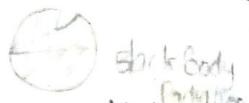


## UNIT - VI

### QUANTUM MECHANICS

Interaction of radiation with matter :-



Black Body Radiation

- \* the electrons in the matter behaves like oscillators with a characteristic frequency.
- \* the oscillators absorb or emit energy in "discrete manner".
- \* To explain Black body Radiation, Max Planck proposed above statement.
- \* According to Huygen's principle, phenomena of Interference, diffraction and polarisation, it was established that light behaves like wave.
- \* According to Einstein photo electric effect, light exhibit particle nature.
- \* these particles are called "PHOTONS" (quantum Packet).
- \* De Broglie assumed that particles like electrons, protons, neutrons etc exhibit wave nature.
- \* The concept of wave nature of material particles was experimentally verified by de Broglie and his group and Thomson and his group.
- \* They discovered the wave nature of electrons through diffraction experiments.

#### Matter Waves :-

- \* According to De Broglie, a wave is associated with a particle in motion called matter wave, which may be regarded as localised with the particle.
- \* the wavelength of the matter wave is given by

$$\boxed{\lambda = \frac{h}{mv} = \frac{h}{P}}$$

Uncertainty principle :-

Heisenberg Uncertainty principle:-

According to Heisenberg, it is impossible to determine the position and momentum of elementary particles simultaneously at arbitrary precision.

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad \left[ \frac{\hbar}{2\pi} = \frac{h}{2\pi} \right] \quad \hbar = \frac{h}{2\pi}$$

Similarly  $\Delta E \Delta t \geq \frac{\hbar}{2}$  where  $E$ -energy  
 $\Delta$ -uncertainty in time

$\Delta L \Delta \theta \geq \frac{\hbar}{2}$  where  $\Delta L$ -uncertainty in Angular momentum  
 $\theta$ -Angle.

Applications of Uncertainty Relation:-

- \* The Uncertainty Relation explains the ground state energy of hydrogen Atom.
- \* It explains the width of the spectral line.
- \* It explains the non existence of electrons in nucleus.
- \* It explains the mass of meson. It is found to be 200 times the mass of electron.

WAVE FUNCTION :-

The trajectory of elementary particles (quantum particles) can be described with the help of wave function.

Wave function can be written as

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

where  $\vec{k}$ -wave vector  $[k = \frac{2\pi}{\lambda}]$

AM Tc TB  
AM AM

When two or more waves with slight differences in frequency overlap, it leads to formation of wave packets.

WAVE PACKET :-

- \* The wave function of matter wave which is confined to small region of space is termed as wave packet and mathematically it can be represented as

$$\Psi(x, t) = \int_{-\infty}^{+\infty} A(k) e^{i(kx - \omega t)} dk$$

## Time dependent Schrodinger Equation :-

The wave function of localised free particles is given by

$$\Psi(x,t) = \int_{-\infty}^{+\infty} A(k) e^{ikx - i\omega t} dk$$

- \* Free particle has only kinetic energy

$$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} \quad \text{--- ①}$$

- \* According to de broglie,  $\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda}$ .

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

we know that  $k = \frac{2\pi}{\lambda}$

$$p = \frac{h}{\frac{2\pi}{k}} \Rightarrow p = \frac{hk}{2\pi}$$

$$P = \hbar k \quad \text{--- ②}$$

- \* According to plank,  $E = h\nu$

$$E = \hbar \frac{2\pi}{\omega} \quad E = \frac{\hbar \omega}{2\pi}$$

$$E = \hbar \omega$$

$$\frac{p^2}{2m} = \hbar \omega$$

$$\frac{\hbar^2 k^2}{2m} = \hbar \omega$$

$$\frac{\hbar k^2}{2m} = \omega$$

$$\omega = \frac{\hbar k^2}{2m}$$

- \* According to wave function  $\Psi(x,t) = \int_{-\infty}^{+\infty} A(k) e^{ikx - i\omega t} dk$

$$\text{Now } \frac{\partial \Psi}{\partial x} = ik \int_{-\infty}^{+\infty} A(k) e^{ikx - i\omega t} dk$$

$$\frac{\partial \Psi}{\partial x} = ik \Psi(x,t)$$

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

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{\hbar^2}{m} \psi(x,t) \quad \text{--- ④}$$

$$-\frac{\hbar^2}{m} \frac{\partial^2 \psi}{\partial x^2}$$

NOW  $\frac{\partial \psi}{\partial t} = -i\omega \psi(x,t)$

$$\boxed{\frac{\partial \psi}{\partial t} = -i\frac{\hbar k^2}{m} \psi(x,t)} \quad \text{--- ⑤}$$

NOW multiply eq ④ with  ~~$i\hbar$~~   $-\frac{\hbar^2}{m}$

$$-\frac{\hbar^2}{m} \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar^2 k^2}{m} \psi(x,t) \quad \text{--- ⑥}$$

NOW multiply eq 5 with  $i\hbar$

$$\text{if } \frac{\partial \psi(x,t)}{\partial t} = \frac{\hbar^2 k^2}{m} \psi(x,t) \quad \text{--- ⑦}$$

From eq ⑥ and eq ⑦

$$\text{if } \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{m} \frac{\partial^2 \psi}{\partial x^2}$$

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

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

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

Schrodinger introduced the potential term (due to forces on particle). In the equation  $-\frac{\hbar^2}{m} \frac{\partial^2 \psi}{\partial x^2} + \underline{V\psi} = i\hbar \frac{\partial \psi}{\partial t}$

We know time dependent Schrodinger equation is

given by

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

In 3-D  $\nabla^2$  -

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

where  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

wave function is  $\psi(x,t) = A e^{i(k_0 x - \omega t)}$

for a free particle :-

$$V=0$$

$$\frac{\partial^2}{\partial m \partial x^2} \psi(x,t) = \frac{\partial^2}{\partial t^2} \psi(x,t)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

$$\frac{1}{2m} \left( -i \frac{\hbar}{\partial x} \right) \left( i\hbar \frac{\partial}{\partial x} \right) \psi = i\hbar \frac{\partial}{\partial t} \psi \quad \text{--- (1)}$$

$$\text{we know that } \frac{P^2}{2m} \psi(x,t) = E \psi(x,t) \quad \text{--- (2)}$$

Comparing Eq's (1) & (2)

- \* In Quantum mechanics, the dynamic variables can be calculated from operators.
- \* the momentum operator :  $\hat{P}_x = -i\hbar \frac{\partial}{\partial x}$
- \* the energy operator :  $\hat{E} = i\hbar \frac{\partial}{\partial t}$
- \* the momentum operator should act on a given wave function, to extract the information regarding the momentum  $\hat{P} \psi = \underline{\underline{\psi}} \rightarrow$  momentum eigen value.
- \*  $\hat{E} \psi = \underline{\underline{\psi}}$  Energy eigen value

for free particle,

$$-\frac{\hbar^2}{8m} \frac{\partial^2}{\partial x^2} \psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \quad \text{--- ①}$$

In 3-D,  $\int -\frac{\hbar^2}{8m} \nabla^2 \psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$   $(-\frac{i\hbar}{\partial x}) (\frac{i\hbar}{\partial x}) \psi = \frac{i\hbar}{\partial t} \psi$

$$E = \frac{P^2}{8m} \psi(x,t) \quad \frac{P^2}{8m} \psi(x,t) = E \psi(x,t)$$

$$\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$\psi = \frac{\sqrt{2}}{a} e^{i\frac{n\pi}{a} x}$$

Hence  $\hat{p} = -i\hbar \frac{\partial}{\partial x}$  - momentum operator

$\hat{E} = i\hbar \frac{\partial}{\partial t}$  - Energy operator.

$$\hat{p} \psi = i\hbar \frac{\partial}{\partial x} \left( \sqrt{\frac{2}{a}} e^{i\frac{n\pi}{a} x} \right) = -i\hbar \frac{\sqrt{2}}{a} \frac{n\pi}{a} e^{i\frac{n\pi}{a} x} = i\hbar \frac{\sqrt{2}}{a} e^{i\frac{n\pi}{a} x}$$

For  $\hat{p} \psi = -i\hbar \frac{\partial}{\partial x} \left( \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \right)$

$$= -i\hbar \sqrt{\frac{2}{a}} \frac{\cos n\pi x}{a}$$

$$\boxed{\hat{p} \psi = i\hbar \frac{\sqrt{2}}{a} n\pi \cos(n\pi x)}$$

$\psi$   
 $E\psi$

## time independent Schrodinger Equation

By using separation of variable concept, we can derive time dependent Schrodinger equation:-

- \* In 1-D, schrodinger wave Eq<sup>n</sup> is given by

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x,t) = \frac{i\hbar}{m} \frac{\partial \psi(x,t)}{\partial t} \quad \text{--- (1)}$$

- \* In 3-D schrodinger wave Eq<sup>n</sup>,

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

- \*  $\psi(x,t) = A e^{i(k_0 x - \omega t)}$

- \* using separation method:-  $\psi(x,t) = \psi(x)\Phi(t)$  --- (2)

- \* substitute Eq<sup>n</sup> 2 with Eq<sup>n</sup> 1

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

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

divide whole equation with  $\psi(x)\Phi(t)$

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

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = \frac{i\hbar}{\Phi(t)} \frac{\partial \Phi(t)}{\partial t}$$

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$$

divide whole Eq<sup>n</sup> with  $\psi(x)$

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

this is independent schrodinger Eq<sup>m</sup>.

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x) = E \Psi(x)$$

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

where  $\hat{H}$  can be written as  $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

\*  $\hat{H}$  is Hamiltonian operator.

hence  $E = \frac{i\hbar}{8m}$

$$E = \frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t}$$

$$\frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t}$$

$$\frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = E$$

$$i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t)$$

$$\phi(t) = C e^{-\frac{Et}{\hbar}}$$

$$\frac{\partial \phi(t)}{\partial t} = E = \frac{i}{\hbar} E \phi(t)$$

$$C e^{\frac{Et}{\hbar}}$$

$$\phi(t) = C e^{-\frac{Et}{\hbar}} \rightarrow \text{eqn used for stationary states}$$

Calculate the eigen values and eigen function in given region of a particle constrained in region where potential is

$$V(x) = 0 \quad -a < x < a$$

$$V(x) = \infty \quad a \geq |x|$$

time independent schrodinger wave equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x)\Psi(x) = E\Psi(x)$$

$$V(x) = 0 \quad \text{in } -a < x < a$$

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

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi = 0$$

here,  $m, E, \hbar$  are constants

$$\boxed{k^2 = \frac{2mE}{\hbar^2}}$$

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0$$



$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi$  is a polynomial, then the general solution

of  $\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi$  is

$$\boxed{\psi(x) = A \cos kx + B \sin kx} \quad \text{--- (1)}$$

- \*  $\psi(x=a) = A \cos ka + B \sin ka = 0$  } since particle doesn't exist
- \*  $\psi(x=-a) = A \cos ka - B \sin ka = 0$  at edges

\*  $A \cos ka = 0$  and  $B \sin ka = 0$

- \* we don't take both  $A = B = 0$  since wave function will be zero.

Case (i) :  $B = 0 \quad \cos ka = 0$

$$ka = \frac{n\pi}{2} \quad (n = \text{odd number})$$

$$\boxed{k = \frac{n\pi}{2a}} \Rightarrow k^2 = \frac{n^2\pi^2}{4a^2}$$

Since  $k^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{4a^2} \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{8ma^2} \quad (n = \text{odd})$$

Case (ii) :  $A = 0 \quad \sin ka = 0$

$$ka = \frac{n\pi}{2} \quad (n = \text{even})$$

$$k = \frac{n\pi}{2a} \rightarrow k^2 = \frac{n^2\pi^2}{4a^2}$$

since  $k^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{4a^2}$

$$\psi(x) = A \cos \frac{n\pi}{2a} x$$

$$\psi(x) = B \sin$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}} \quad n = \text{even}$$

when  $B=0 \quad \cos ka = 0 \quad \psi_{\text{odd}}(x) = A \cos \frac{n\pi}{2a} x$ . when  $n$  is odd

when  $A=0 \quad \sin ka = 0 \quad \psi_{\text{even}}(x) = B \sin \frac{n\pi}{2a} x$  when  $n$  is even

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2} \quad n = 1, 2, 3, 4, \dots$$

when  $n$  is odd,  $\Psi_{\text{odd}} = \sqrt{\frac{1}{a}} \cos \frac{n\pi x}{2a}$ ,

when  $n$  is even  $\Psi_{\text{even}} = \sqrt{\frac{1}{a}} \sin \frac{n\pi x}{2a}$ .

$$A = \sqrt{\frac{1}{a}}$$

$$* E_n = \frac{n^2 \pi^2 \hbar^2}{8m(2a)^2}$$

$$E_1 = \frac{\pi^2 \hbar^2}{8ma^2} \quad E_2 = 4 \frac{\pi^2 \hbar^2}{8ma^2} \quad E_3 = 9 \frac{\pi^2 \hbar^2}{8ma^2} \quad E_4 = 16 \frac{\pi^2 \hbar^2}{8ma^2}$$

$$E_{100} = (100)^2 \frac{\pi^2 \hbar^2}{8ma^2} \quad E_{101} = (101)^2 \frac{\pi^2 \hbar^2}{8ma^2} \dots$$

$$\Delta E = E_{101} - E_{100} = 201 \frac{S}{(2a)^2} \quad [ \because S = \frac{\pi^2 \hbar^2}{8m} ]$$

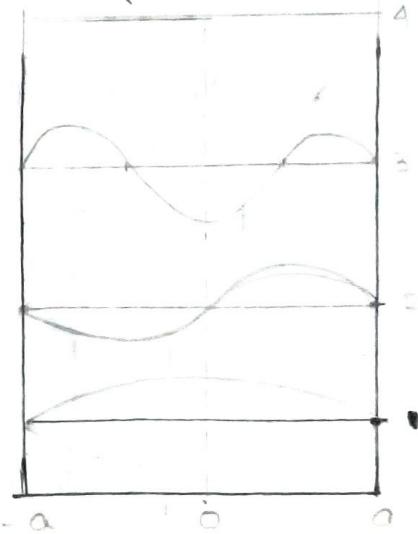
$$* \alpha = -a \quad \Psi(x) = A \cos \frac{n\pi x}{2a}$$

$$A \cos n\pi/2 = 0$$

$$\alpha = 0 \quad \Psi(x) = A \cos 0$$

$$T_0 / T_1 = 5 \sin \frac{n\pi x}{2a}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{8m(2a)^2}$$



\* As  $n$  increases discreteness decreases, it become continuous, so quantum problem behaves as classical problem

\* If a particle is contained to a region of  $a$  to  $L$ .

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

$$\Psi_{\text{even}} = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{L}$$

For  $n$  odd taking into account from  $x=0$

$$x = \frac{2n+1}{2} \frac{\pi L}{n}$$

## Normalisation Functions :-

$\psi$  represents trajectory of a particle

$$x(t) = \sin t \quad x(t) = \cos t$$

$$\dot{x}(t) = \sin t \quad \dot{x}(t) = \cos t$$

we have wave function,  $\psi(x,t) = A e^{i(kx - \omega t)}$

we have wave packet,  $\psi(x,t) = \int A e^{i(kx - \omega t)} dz$

\* The probability of finding particle in mode is given by

$$P = \int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$P = \int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

\*  $\psi = N \sin\left(\frac{n\pi x}{L}\right)$  is a normalised function - ①

$$P = N^2 \int_{-\infty}^{\infty} \sin^2 \frac{n\pi x}{L} dx = N^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$$

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

$$P = \frac{N^2}{2} \left[ x - \frac{\sin \frac{n\pi x}{L}}{\frac{n\pi}{L}} \right]_0^L = 1$$

$$P = \frac{N^2}{2} L = 1 \Rightarrow N = \sqrt{\frac{2}{L}}$$

from ① where  $N$  is normalised value

$$\boxed{\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}$$

- Normalised function.

Density of Energy states:-

$$* In 1-D \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$* In 3-D \quad E_n = (n_x^2 + n_y^2 + n_z^2) \frac{\pi^2 \hbar^2}{8mL^2}$$

$$\text{Volume} = \frac{4}{3}\pi n^3 - \frac{4}{3}\pi n^3$$

where  $n$  is energy level



$$n^2 = \frac{8mL^2 E}{\pi^2 \hbar^2}$$

$$n^3 = \left( \frac{8mL^2 E}{\pi^2 \hbar^2} \right)^{3/2}$$

\* Energy values won't be negative, so levels are all in first volume = octant only.

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

$$\text{volume} = \frac{1}{6} \pi \left( \frac{8mL^2 E}{\pi^2 \hbar^2} \right)^{3/2}$$

\* For unit volume of each level, & total volume be in then

$$\text{No. of energy level} = N(E) = \frac{\text{volume of total surface}}{\text{volume of each layer}}$$

\* for total volume = 1 & volume of each level = 1

then

$$N(E) = \frac{1}{6} \pi \left( \frac{8mL^2 E}{\pi^2 \hbar^2} \right)^{3/2}$$

\*

$$N(E) = \int D(E) dE$$

\*

$$D(E) = \frac{d}{dE} N(E)$$

where  $D(E) \rightarrow$  density of energy level

$$D(E) = \frac{1}{6} \pi \left( \frac{8mL^2}{\pi^2 \hbar^2} \right)^{3/2} \frac{3}{8} E^{1/2}$$

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

## Fermi level :-

\* the highest occupied energy level at absolute zero temp. (OK) is called "FERMI LEVEL".

\* At absolute zero, the fermi energy represents the energy which divides the filled states from the empty states.

\* The function is given by

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

where E - energy of particle

$E_F$  - Fermi energy

3s	1
3p	1L + 1L
3s	1L
1s	1L
	$Na = 1s^2 2s^2 2p^6 3s^1$

\* The Above equation gives the probability that particular quantum state at part energy E is filled or not

\* If  $f(E)=1$ , that means energy state is occupied by electron

\* If  $f(E)=0$ , means Energy state is empty.

\* when  $E_F=E$   $f(E)=1/2$

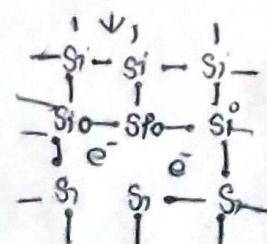
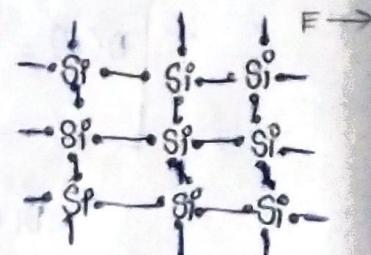
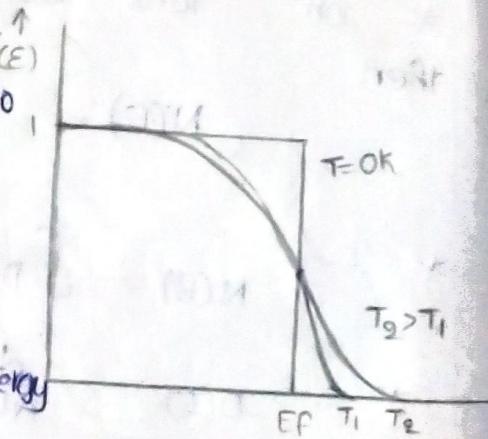
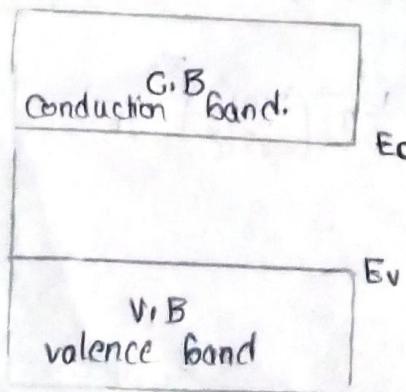
some of electrons ( $1/2$  no) are excited to empty levels.

Note:- The electrons near to Fermi level are participated in excitation.

## Band Theory of solids

\* In solids, instead of single energy levels, energy bands will form.

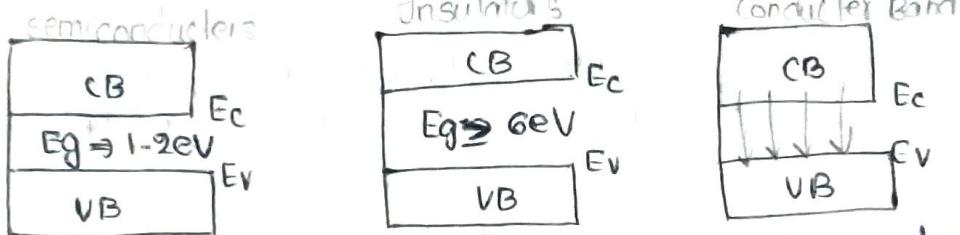
\* The band structure can be shown in the figure



\* Quantum mechanics explained the existence of forbidden energy band between two bands.

\* If the width of forbidden band between valence band and conduction band is in order of 6eV or more, the excited electrons (as for conduction) not exist. such materials are called "INSULATORS". [6eV]

\* If the width of forbidden band is in order of 1-2eV a few electrons which are near to the Fermi level can excited to the conduction Band. Such materials are called SEMICONDUCTORS.



\* In the conductors, the conduction band overlaps on the valence band.

Concentration of electrons and holes in a SEMICONDUCTOR.

We know density of energy states is given by

$$D(E) = \frac{L^3}{4} \cdot \frac{1}{h^3 \pi^2} (\alpha m)^{3/2} E^{1/2}$$

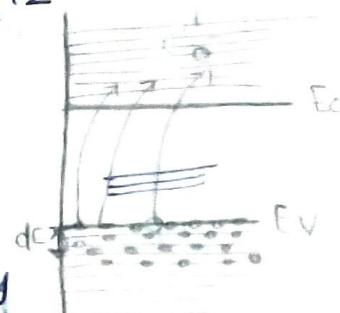
$$\frac{2}{\sqrt{3}} \cdot \frac{2}{\sqrt{4}} \cdot \frac{6}{\sqrt{3}} \cdot \frac{2}{\sqrt{4}} \cdot \frac{2}{\sqrt{3}} \cdot \frac{2}{\sqrt{4}}$$

The No. of states is given by

$$N(E) = D(E) dE$$

No. of occupied states is given by

$$N(E) = D(E) dE \times f(E)$$



Number of states per unit volume is given by in range of energy E and E+DE is

$$dn_0 = \frac{N(E)}{V} = \frac{1}{4\pi^2 h^3} (\alpha m)^{3/2} (E - E_c)^{1/2} f(E)$$

$$n_b = \int_{E_c}^{\infty} dn_0 = \int_{E_c}^{\infty} \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \frac{(E - E_c)^{1/2}}{e^{(E - E_f)/k_B T} + 1} dE$$

$$\frac{(\hbar)^3}{8\pi^3 h^3} \frac{8\sqrt{2} \pi m^{3/2}}{4\pi k_B T^3} \frac{1}{e^{(E - E_f)/k_B T} + 1}$$

since  $e^{(E-E_f)/k_B T} \gg 1$  we neglect this term. 1

$$n_0 = \int_{E_C}^{\infty} \frac{8\sqrt{2}\pi m_n^{3/2}}{h^3} \frac{1}{2} \frac{(E-E_C)}{e^{E/k_B T}, e^{-E_F/k_B T}} dE$$

$$n_0 = \int_{E_C}^{\infty} \frac{8\sqrt{2}\pi m_n^{3/2}}{h^3} \frac{e^{E_F/k_B T}}{e^{E/k_B T}} \times \frac{e^{E_C/k_B T}}{e^{E_C/k_B T}} \frac{1}{2} (E-E_C) dE$$

$$n_0 = \int_{E_C}^{\infty} \frac{8\sqrt{2}\pi m_n^{3/2}}{h^3} e^{E_F/k_B T} e^{-E_C/k_B T} e^{\frac{(E_C-E)}{k_B T}} \frac{1}{2} (E-E_C) dE$$

let  $\frac{E_C - E}{k_B T} = x_C$

$$E_C - E \leftarrow x_C k_B T$$

$$\frac{E - E_C}{k_B T} = x_C$$

$$E - E_C = x_C k_B T$$

$$(dE = dx_C k_B T)$$

$$n_0 = \frac{8\sqrt{2}\pi m_n^{3/2}}{h^3} e^{-(E_C-E_F)/k_B T} \int_0^{\infty} \frac{1}{2} \frac{1}{(k_B T)^{1/2}} (k_B T)^{1/2} e^{-x_C(k_B T)} dx_C$$

$$n_0 = \frac{8\sqrt{2} m_n^{3/2}}{h^3} (k_B T)^{3/2} \frac{\sqrt{\pi}}{2} e^{-\frac{(E_C-E_F)}{k_B T}}$$

Electron Concentration:  $n_0 = \frac{8\sqrt{2} m_n^{3/2}}{2} \frac{k_B T}{h^2} e^{-(E_C-E_F)/k_B T}$

$$n_0 = N_C e^{-(E_C-E_F)/k_B T}$$

Hole Concentration:-

$$P_0 = N_V e^{-(E_F-E_H)/k_B T}$$

$$N_V = \frac{8\pi m_p^{3/2}}{2} \frac{k_B T}{h^2} m_n^{1/2} \text{ effective mass of electron}$$

$$m_p^{1/2} \text{ effective mass of hole.}$$

## LAW OF MASS ACTION :-

# the no. of electrons per unit volume in the conducting semiconducting band is given by  $n_e = \frac{8}{3} \left( \frac{\pi m_n^* k_B T}{h^2} \right)^{3/2} e^{-(E_c - E_F)/k_B T}$

# The no. of holes per unit volume in the valence band is given by  $n_h = \frac{8}{3} \left( \frac{\pi m_p^* k_B T}{h^2} \right)^{3/2} e^{-(E_F - E_v)/k_B T}$

$$n_0 P_0 = \frac{8}{3} \left( \frac{\pi^2 m_p^* m_n^*}{h^3} \right)^{3/2} T^3 e^{-(E_c - E_v)/k_B T}$$

$$\boxed{n_0 P_0 = A T^3 e^{-(E_c - E_v)/k_B T}}$$

\* The product  $n_0 P_0$  is seem to be independent of position of Fermi level and has same values for intrinsic semiconductors (for pure semiconductors) and for extrinsic (impure)

$$n_0 P_0 = n_i P_i$$

since pure conductor ( $n_i = P_i$ )

$$\boxed{n_0 P_0 = n_i^2 = P_i^2}$$

$$n_i^2 = P_i^2 = A T^3 e^{-(E_c - E_v)/k_B T}$$

where  $E_g \approx$  energy gap

$$n_i^2 = P_i^2 = A T^3 e^{-E_g/k_B T}$$

$$n_i = P_i = A^{1/2} T^{3/2} e^{-\frac{E_g}{2k_B T}}$$

at 300K,

For Silicon (Si)  $E_g = 1.1 \text{ eV}$

$$\boxed{n_i = P_i = 1.6 \times 10^{10} \text{ atom/cm}^3}$$

For Germanium (Ge)  $E_g = 0.7 \text{ eV}$

$$\boxed{n_i = P_i = 8.5 \times 10^{13} \text{ atom/cm}^3}$$

$n_i$  - no. of electrons in conduction band

$P_i$  - no. of holes in Valence band

calculate Fermi level position in Intrinsic semiconductors

$$n_i = p_i \text{ (for intrinsic)}$$

$$n_0 = p_0$$

$$N_c e^{-(E_C - E_F)/k_B T} = N_V e^{-(E_F - E_V)/k_B T}$$

$$N_c \log e^{-(E_C - E_F)/k_B T} = N_V \log e^{-(E_F - E_V)/k_B T}$$

$$\cancel{-N_c} \frac{(E_C - E_F)}{k_B T} = -N_V \frac{E_F - E_V}{k_B T}$$

$$\cancel{N_c (E_C - E_F)} = \cancel{N_V (E_F - E_V)}$$

$$N_c E_C - N_c E_F = N_V E_F - N_V E_V$$

~~since~~ since ( $N_c = N_V$ )

$$e^{-(E_C - E_F)/k_B T} = e^{-(E_F - E_V)/k_B T}$$

$$(E_C - E_F)/k_B T = \frac{E_F - E_V}{k_B T}$$

$$E_C - E_F = E_F - E_V$$

$$E_F = \frac{E_C + E_V}{2}$$

Position of Fermilevel in Intrinsic Semiconductors

Velocity And Effective mass:-

\* When a electron is accelerated inside a crystal, its mass is generally appears different from free electron mass and is usually referred as "effective mass of electron".

\* According to deBroglie, the particle velocity 'v' is equal to the Group velocity of wave packet represented by an electron is given by

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

$$v_g = \frac{dw}{dk}$$

$$E = \hbar \omega$$

$$E = \hbar \omega$$

$$\frac{dE}{dk} = \hbar \frac{d\omega}{dk}$$

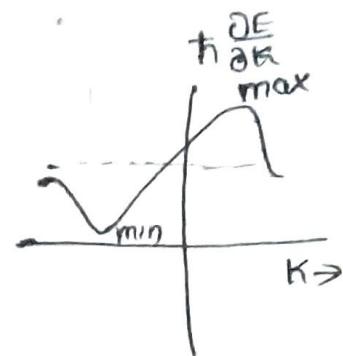
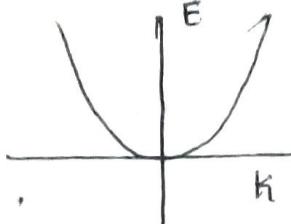
$$\left[ \frac{d\omega}{dk} = \frac{1}{\hbar} \left( \frac{dE}{dk} \right) \right]$$

$$\frac{d\omega}{dk} = \frac{1}{\hbar} \left( \frac{dE}{dk} \right)$$

$$F = \hbar \cdot$$

$$c = \lambda \nu$$

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



\* Let an  $\bar{e}$  is subjected to applied electric field with strength  $E$ , for a time interval  $t$ ,

\* If velocity of  $\bar{e}$  is  $v$ , & distance travelled by  $\bar{e}$  in  $t$  then  $\frac{dt}{dt}$  time interval 'dt' is given by

$$\text{distance} = v dt$$

\* ~~Electric field is given by~~

\* Energy gained by an electron is given by  $dE$

$$\left[ dE = (e\bar{E}) (v dt) \right] \Rightarrow dE = (e\bar{E}) \frac{1}{\hbar} \frac{\partial E}{\partial k} dt$$

where  $dE$  is energy gained by  $\bar{e}$  in time  $dt$

\* Acceleration of free electron is given by

$$F = ma = eE$$

$$\therefore a = \frac{eE}{m} \quad \text{--- (1)}$$

$$\frac{dv}{dt} = \frac{E}{m}$$

$$dv = \frac{E}{m} dt$$

$$\frac{d^2v}{dt^2} = \frac{1}{m} \frac{dE}{dk} dt$$

$$a = \frac{d}{dt} \left( \frac{1}{\hbar} \frac{\partial E}{\partial k} \right) = \frac{1}{\hbar} \frac{d}{dt} \left( \frac{\partial E}{\partial k} \right)$$

$$\boxed{a = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \frac{dk}{dt}}$$

$$\text{we know } dE = \frac{(e\bar{E})}{\hbar} \frac{\partial E}{\partial k} dt$$

$$\frac{dk}{dt} = \frac{e\bar{E}}{\hbar}$$

$$\boxed{a = \frac{1}{\hbar} \frac{e\bar{E}}{\hbar} \frac{\partial^2 E}{\partial k^2}}$$

$$a = \frac{eE}{h^2} \frac{\partial^2 E}{\partial k^2}$$

where  $\frac{\partial E}{\partial k}$  value at maximum

$$w kT \quad a = \frac{eE}{m}$$

$$\frac{eE}{m} = \frac{\partial E}{h^2} \frac{\partial^2 E}{\partial k^2}$$

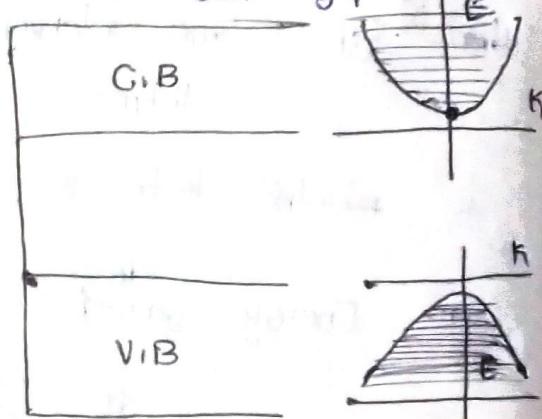
$$m^* = \frac{h^2}{(\frac{\partial^2 E}{\partial k^2})}$$

effective mass

- \* For a free  $e^-$   $m^* = m$
- \* For an intrinsic semiconductors, no. of electrons = no. of holes
- \* Germanium, Silicon have indirect band gaps.
- \* more 3ev, behaves as insulator.

Ge-0.7ev Si-1.1ev

- \* when energy given to atom to emit  $e^-$ , if total energy is consumed to emit electron from V.B is called "direct Band"
- \* when energy provided to atom is used to heat lattice called "Indirect Band"
- \* In intrinsic semiconductors, no. of  $e^-$ s = no. of holes in valency band in all the temperatures



$$n_p = n_i$$

$$N_C e^{-(E_C - E_F)/k_B T} = N_V e^{-(E_F - E_V)/k_B T}$$

$$\frac{N_C}{N_V} = e^{(E_F + E_V + E_C - E_{F_i})/k_B T}$$

$$\left(\frac{m_n^*}{m_p^*}\right)^{3/2} = e^{(E_C + E_V - E_{F_i})/k_B T}$$

Applying ln on B.T

$$(E_C + E_V - E_{F_i}) = k_B T \ln \left( \frac{m_n^*}{m_p^*} \right)^{3/2}$$

$$E_{Fp} = \left( \frac{E_C + E_V}{2} \right) - \frac{k_B T}{2} \ln \left( \frac{m_n^*}{m_p^*} \right)^{3/2}$$

$$(or)$$

$$E_{Fp} = \left( \frac{E_C + E_V}{2} \right) + \frac{k_B T}{2} \ln \left( \frac{m_p^*}{m_n^*} \right)^{3/2}$$

\* If effective mass of hole = effective mass of electron, Fermi level will exactly at the middle of the forbidden gap.

Position of Fermi level in Extrinsic for Semiconductors.

Position of Fermi level in Extrinsic for Semiconductors.

$n_0 = N_c e^{-(E_C - E_F)/k_B T}$  ( $e^-$  charge density in N type)

$$P_0 = N_V e^{-(E_F - E_V)/k_B T}$$

$$* \frac{n_0}{P_0} = \frac{N_c}{N_V} e^{-(E_C + E_V - 2\alpha f_n)/k_B T}$$

$$\frac{n_0}{P_0} = \frac{n_0 \times n_0}{P_0 \times P_0} = \frac{n_0^2}{P_0 \times n_0} = \frac{n_0^2}{n_i^2} \quad [ : n_i = P_0 \text{ in intrinsic semiconductors} ]$$

$$* \frac{n_0^2}{n_i^2} = \frac{N_c}{N_V} e^{-(E_C + E_V - 2\alpha f_n)/k_B T}$$

$$+ (E_C + E_V - 2\alpha f_i)/k_B T$$

$$\frac{N_c}{N_V} = e$$

$$\frac{n_0^2}{n_i^2} = e^{\frac{(E_C + E_V - 2\alpha f_i)}{k_B T}} e^{-\frac{(E_C + E_V - 2\alpha f_n)}{k_B T}}$$

$$\frac{n_0^2}{n_i^2} = e^{\frac{2(f_n - f_i)}{k_B T}}$$

$$n_0^2 = n_i^2 e^{\frac{2(f_n - f_i)}{k_B T}}$$

$f_n$  - Fermi level of N type

$f_i$  - Fermi level of intrinsic

$$n_0 = n_i e^{\frac{(f_n - f_i)}{k_B T}}$$

$$n_0 \gg n_i$$

$n_0$  - electron charge concentration in N type.

Since  $n_i > n_0$

$$E_{fn} > E_{f0}$$

\* Since no. of electrons ( $n_0$ ) in conduction band of N type semiconductor is greater than  $n_i$ .

\* The Fermi level in N type semiconductor is close to conduction band.

\* Similarly for p type semiconductors,

$$P_0 = P_0 e^{(E_{fn} - E_F)/k_B T}$$

the Fermi level close to valence band.

Exact position of Fermilevel in N type semiconductor can be made if

$$N_D = N_c e^{-(E_C - E_{fn})/k_B T}$$

$$\ln\left(\frac{N_D}{N_c}\right) = -\frac{E_C + E_{fn}}{k_B T}$$

$$-E_C - E_{fn} = k_B T \ln\left(\frac{N_D}{N_c}\right)$$

$$E_{fn} = E_C + k_B T \ln\left(\frac{N_D}{N_c}\right) \quad \text{--- (1)}$$

$$E_{fn} = E_C - k_B T \ln\left(\frac{N_c}{N_A}\right)$$

$$N_A = N_V e^{-(E_{fp} - E_V)/k_B T}$$

$$\ln\left(\frac{N_A}{N_V}\right) = -\frac{E_{fp} + E_V}{k_B T}$$

$$-E_{fp} - E_V = k_B T \ln\left(\frac{N_A}{N_V}\right)$$

$$E_{fp} = E_V - \ln\left(\frac{N_A}{N_V}\right) k_B T$$

$$E_{fp} = E_V + \ln\left(\frac{N_A}{N_D}\right) k_B T \quad \text{--- (2)}$$

Adding ① & ②

$$E_{Fn} + E_{Fp} = E_C + k_B T \ln\left(\frac{N_D}{N_C}\right) + E_V + \ln\left(\frac{N_C}{N_A}\right)$$

$$E_{Fn} + E_{Fp} = E_C + E_V + k_B T \ln\left(\frac{N_D}{N_A}\right)$$

Transistor is used to control flow of  $e^-$ s.

Si Ge In  
Ga As direct band gap

### Hall Effect

$$F_B = q(E \times B)$$

$$F_E = qE$$

$$qE = V(q \times B) \quad [ \because B \& E \perp n ]$$

$$qE = qVB$$

$$V_B = \frac{V_H}{w} \quad w - \text{thickness of semiconductor}$$

$$V_H = \frac{q_e B w}{neA} \quad \text{① = naive } \frac{q}{neA}$$

$$V_H = \frac{\frac{q}{neA} B w}{\frac{q}{neA} B w} = \frac{q}{ne^2 t} B \psi - \frac{IB}{net}$$

$$V_H = \frac{IB}{net} \quad R_H = \frac{1}{ne} = \frac{V_H t}{IB} \quad \text{IL} = R_H \text{ IL}$$

Exception values:  $\langle P_x \rangle = \int \psi^* (-i\hbar \frac{\partial}{\partial t}) \psi$

$$\int \psi^* \psi dz = 1$$

$$\psi = \sqrt{\frac{1}{L}} \sin \frac{n\pi z}{L}$$

