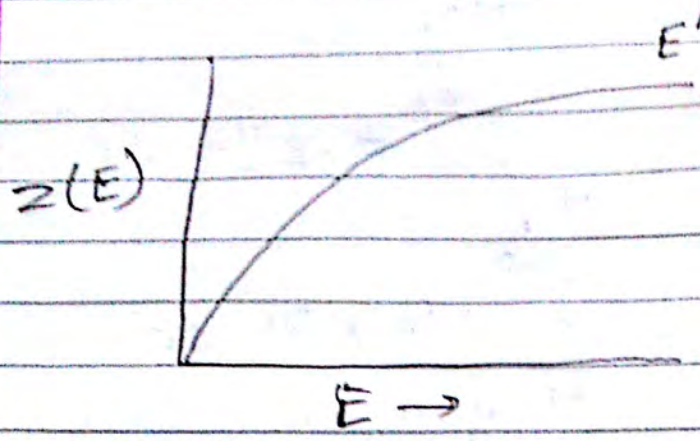
$= CE^{1/2} dE$

where $C = \frac{4\pi V}{h^3} (2m)^{3/2}$



Total no. of e^-,

$$N = \int_0^{E_f} Z(E)\, dE$$

E_f = fermi energy and it is defined as maximum K.E which e^-s can have at absolute zero of temp.

$$\therefore N = \int_0^{E} CE^{1/2} dE$$

$$= C \frac{2}{3} E_f^{3/2}$$

$$\therefore E_f = \left(\frac{3N}{2C}\right)^{2/3}$$

$$= \left[\frac{3N}{2(4\pi V)(2m)^{3/2}} h^3\right]^{2/3}$$

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

Here $\frac{N}{V} = n$ (density of e^-)

$$\therefore \boxed{E_f = \frac{h^2}{2m} \cdot \left(\frac{3n}{8\pi}\right)^{2/3}}$$

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Average Energy of free e⁻;

$$\overline{E_0} = \frac{1}{N}\int_0^{E_F} E\,Z(E)\,dE$$

$$\overline{E_0} = \frac{1}{N}\int_0^{E_f} E\,CE^{1/2}\,dE$$

$$= \frac{C}{N}\int_0^{E_F} E^{3/2}\,dE$$

$$= \frac{3}{2}E_F^{-3/2}\,\frac{2}{5}E_F^{5/2}$$

$$\boxed{E_0 = \frac{3}{5}E_F}$$

Effective mass of e⁻

One e⁻ in the crystal interacts with the crystal lattice therefore its behaviour towards external force is different from that of a free electron. This deviation of e⁻ behaviour is taken into account by considering the e⁻s to have effective mass (m^*) rather than its free space mass 'm'. The effective mass m^* depends on the nature of the crystal lattice and varies with the direction of motion of e⁻s in the lattice.

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Let an e^- move when external field 'E' is applied. Then the force acting on the e^- will be 'eE'

Then work done by the force. $= eE\,dx$

$$= eE\,v\,dt$$

$$= eE\,v_g\,dt \quad \text{—(1)}$$

(where v_g = group vel. = v (particle velocity))

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

$$dE = \frac{h}{2\pi}\,d\omega = \frac{h}{2\pi}\frac{d\omega}{dk}\,dk$$

$$= \frac{h}{2\pi}\,v_g\,dk \quad \text{—(2)}$$

from (1) and (2)

equate eqn (1) and (2)

$$eE\,v_g\,dt = \frac{h}{2\pi}\,v_g\,dk$$

$$\Rightarrow \frac{dk}{dt} = \frac{2\pi eE}{h} \quad \text{—(3)}$$

from (2), $v_g = \frac{2\pi}{h}\frac{dE}{dk}$

$$\frac{dv_g}{dt} = \frac{2\pi}{h}\frac{d^2E}{dk\,dt}$$

$$= \frac{2\pi}{h}\frac{d^2E}{dk^2}\frac{dk}{dt}$$

on putting value of $\frac{dk}{dt}$ from (3)

$$\therefore \frac{dv_g}{dt} = \left(\frac{2\pi}{h}\right)^2 \frac{d^2E}{dk^2}\,eE$$

Again $v_g = v$

$$\therefore \frac{dv}{dt} = \left(\frac{4\pi^2}{h^2}\frac{d^2E}{dk^2}\right)eE$$

$$\frac{dv}{dt} = \frac{1}{m^*}eE$$

where, $\frac{1}{m^*} = \left(\frac{4\pi^2}{h^2}\frac{d^2E}{dk^2}\right) = \frac{1}{m^*}$

$$\frac{dv}{dt} = \frac{1}{m^*}eE$$

↓ acc^n ↓ mass ↓ force

Conductivity :-

$$\sigma = n_e e\mu_e + n_h e\mu_h$$

where n_e = e^- conc.

n_h = hole conc.

μ_e = e^- mobility

μ_h = hole mobility

Resistivity :-

$$\rho = \frac{1}{\sigma}$$

For intrinsic semiconductors

$$n_e = n_h = n_i$$

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

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Concentration of free e^- & holes in semiconductors.

Let the no. of e^- per unit volume in the energy range E & $E+dE$ is given by $n(E) = g(E) f(E) dE$

where $g(E)$ = no. of available quantam states of e^-.

$f(E)$ = fermi function.

$$= \frac{1}{e^{(E-E_F)/kt} + 1}$$

where E_F = fermi energy.

$\because$ Conduction band varies from E_g to ∞

$\therefore$ Conc. of e^- in conduction band is,

$$n_e = \int_{E_g}^{\infty} g(E) f(E) dE$$

$$= \int_{E_g}^{\infty} \frac{g(E)}{e^{(E-E_F)/kt} + 1} dE$$

$\because (E-E_F)/kt >> 1$

$$n_e = \int_{E_g}^{\infty} g(E) e^{-(E-E_F)/kt} dE$$

$$\therefore n_e = K_e e^{-(E_g - E_F)/kt}$$

Similarly,

$$n_h = K_h e^{-(E_g - E_F')/kt}$$

for intrinsic semiconductors,

$$n_e = n_h$$

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X ∴ we can assume, that if $k_e = k_h$

$$E_g - E_f = E_g - E_{f'}$$

$$E_g = E$$

$$K e^{-(E_g - E_f)/kt} = k_h e^{-(E_g - E_{f'})/kt}$$

Electron hole cone. in intrinsic semiconductor.

Rate of combination

$$R = \gamma n_e n_h$$

where γ = Const. of proportionality

Under eqⁿ,

rate of generation = rate of combination

$$\therefore g = R = n_e n_h$$

In intrinsic,

$$n_e = n_h = n_i$$

$$\therefore g = R = \gamma n_e n_h = \gamma n_i^2$$

$$\therefore \boxed{n_i^2 = n_e n_h}$$

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Module IV

Polar and non-polar molecules

The molecules in which center of gravity of +ve and -ve charges coincide are known as non-polar molecule.
Dipole moment of such molecules is zero.
H_2, O_2, CO_2, CH_4, C_6H_6.
These molecules have linear symmetrical structure.
The molecules in which center of gravity of positive and negative charges do not coincide are known as polar molecules. Since center of gravity of +ve and -ve charges are separated by a distance of molecular dimension, they form an electric dipole. Therefore net dipole moment of such molecules is non-zero. Ex- H_2O, $CHCl_3$, C_6H_5Cl.
Such molecules do not have symmetrical structure.

Dielectrics

Insulators are materials which have no free electron therefore they do not conduct electric current in presence of electric field. The insulators dense behaviour gets modified in the presence of external electric field

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are known as Dielectrics. Dielectrics are special types of insulators which are highly resistant to flow of electric current in them.

Dielectric Polarisation :-

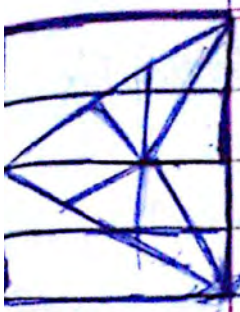
When a dielectric is placed in external electric field, its molecule acquire an electric dipole moment along the external field. this phenomenon in which dipole moment align along the direction of electric field is known as dielectric polarization.

Dielectric constant.
It is represented by K or ε_r.
It is also called relative permitivity

$$\varepsilon_r = K = \frac{\varepsilon}{\varepsilon_0}$$

Where ε_0 = permitivity of free space.
ε = " " material

Electric polarisation vector:
It is represented by "$\vec{P}$". It is also called dipole moment per unit volume. It is defined as vector field that expresses the density of permanent or induc



dipole moment in dielectric material, Its unit is C/m^2. $\vec{P}$ is proportional to strength E of external electric field.

$$\vec{P} \propto \vec{E}$$
$$= \chi_e \vec{E}$$

where χ_e = Electric susceptibility

Electric displacement vector ($\vec{D}$)

$$\vec{D} \propto \vec{E}$$
$$\vec{D} = \epsilon \vec{E}$$

or let σ_b and σ_f are surface charged density of bound and free charges then

$$\boxed{\vec{P} = \sigma_b}$$
$$\boxed{\vec{D} = \sigma_f}$$

$$\vec{P} = \alpha \vec{E}$$

where α = Electric polarizability of dielectric material.

Relation b/w $\vec{D}$, $\vec{E}$ & $\vec{P}$

Consider electric polarisation of dielectric slab insulated b/w plates of capacitor. Let σ_f and σ_b are surface charged density of free and bound charges present on capacitor plate and dielectric slab respectively.

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Let E_f & E_b are the corresponding electric field strength of free charges and bound charges then the magnitude of E_f and E_b are given by

$$E_f = \frac{\sigma_f}{\varepsilon_0}$$

$$E_b = \frac{\sigma_b}{\varepsilon_0}$$

Since E are opp. directed hence the net electric field is given by.

$$E = E_f - E_b$$

~~$\sigma_f - \sigma_b$~~

$$= \frac{\sigma_f}{\varepsilon_0} - \frac{\sigma_b}{\varepsilon_0}$$

or,

$$\sigma_f - \sigma_b = \varepsilon_0 E$$

or,

$$\boxed{D - P = \varepsilon_0 E}$$

In vector form,

$$\vec{D} - \vec{P} = \varepsilon_0 \vec{E}$$

or,

$$\vec{D} = \vec{P} + \varepsilon_0 \vec{E}$$

In above relation :-

1) D is related to free charges thus it can be represented by lines of electric displacement.
2) The lines of P begins and ends on bound charges.
3) E is related to both free charges

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and bound charges.

Relationship b/w χ_e & K.

↓
Electric susceptibility
and dielectric const.

$\therefore \vec{D} = \varepsilon_0 E + \vec{P}$ — (1)

Also $\vec{D} = \varepsilon \vec{E}$ — (2)

$\vec{P} = \chi_e \vec{E}$ — (3)

Putting (2) & (3) in (1)

$\varepsilon \vec{E} = \varepsilon_0 E + \chi_e E$ — (4)

Also,

$K = \frac{\varepsilon}{\varepsilon_0}$

$\Rightarrow \varepsilon = \varepsilon_0 K$ — (5)

Putting (5) in (4)

$\varepsilon_0 K E = \varepsilon_0 E + \chi_e E$

or, $\boxed{K = 1 + \frac{\chi_e}{\varepsilon_0}}$

or, $\boxed{\chi_e = (K-1)\varepsilon_0}$

or, $\vec{P} = \chi_e \vec{E}$

$\therefore \boxed{\vec{P} = (K-1)\varepsilon_0 \vec{E}}$

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Gauss Law in Dielectrics

This law states that the surface integral of electric displacement vector $\vec{D}$ is equal to free charges enclosed in the surface over a closed surface.

Mathematically,

$$\oint \vec{D} \cdot d\vec{s} = q_f$$

where $\vec{D}$ = Electric displacement vector

q_f = free charge

Proof:- Let q_f and q_b are free and bound charges on the capacitor plate and dielectric slab respectively then acc. to gauss law

$$\oint E_0 \, ds = \frac{1}{\varepsilon_0} \cdot (q_f - q_b) \quad \text{---(1)}$$

Let E & E_0 be the electric field strength on the capacitor plate in the absence and presence of dielectric slab.

then dielectric constant $K = \frac{E_0}{E}$ ---(2)

Also, $E_0 = \frac{q_f / A}{\varepsilon_0}$

$$\therefore K = \frac{q_f}{A \varepsilon_0 E}$$

or, $$E = \frac{q_f}{A \varepsilon_0 K}$$

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$$\text{or, } E_f - E_b = \frac{q_f}{A\epsilon_0 k}$$

or,

$$\frac{\sigma_f}{\epsilon_0} - \frac{\sigma_b}{\epsilon_0} = \frac{q_f}{A\epsilon_0 k}$$

$$\text{or, } \frac{q_f/A}{\epsilon_0} - \frac{q_b/A}{\epsilon_0} = \frac{q_f}{A\epsilon_0 k}$$

$$\text{or, } \frac{q_f}{A\epsilon_0} - \frac{q_b}{A\epsilon_0} = \frac{q_f}{A\epsilon_0 k}$$

$$\text{or, } \frac{q_f}{A\epsilon_0}\left(1 - \frac{1}{k}\right) = \frac{q_b}{A\epsilon_0}$$

$$\text{or, } q_f - \frac{q_f}{k} = q_b$$

$$\text{or, } q_f - q_b = \frac{q_f}{k} \quad \text{— (3)}$$

putting in eq (1)

eq. (1) becomes

$$\oint E \cdot ds = \frac{1}{\epsilon_0}\frac{q_f}{k}$$

$$\text{or, } \oint \underbrace{\epsilon_0 E k}_{\vec{D}} ds = q_f$$

$$\text{or, } \boxed{\oint \vec{D} \cdot ds = q_f}$$

Type of magnetic materials

1) Diamagnetic materials → These materials are

Slighty Repel by magnetic field and Material does not retain magnetic properties when external field is removed. In this all e⁻s are paired and therefore they have no permanent net magnetic Moment per atom. They have very weak Susceptibility. for eg Copper, Silver, gold.

2) Paramagnetic Materials → In this some atoms of the material have net magnetic moment due to unpaired e⁻s in partially filled orbitals. Paramagnetic properties are due to the presence of these unpaired e⁻s and form Realignment of e⁻s. Caused by ext. Magnetic field. These materials are slightly attracted by M.F and materials dont loose these magnetic properties when ext. field is removed. They have positive Susceptibility. For eg. Magnesium, Molybdenum, Lithium.

3) Ferromagnetic Materials → They have large and positive Susceptibility due to pres of ext. M.F. They exhibit strong attraction to a magnetic field and are able to retain their Magnetic prop. even after ext. field is removed. These mats have very few unpaired e⁻s. for eg iron, Nickel, cobalt.

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4) Ferrimagnetic materials:-
In these materials magnetic structure is composed of two magnetic sub lattices whose spin moment are oriented in opp. direction, for eg. FeO, Fe_2O_3, Fe_3O_4

5) Antiferromagnetic Materials :-
In this two sub lattices have exactly equal and opp. spin orientation therefore the net magnetic moment of these materials is zero. for eg. FeS,

Clausius - Mosotti Equation

For non-polar dielectrics, Molecular Electric field is given by,

$$\vec{E_m} = \left(\alpha + \frac{P}{3\varepsilon_0} \right)$$

This eqn give the relationship between molecular polarisability α and dielectric constant K. It is valid for non polar molecules.

$$\vec{E_m} = \vec{E} + \frac{P}{3\varepsilon_0}$$

where $\vec{P}$ = polarisation

If p_m is induced dipole moment then

$$p_m = \alpha \vec{E_m}$$

If is no of molecules per unit vol. then polarisation $\vec{P}$ is.

$$\vec{P} = N p_m.$$

or, $\vec{P} = N\alpha \vec{E_m}$

$$= N\alpha \left(\vec{E} + \frac{\vec{P}}{3\varepsilon_0} \right)$$

$\because P = (K-1)\varepsilon_0 \vec{E}$

$$(K-1)\varepsilon_0 E = N\alpha \left(E + \frac{(K-1)\varepsilon_0 E}{3\varepsilon_0} \right)$$

or, $(K-1)\varepsilon_0 = N\alpha \left[1 + \frac{(K-1)}{3} \right]$

or, $(K-1) = \frac{N\alpha}{\varepsilon_0} \left[\frac{3 + K - 1}{3} \right]$

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$$\text{or,}\quad (K-1) = \frac{N\alpha}{3\varepsilon_0}\left(K+2\right)$$

$$\text{or,}\quad \boxed{\alpha = \frac{3\varepsilon_0}{N}\,\frac{(K-1)}{(K+2)}}$$

Clausius Mosotti Equation.