

Quantum mechanics:-

* Quantum mechanics (physics) ^{introduced} due to failure of ^{classical} physics

failure of classical physics: To explain

* Blackbody radiation

* Specific heat of solids.

* Stability of atom.

* Photoelectric effect.

* Motion of subatomic

* Compton effect

particles like electron,

* X-ray spectrum

proton etc.,

Quantum mechanics:-

Quantum mechanics is the branch of science physics that deals with the behaviour of matter and light on a subatomic

and atomic level

* It explains about the properties of electrons, protons, neutrons etc.,

Light-matter interaction:-

$$m_e = 9.1 \times 10^{-31} \text{ kg}$$

$$m_p = 1.67 \times 10^{-27} \text{ kg}$$

* classically, light-matter interactions are result of an oscillating electromagnetic field resonantly interacting with charged particles in the matter (i.e. electrons) most often bound electron.

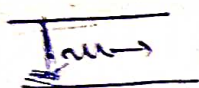
Planck's radiation:



$$E = nh\nu$$

$$n = 1, 2, 3, \dots$$

②



$$E_2 - E_1 = h\nu$$

$$h = 6.626 \times 10^{-34} \text{ J.s}$$

$$E = h\nu$$

$$E = h\nu$$

$$u(\nu) = \frac{8\pi h\nu^3}{c^3} \left(\frac{1}{e^{h\nu/k_B T} - 1} \right) \quad \text{Planck's radiation law}$$

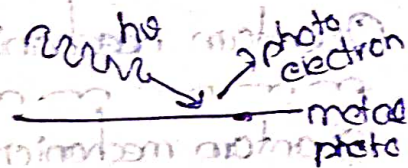
Photo-electric effect:

When light wave of sufficient energy incident on a metal then electrons are ejected from its surface. This phenomenon is known as photoelectric effect & the ejected electrons are known as photo electrons.

The photo electric effect observed

when the incident radiation is greater

than (a) equal to the work function of metal (Na, K, Zn, Cs)



$$h\nu = \phi_0 + (K.E)_{\text{max}} \quad \rightarrow \text{Einstein photoelectric equation}$$

ϕ_0 - work function of a metal

$$A_0 = \frac{hc}{\lambda_0}$$

$h\nu$ - Incident photon energy

$K.E$ - K.E of photo electron. (ejected photo electron)

$$h\nu = h\nu_0 + \frac{1}{2} m v_{\text{max}}^2$$

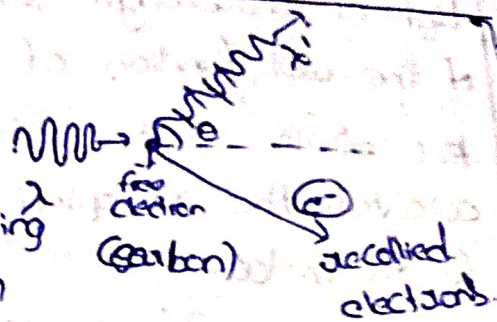
Threshold frequency.

$K.E$ of photo electron & freq. of the incident photon.

photoelectrons emitted $\propto$ Intensity of the incident radiation.

* Compton Effect: - [X-rays] :-

The decrease in energy (or decrease in wavelength) of X-rays after scattering from the object is called Compton effect (ex carbon)



The loss in energy comes in the form of recoiled electrons

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{m_0 c} (1 - \cos\theta) \quad \text{--- (1)}$$

h - Planck constant

m_0 - mass of rest electron

c - velocity of light

θ - angle of scattering

$$\Delta\lambda = 0.024 \text{ \AA} (1 - \cos\theta)$$

$$E = \frac{1.24}{\lambda \text{ \AA}} \text{ eV}$$

* Radiation - wave nature (a) particle nature

- Reflection
- Refraction
- Polarization
- Diffraction

- Reflection
- Refraction
- Photoelectric effect
- Compton effect

$$\phi_{Ba} = 2.5 \text{ eV}$$

$$\phi_{Ba} = 4.2 \text{ eV}$$

Visible light 400nm - 700nm

$$\lambda_1 = 400 \text{ nm} = 4000 \text{ \AA} \Rightarrow E = h\nu = \frac{hc}{\lambda}$$

$$\lambda_2 = 700 \text{ nm} = 7000 \text{ \AA} \quad 1 \text{ eV} = 1.609 \times 10^{-19} \text{ J}$$

λ - μm (E - eV)

$$E (\text{eV}) = \frac{1.24}{\lambda \mu\text{m}}$$

$$E = \frac{1.24}{0.4} = 3.1$$

$$E = \frac{1.24}{0.7} = 1.77$$

$$E = \frac{1.24}{\lambda \mu\text{m}}$$

- * Light of wavelength $2000 \text{ \AA}$ falls on a metal surface. If the work function of the surface is 4.2 eV . What is the K.E of the fastest photoelectrons emitted. And also calculate the stopping potential and threshold wavelength for the metal.

$$\lambda = 2000 \text{ \AA}$$

$$K.E = h\nu - \phi_0$$

$$= \frac{1.24}{0.2} - 4.2$$

$$K.E = 2 \text{ eV}$$

$$\phi_0 = \frac{hc}{\lambda_0} \Rightarrow \lambda_0 = \frac{hc}{\phi_0} = 0.295 \mu\text{m}$$

Threshold frequency $\nu = \frac{c}{\lambda} = \frac{3 \times 10^8}{0.295 \mu\text{m}}$

$$G(\text{eV}) = \frac{1.24}{\lambda(\mu\text{m})}$$

- * A photo of wavelength $10 \text{ \AA}$ strikes an electron and is scattered at an angle of 150° to its original dir. find the wavelength of the photon after collision.

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos\theta)$$

$$\frac{h}{m_0c} = 0.024 \text{ \AA}$$

$$\Delta\lambda = 0.024 \text{ \AA} (1 - \cos\theta)$$

$$\theta = 150^\circ$$

$$\Delta\lambda = 0.044 \text{ \AA}$$

$$\lambda' = \lambda + \Delta\lambda = 10.044 \text{ \AA}$$

$$1.8 = \frac{1.24}{\lambda_0} = 3$$

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$$\frac{1.24}{\lambda_0} = 3$$

Dual nature of radiation/matter:-

* It is discussed by Louis de Broglie

* A wave is associated with the moving matter particle. We call that wave as "matter wave".

Ex: electrons, protons

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

p - momentum of particle (mv)

↳ wave length of matter wave.

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

→ de-broglie relation.

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

$$p = mv$$

$$k = \frac{p}{\hbar}$$

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

$$k = \frac{p^2}{2m} \Rightarrow \sqrt{2mk}$$

$$k \cdot e = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mk \cdot e} = \sqrt{2 \times 9.1 \times 10^{-31} \times 1000 \times 1.6 \times 10^{-19}} = 1.7 \times 10^{-24}$$

$$E = h\nu = \frac{hc}{\lambda} \rightarrow \text{Energy of a photo.}$$

$$\lambda = \frac{h}{\sqrt{2mk}}$$

$$\lambda \propto \frac{1}{\sqrt{m}}$$

Heisenberg uncertainty principle:-

* Take two pairs of canonically conjugate variables.

$$\Delta x = 0$$

$$\Delta x \Delta p = h$$

$$\Delta p \rightarrow \infty$$

position momentum
 x p_x

$$\Delta x \Delta p_x \approx h$$

$$\Delta y \Delta p_y \approx h$$

$$\Delta z \Delta p_z \approx h$$

* no two canonically conjugate variables can't be measured simultaneously

$$\Delta E \cdot \Delta t = h / 2\pi$$

$$\Delta t \cdot \Delta E = h / 2\pi$$

* It is impossible to determine both position and momentum of a electron in an atom simultaneously and accurately

$\Delta x \rightarrow$ uncertainty in position

$\Delta p \rightarrow$ uncertainty in momentum.

if $\Delta x = 0$

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

$$\Delta x = \frac{h}{\Delta p} = 0$$

Quantum mechanics explains all effects like black-body radiation

$x \quad p_x$

$y \quad p_y$

$z \quad p_z$

$$\Delta x \Delta p_x \approx \frac{h}{2}$$

$$\Delta y \Delta p_y \approx \frac{h}{2}$$

$$\Delta E \Delta t \approx \frac{h}{2} \rightarrow \text{(use in spectral width of source)}$$

$$\Delta \phi \Delta L_z \approx \hbar$$

$\downarrow \quad \downarrow$
angle $(z\text{-component of angular momentum})$

Applications

→ We measure the spectral width ($\Delta \lambda$)

→ we can measure ground state energy of hydrogen atom

$$1s \rightarrow (-13.6 \text{ eV})$$

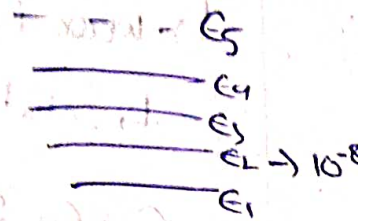
→ we can measure the mass of the meson
 $m = 200 m_e$

→ we prove that the non-existence of e^- inside the nucleus.

An electron in the $n=2$ state of hydrogen remains there on the average of about 10^{-8} s before making a transition to $n=1$ state. Estimate the uncertainty in the energy of the $n=2$ state. What fraction of the transition energy is this? What is the

wavelength and width of this line in the spectrum by hydrogen atom

$$E_n = -\frac{13.6 \text{ (ev)}}{n^2} \quad n=1,2,3,\dots$$



$$E_1 = -13.6 \text{ ev}$$

first excited state

$$n=2 \Rightarrow E_2 = -\frac{13.6}{4} = -3.4 \text{ ev}$$

Estimate in uncertainty

$$\Delta E \cdot \Delta t \approx h$$

$\Delta t \rightarrow 10^{-8} \text{ s}$

$$\Delta E = \frac{h}{10^{-8} \text{ s}} = \frac{6.626 \times 10^{-34}}{10^{-8}} \text{ J}$$

$$\Delta E = \frac{6.626 \times 10^{-26} \text{ J}}{1.602 \times 10^{-19}} \text{ (ev)}$$

$$E_2 - E_1 = -3.4 \text{ ev} + 13.6 \text{ ev} = 10.2 \text{ ev}$$

$\Delta E \approx 10^{-8}$

$$\frac{\Delta E}{E} = \frac{4.14 \times 10^{-7} \text{ ev}}{10.2 \text{ ev}} = 4.06 \times 10^{-8}$$

$$\lambda (\text{nm}) = \frac{1.24}{E (\text{ev})}$$

$$\lambda = \frac{1.24}{10.2} = 0.121 \text{ nm} = 121 \text{ nm}$$

$$\Delta \lambda = \frac{\Delta E}{E} \lambda = 4.06 \times 10^{-8} \times 121 \times 10^{-9} = 4.91 \times 10^{-16} \text{ nm}$$

$$\frac{\Delta E}{E} = -\frac{hc}{\lambda^2} \Delta \lambda = -\frac{\Delta \lambda}{\lambda}$$

Wave is associated

↳ wave function $\rightarrow \psi(x, t)$ $\psi(y, t)$

↳ solution of wave equation $\psi(z, t)$

$$G = E_0 \sin(kz - \omega t)$$

$$\Delta p(z, t) = \Delta p_{\max} \cos(kz - \omega t)$$

$$S_{\max}(z, t) = A \cos C(kz - \omega t)$$

* We need a wave function to represent a particle in quantum mechanics.

* If we know the wave function then it's easy to retrieve information.

* It is represented as $\psi(x, t)$

ψ^* $\rightarrow$ complex conjugate of ψ

$\psi^* \psi$ $\rightarrow$ probability of finding the particle in unit volume

Normalized condition:-

$$\int_{-\infty}^{+\infty} \psi^* \psi d\tau = 1$$

ψ - wave function

Total probability

$\int \psi^* \psi d\tau \rightarrow$ total probability of finding a particle

Operator:-

* In Q.M. every quantity has some physical operator.

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

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

$$\vec{\nabla} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \quad (\text{Del operator})$$

$$\hat{p} = -i\hbar \vec{\nabla} = -i\hbar \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right)$$

$$= -i\hbar \hat{i} \frac{\partial}{\partial x} - i\hbar \hat{j} \frac{\partial}{\partial y} - i\hbar \hat{k} \frac{\partial}{\partial z}$$

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

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

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

$\hat{p}_x$ $\hookrightarrow$ x-component of the momentum operator.

$\hat{p}_y$ $\hookrightarrow$ y-component of the momentum operator.

$\hat{p}_z$ $\hookrightarrow$ z-component of the momentum operator.

$$\hat{E} (\text{Energy operator}) = -i\hbar \frac{\partial}{\partial t}$$

$$K.E. = -\frac{\hbar^2}{2m} \nabla^2$$

$$K.E. = \frac{p^2}{2m} = \frac{(i\hbar \nabla)^2}{2m} = -\frac{\hbar^2 \nabla^2}{2m}$$

Hamiltonian operator:

* (Total energy operator)

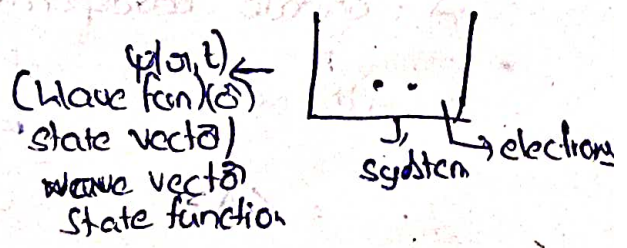
$$K.E. + P.E. \Rightarrow \left[-\frac{\hbar^2 \nabla^2}{2m} + V(x) \right]$$

$\rightarrow \hat{A} \cdot \psi = a \cdot \psi$ (operator operates on a wave function)
 $\hookrightarrow$ eigenvalue

Q

* When sub-atomic particles then wave is associated with it.

* This wave function may represent $\vec{E}, \vec{B}, \Delta \vec{p}$,



ψ - is a fun of spatial and time-coordinates.

$$\psi(z,t) = \psi_0 \cos(kz - \omega t) \\ = \psi_0 e^{i(kz - \omega t)}$$

$$\psi^*(z,t) = \psi_0 e^{-i(kz - \omega t)} \text{ (complex conjugate)}$$

$\psi^* \psi$ - (probability density) of finding a particle / System in unit volume)

$\psi^* \psi d\tau$ - " " " " " " in a elementary volume $d\tau$ (1/v)

Total probability density = $\int \psi^* \psi d\tau$

Normalized condition $\int_{-\infty}^{\infty} \psi^* \psi d\tau = 1$ 

Expectation value of an observable:

- g' - u' n

* The expectation value of any parameter.

Ex: Simple pendulum experiment

$$\begin{array}{c} g_1 \text{ --- } g_n \text{ (observable)} \\ g_1 + g_2 \text{ --- } g_n \\ \hline n \end{array} = \text{expectation value (average of all values)}$$

* It is represented as $\langle A \rangle$

* And defined as
$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{A} \psi d\tau}{\int_{-\infty}^{\infty} \psi^* \psi d\tau}$$

$\hat{A}$ - operator corresponding to the observable

ψ is normalized
$$\int_{-\infty}^{\infty} \psi^* \psi d\tau = 1$$

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi d\tau$$

$A\psi = a\psi \rightarrow$ Eigen value equation.

$$\hat{G}_x = \frac{\partial}{\partial x} e^{ikx} = ik e^{ikx}$$

$$\hat{A}\psi = a\psi$$

$\hookrightarrow$ eigen value. (possible values of an observable.)

$\hat{G}_x: g_1, \dots, g_n$ are eigen values.

$$\hat{G}_x: \langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* (-i\hbar \frac{\partial}{\partial x}) \psi dx$$

$\hookrightarrow$ expectation value of the x-component of the momentum.

position vector $\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi dx$

observable

operator

p_x

$-i\hbar \frac{\partial}{\partial x}$

p_y

$-i\hbar \frac{\partial}{\partial y}$

p_z

$-i\hbar \frac{\partial}{\partial z}$

$\hat{c}$

$i\hbar \frac{\partial}{\partial t}$

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

$$\vec{\nabla} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$$

$K.E + P.E$

$$\downarrow$$

$$\frac{-\hbar^2 \nabla^2}{2m} + V = \text{hamiltonian}$$

$\hat{H}$

$\int$ Schrodinger time independent wave equation :-

3-dim wave eq $\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}$

$$\textcircled{a} \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi(x) = E \psi(x) \quad \left[\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \right] \hookrightarrow \text{wave equation.}$$

$\hookrightarrow$ STI wave

consider free particle $V=0$

$$\textcircled{a} \left[-\frac{\hbar^2}{2m^2} \nabla^2 \right] \psi(x) = E \psi(x) \Rightarrow \text{STI wave for free particle.}$$

Prob A particle constrained to move along x-axis in the domain $0 \leq x \leq L$ has a wave function $\psi(x) = \sin\left(\frac{n\pi x}{L}\right)$ where n is an integer. Normalize the wave function and evaluate the expectation

$$\psi(x) = N \cdot \sin\left(\frac{n\pi x}{L}\right) \quad \psi^*(x) = N \sin\left(\frac{n\pi x}{L}\right)$$

$\hookrightarrow$ Normalization constant $\psi^* \psi = |\psi|^2$
 $\psi \rightarrow$ wave fun

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1 \quad (N \cdot L)$$

$$\int_0^L \psi^* \psi dx = 1 \Rightarrow \int_0^L N^2 \sin^2 \frac{n\pi x}{L} dx = 1$$

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

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

$$\frac{N^2}{2} \left(\int_0^L dx - \frac{\sin \frac{2n\pi x}{L}}{\frac{2n\pi}{L}} \right) \Big|_0^L = 1$$

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

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

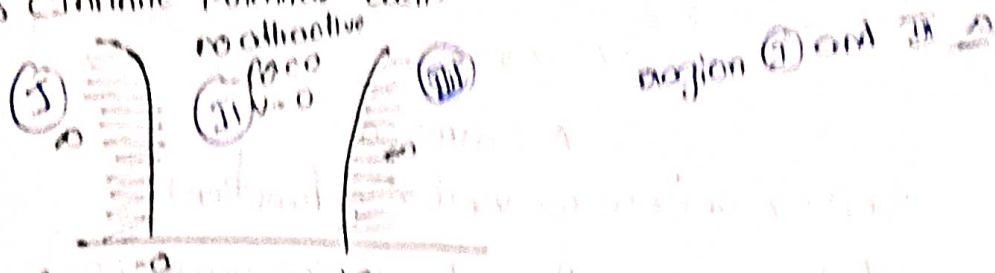
$$\langle p_x \rangle = \int_0^L \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi dx$$

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

$$= \frac{2}{L} i\hbar \int \sin^2 \left(\frac{n\pi}{L} x \right) dx$$

1-D eigen value problem:

We will discuss for a square well potential with rigid walls (infinite potential well).



potential function for $V(x) = 0$, $-a < x < a$

potential function for $V(x) = \infty$, $|x| > a$

$$\Delta \psi = 0$$

$$|x| < a \quad V = 0$$

Schrodinger time independent equation

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

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + 0 \right] \psi = E \psi$$

$$\text{Eq } -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \rightarrow \boxed{1} \quad k^2 = \frac{2mE}{\hbar^2} \quad (1)$$

Assume the solution to above eq $\psi(x) = A \sin kx + B \cos kx$

$$\text{at } x = \pm a \quad V(x) = \infty \quad \psi(x) = 0$$

$$\psi(a) = 0 = \psi(-a) \quad (\text{Boundary condition})$$

$$\psi(a) = 0 = A \sin ka + B \cos ka \rightarrow (2)$$

$$\psi(-a) = A \sin(-a) + B \cos(-a)$$

$$= -A \sin ka + B \cos ka \rightarrow (3) \quad \cos(-a) = \cos a$$

$$\sin(-a) = -\sin a$$

$$(1) \cdot (3) \quad \psi(a) + \psi(-a)$$

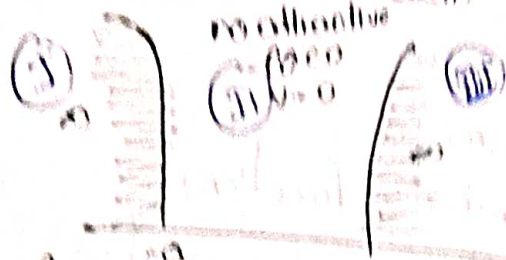
$$\Rightarrow A \sin ka + B \cos ka - A \sin ka + B \cos ka$$

$$\Rightarrow 2 B \cos ka = 0$$

$$\Rightarrow B \cos ka = 0$$

1-D eigen value problem:

We consider electron in a square well potential with rigid walls (infinite attractive well).



Region (I) and (III)

Potential function for $V(x) = 0$, $-a < x < a$

Potential function for $V(x) = \infty$, $|x| > a$

$$A\psi = E\psi$$

$$|x| < a \quad V=0$$

Schrodinger's time independent equation for

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right] \psi(x) = E \psi(x) \quad \text{Region (II) } V=0$$

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 0 \right] \psi = E \psi$$

$$\text{Eq } -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \Rightarrow \frac{d^2 \psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi$$

$$\frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \rightarrow |k| \quad k^2 = \frac{2mE}{\hbar^2} \quad (1)$$

Assume the solution to above eq $\psi(x) = A \sin kx + B \cos kx$

$$\text{at } x = \pm a \quad V(x) = \infty \quad \psi(\pm a) = 0$$

$$\psi(a) = 0 = \psi(-a) \quad (\text{Boundary condition})$$

$$\psi(a) = 0 = A \sin ka + B \cos ka \rightarrow (1)$$

$$\psi(-a) = A \sin(-a) + B \cos(-a)$$

$$= -A \sin ka + B \cos ka \rightarrow (2) \quad \cos(-\pi) = \cos \pi$$

$$\sin(-\pi) = -\sin \pi$$

$$(1) - (2) \quad \psi(a) + \psi(-a)$$

$$\Rightarrow A \sin ka + B \cos ka - (-A \sin ka + B \cos ka)$$

$$\Rightarrow 2B \cos ka = 0$$

$$\Rightarrow B \cos ka = 0$$

② ③

$$A \sin ka + B \cos ka = 0$$

$$-A \sin ka + B \cos ka = 0$$

$$2A \sin ka = 0$$

$$A \sin ka = 0$$

$$\psi(x) = A \sin kx + B \cos kx \text{ (wave function)}$$

if $A=0$, $B=0$ then $\psi=0$ (not acceptable)

possible conditions are

① $A \neq 0$, $B \neq 0$ then $B \cos ka = 0$

$$\cos ka = 0$$

$$ka = \frac{n\pi}{2}$$

where $n = 1, 3, 5, 7, \dots$
($2n+1$)

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

from eq ① $k^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{4a^2}$

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

energy eigen values of particles

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

$n = 1, 3, 5, 7, \dots$

$$\psi = A \sin ka + B \cos ka$$

$$A \neq 0 \quad B = 0$$

$$A \sin ka = 0$$

$$ka = \frac{n\pi}{2}$$

$n = 2, 4, 6, 8, \dots$

$$k = \frac{n\pi}{2a}$$

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

We determine A and B by using normalized condition

$$\int_{-a}^a \psi^2(x) dx = 1 \quad \psi^* \psi = \psi^2$$

$$\int_{-a}^a (A \sin kx)^2 dx = 1 \Rightarrow \int_{-a}^a A^2 \sin^2 kx dx = 1$$

$$\Rightarrow A^2 \left[\int_{-a}^a \frac{1 - \cos 2kx}{2} dx \right] = 1$$

$$\frac{A^2}{2} \left[\int_{-a}^a (1 - \cos 2kx) dx \right] = 1$$

$$\frac{A^2}{2} \left[x \right]_{-a}^a = 1$$

$$\frac{A^2}{2} [2a] \Rightarrow A^2 a = 1$$

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

$$\int_{-a}^a \psi^2 dx \quad \psi = B \cos kx$$

$$\int_{-a}^a B^2 \cos^2 kx dx = \int_{-a}^a B^2 \left(\frac{1 + \cos 2x}{2} \right) dx$$

$$= \frac{B^2}{2} \int_{-a}^a (1 + \cos 2x) dx$$

$$= \frac{B^2}{2} \left[x + \frac{\sin 2x}{2} \right]_{-a}^a$$

$$= \frac{B^2}{2} \left[2a + \frac{1}{2} [2 \sin 2a] \right]$$

$$= \frac{B^2}{2} [2a + \sin 2a]$$

$$= \frac{B^2}{2}$$

$$\sin \frac{n\pi}{2a}$$

$$\frac{2a}{n\pi} \sin \left(\frac{n\pi}{2} \right)$$

$$\left[2a + \frac{\sin \frac{n\pi}{2}}{\frac{n}{2}} \right]$$

$$\frac{2}{n\pi} \sin \left(\frac{n\pi}{2} \right)$$

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

$$\psi_1(x) = \frac{1}{\sqrt{a}} \sin \left(\frac{n\pi}{2a} \right) x \quad n = 2, 4, 6, \dots$$

$$= \frac{1}{\sqrt{a}} \sin \left(\frac{n\pi}{2a} \right) x \quad n = 1, 3, 5, \dots$$

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

$n=1$ Ground state

$$E_1 = \frac{\pi^2 \hbar^2}{8ma^2}$$

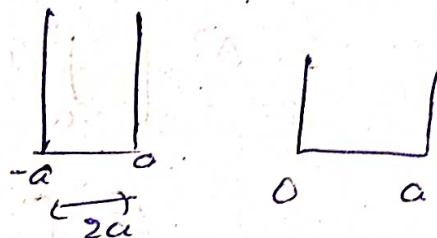
$$\psi_1(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a}x\right)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{8ma^2} = \frac{n^2 \pi^2 \hbar^2}{2m\omega^2}$$

$\omega = 2a = \text{width of the box}$

$$V(x) = 0 \quad 0 \leq x \leq a$$

$$= \infty \quad \text{otherwise } |x| > a$$



$$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34} \text{ J}\cdot\text{sec}$$

$$E_2 - E_1 = \frac{2^2 \pi^2 \hbar^2}{2m\omega^2} - \frac{1^2 \pi^2 \hbar^2}{2m\omega^2} = \frac{3\pi^2 \hbar^2}{2m\omega^2}$$

$$= \frac{3 \times (3.14)^2 \times (1.055 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times 10^{-20} \times 1.609 \times 10^{-14}}$$

$$= 113.27 \text{ eV}$$

$$E_2 - E_1 = h\nu \Rightarrow \nu = \frac{E_2 - E_1}{h} = \frac{113.27 \text{ eV}}{h} = \frac{1.609 \times 10^{-19} \times 113.27 \text{ eV}}{6.626 \times 10^{-34}}$$

$$\nu\lambda = \nu \Rightarrow \lambda = \frac{c}{\nu} = \frac{3 \times 10^8}{2.7 \times 10^{16}} = 1.1 \times 10^{-8} \text{ m}$$

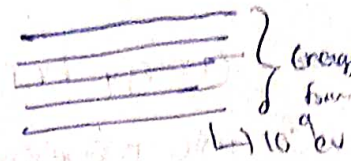
$$\boxed{\lambda = 11 \text{ nm (UV region)}}$$

* A electron in a one-dimensional infinite well defined.
(a) ν and λ

Pauli's exclusive principle:- No two electrons in a given interacting system can have same quantum state and hence same energy.

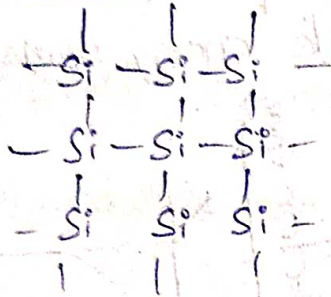
Semi-conductors.

* Band theory of solids: Group of closely spaced energy levels.



Band formation:

Si-crystal



$L=0 \rightarrow s$

$L=1 \rightarrow p$

$L=2 \rightarrow d$

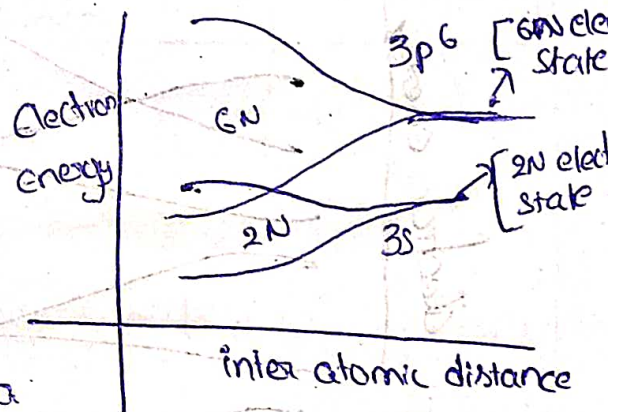
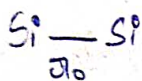
$L=3 \rightarrow f$

* Atomic number $Z = 14$ with electronic configuration

$1s^2 2s^2 2p^6 3s^2 3p^2$

bound very tightly

Valency shell electrons

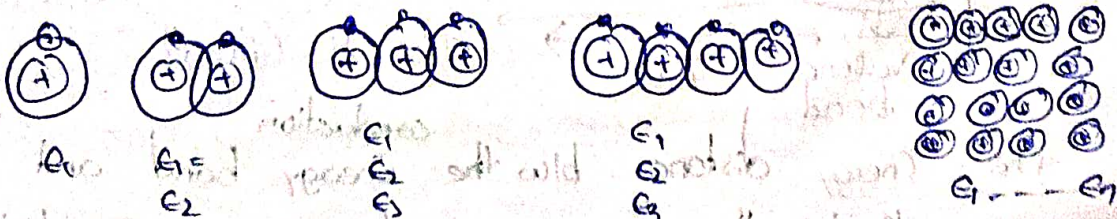
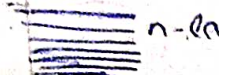


* consider an atom electron in a particular atom. And this electron has energy level E_1

• When we brought two atom together then the wave functions of two atom overlap and therefore the energy corresponds to these wavefunction splits into two energy.

* When we brought N atoms then N -energy levels formed

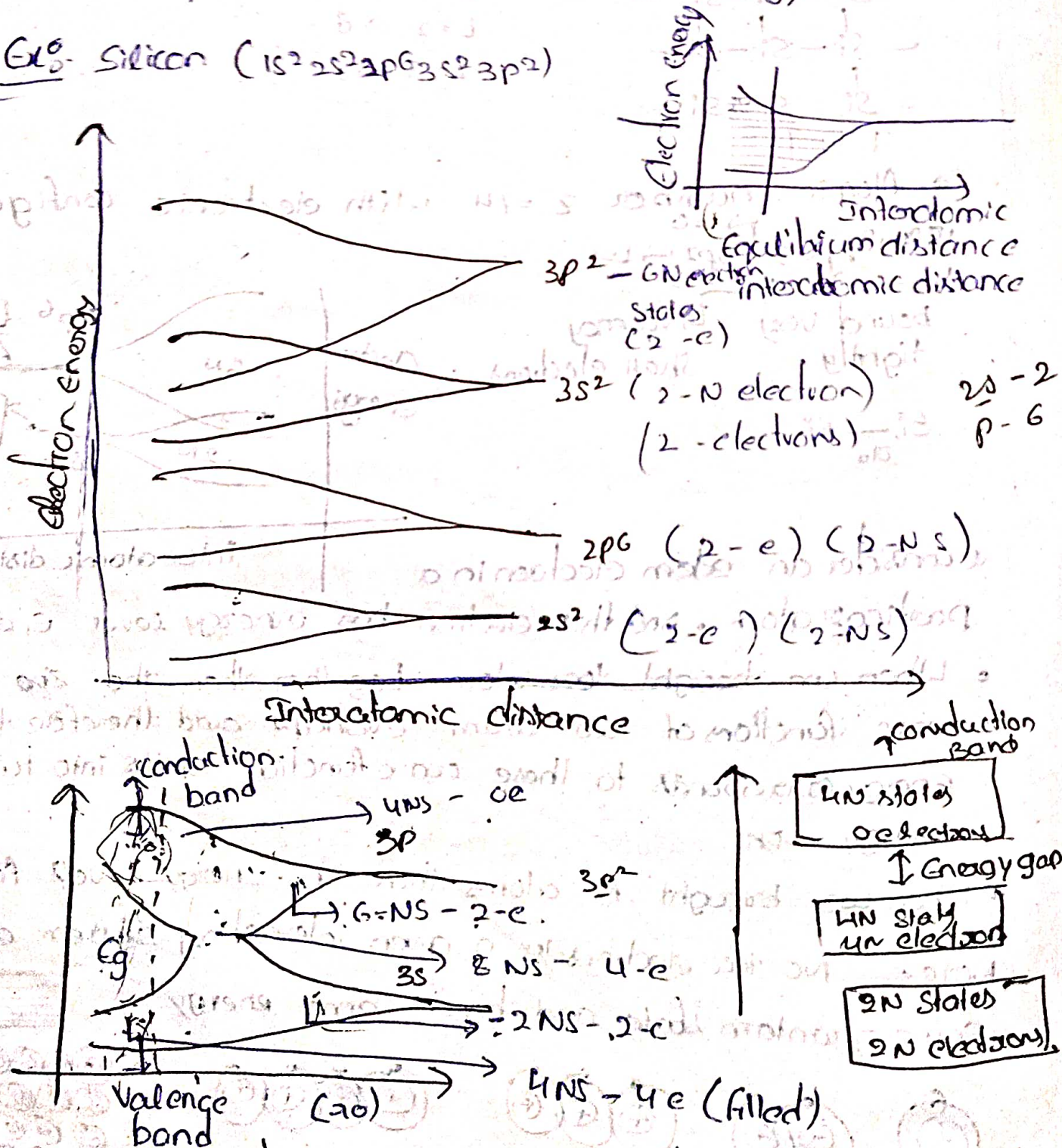
Note: No two electrons in a given interacting system can have same quantum state and hence same energy



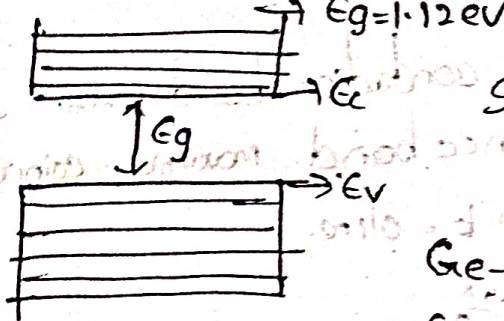
Here we know that solid is a collection of n -atoms that means n -bands energy levels

- Collection of energy levels is energy bands.
- Energy band is formed by splitting of one energy level into n -energy level.
- Pushing the atoms together, the initial quantized energy level will split into a band of discrete energy levels.

Ex: Silicon ($1s^2 2s^2 2p^6 3s^2 3p^2$)



The energy distance b/w the conduction band and valence band in the energy

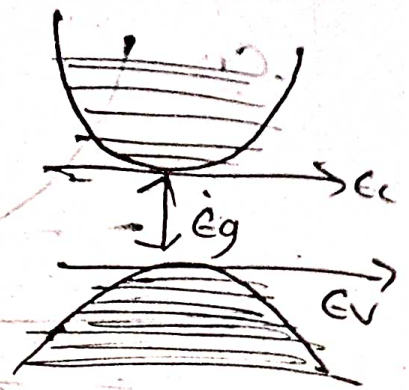


Semi-conductor
(1-2 eV) E.G.

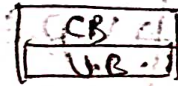
Ge - 0.67 eV $\approx$ 0.7 eV

Si - 1.12 eV

GaAs $\rightarrow$ 1.42 eV



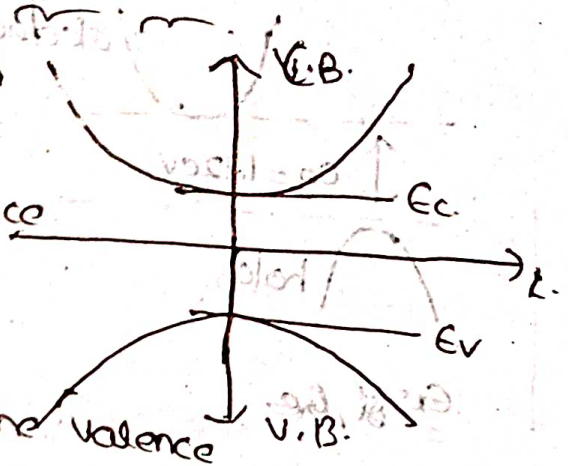
Metal & conductor: $\approx$ 0 eV



Insulators: $E_g > 3$ eV. e.g. plastic, rubber, wood, glass, resin.

Semi-conductors are also insulators at $T=0$ K.

At $T=0$ K the conduction band is empty means all the valence electrons present will be in valence band only.



Conduction in the conductor is possible when the electrons in the valence band become free (move from V.B. to C.B.) (or) bring few e^- to the C.B. at $T=0$ K. The electrons transmission not occurs.

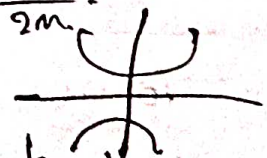
Types of semiconductors based on band gaps:-

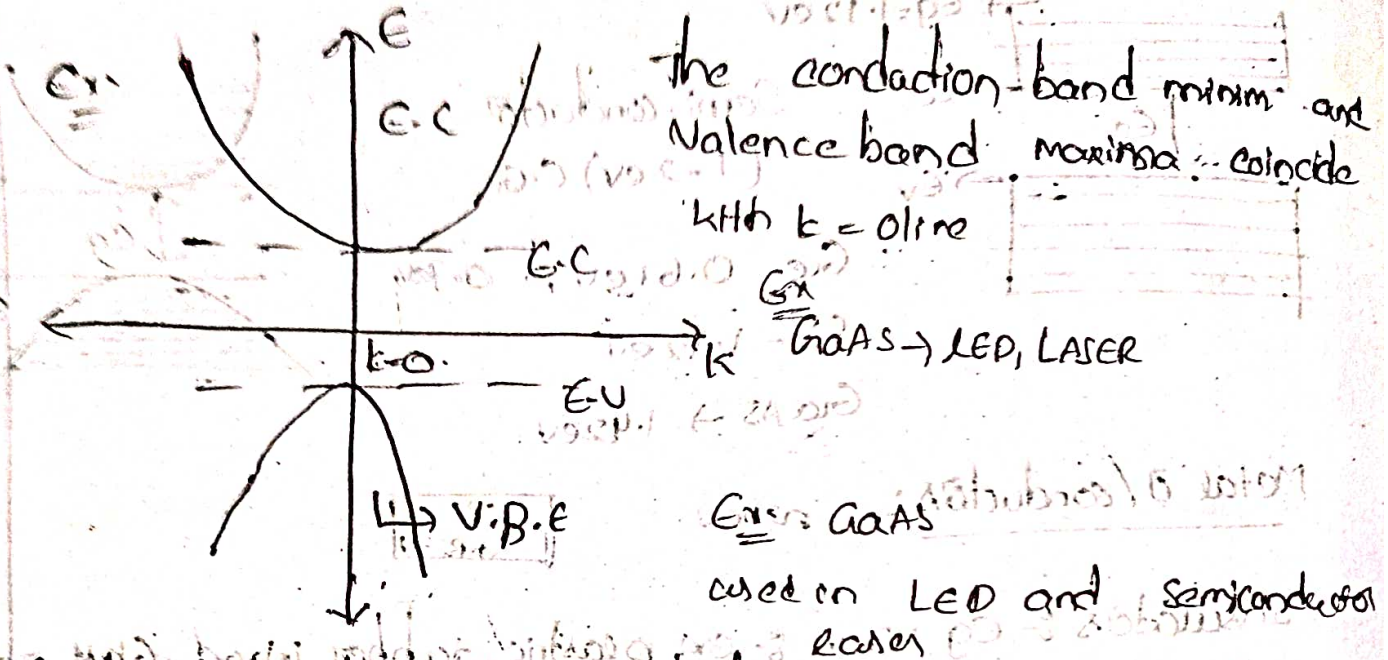
1. Direct band gap semi-conductors:-

By the quantum mechanics $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

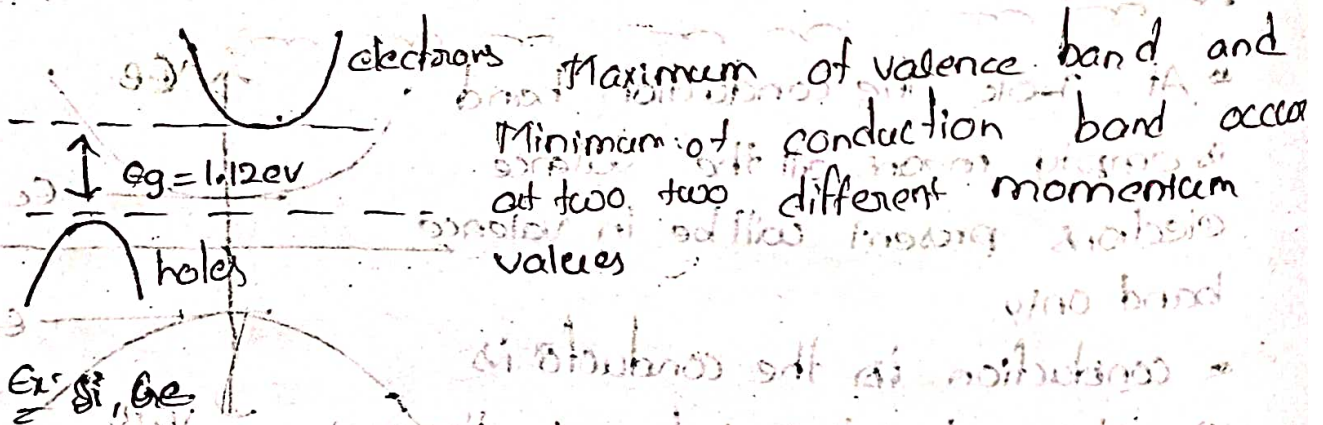
$\Rightarrow E \propto k^2$ (Equation of parabola)

$\therefore$ lower parabola represents the valence band and upper parabola represents conduction band.





Indirect bandgap Semi-conductor:-



Density of states function:- The number of quantum states between E and $E+dE$ is

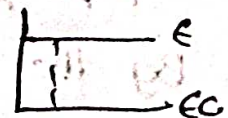
$$g(E)dE = \frac{4\pi a^3}{h^3} (2m)^{3/2} \sqrt{E} dE$$

$$g(E) = \frac{4\pi}{h^3} (2m)^{3/2} \sqrt{E}$$

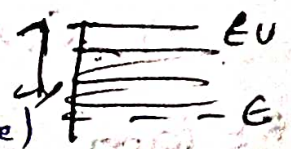


The density of quantum states function of energy

for C.B. $g(E) = \frac{4\pi}{h^3} (2m_e^*)^{3/2} \sqrt{E - E_c}$



for V.B. $g(E) = \frac{4\pi}{h^3} (2m_h^*)^{3/2} \sqrt{E_v - E}$



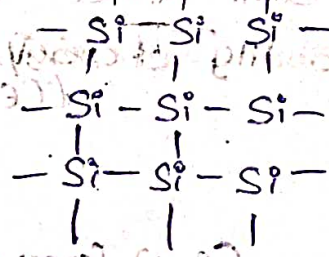
m_e^* - sufficient mass of electron (effective)
 m_h^* - sufficient mass of hole

Intrinsic Semiconductor:- Pure form of semi-conductor.

• pure form (No impurities & no defects).

Ex: Si - $1s^2 2s^2 2p^6 3s^2 3p^2$

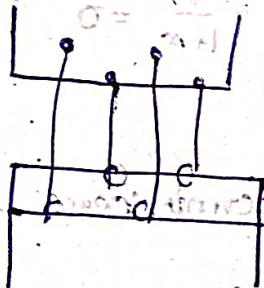
• The energy need to break the bond is the Energy gap



• Intrinsic Si at $T=0\text{K}$ act as insulator

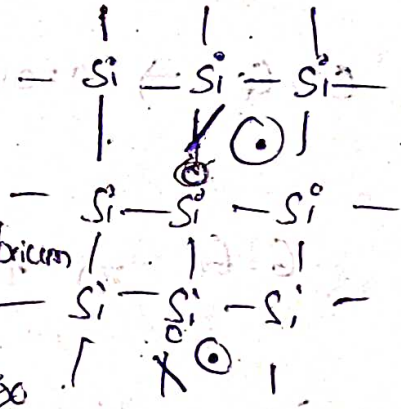
• If we increase the temp, the silicon atoms start vibrating, and generates phonons (heat waves / sound). $\text{The phonons Propagating in a same direction form a giant phonon. These have the great more energy than energy gap. Therefore the bond breaks.}$

• Absence of bound electron is called hole.



$n_e = n_h$ in a sem-con

$n_i = n_0 = p_0$ (Thermal Equilibrium State) (Intrinsic carrier concentration) (no of ~~the~~)



Thermal equilibrium state:-

• No Magnetic field.

• No light exposure

• No potential difference

• No temp gradient

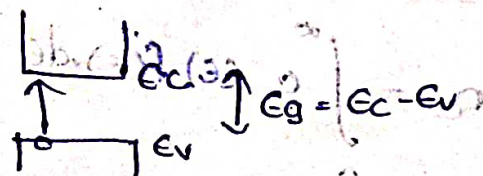
• No electric field



Carrier concentration in Intrinsic semi-conductors:-

Intrinsic semi-conductors:-

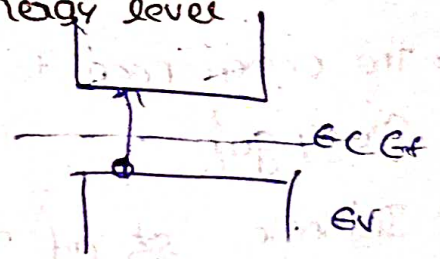
Bond energy $\approx$ Energy gap



Fermi-energy level :- The highest occupied energy level at absolute zero (0K) temperature is called as Fermi level.

Fermi-Dirac distribution function :- for finding the probability of energy occupancy at a given energy level.

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



$E_f \rightarrow$ Fermi-energy

$T = 0 \text{ K}$

$\Rightarrow$

$$f(E) = \frac{1}{1 + e^{-\frac{0}{0}}} = \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0} = 1$$

$E < E_f$

$E - E_f < 0$

$$= \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0} = 1 \text{ (probability function)}$$

$E > E_f \Rightarrow T = 0 \text{ K}$

$\Rightarrow$

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

$E - E_f > 0$

$= \frac{1}{1 + \infty} = 0$

$E = E_f$

$\Rightarrow$

$T = 0 \text{ K}$

$f(E) =$

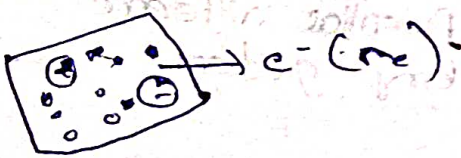
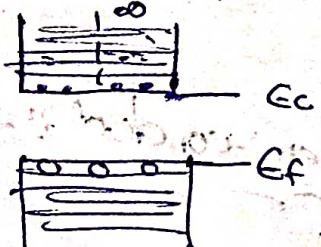
$$\frac{1}{1 + e^0} = \frac{1}{2}$$

$= \frac{1}{2}$

(Fermi energy state)

* Reference imaginary level (Fermi-level).

Thermal-equilibrium electron concentration in intrinsic semiconductor



$$n_e = \frac{\hbar^2}{2\pi^2} \frac{d^2 E}{dk^2}$$

$$n_e = \int_{E_c}^{\infty} g_c(E) f(E) dE$$

The electron concentration under thermal equilibrium condition in intrinsic semi-conductor is obtained by multiplying the density of states function with the Fermi-Dirac distribution function and then integrating under the appropriate limits.

$$n_e = \int_{E_c}^{\infty} g_c(E) f(E) dE$$

$$f(E) = \frac{1}{1 + e^{\frac{E - E_f}{k_B T}}} \Rightarrow \text{as } E > E_f \Rightarrow E - E_f > 0$$

$$\frac{1}{1 + e^{\frac{E - E_f}{k_B T}}} \gg 1$$

$$\Rightarrow f(E) = e^{-\frac{(E - E_f)}{k_B T}}$$

$$n_0 = \int_{E_c}^{\infty} \frac{4\pi (2m_e)^{3/2}}{h^3} \sqrt{E - E_c} \cdot e^{-\frac{(E - E_f)}{k_B T}} dE$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} \int_{E_c}^{\infty} (E - E_c)^{1/2} e^{-\frac{(E - E_f)}{k_B T}} dE$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} \int_{E_c}^{\infty} (E - E_c)^{1/2} e^{-\frac{(E - E_c + E_c - E_f)}{k_B T}} dE$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} e^{-\frac{(E_c - E_f)}{k_B T}} \int_{E_c}^{\infty} (E - E_c)^{1/2} e^{-\frac{(E - E_c)}{k_B T}} dE$$

$$\text{Let } \eta = \frac{E - E_c}{k_B T} \Rightarrow E - E_c = k_B T \eta$$

$$dE = k_B T d\eta$$

$$\text{at } E = E_c \quad \frac{E - E_c}{k_B T} \Rightarrow \eta = 0$$

$$\text{at } E = \infty \quad \eta = \infty$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} \cdot e^{-\frac{(E_c - E_f)}{k_B T}} \int_0^\infty (E - E_c)^{1/2} e^{-\frac{(E - E_c)}{k_B T}} dE$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} \cdot e^{-\frac{(E_c - E_f)}{k_B T}} \int_0^\infty (k_B T)^{1/2} \eta^{1/2} e^{-\eta} k_B T d\eta$$

$$= \frac{4\pi (2m_e)^{3/2}}{h^3} (k_B T)^{3/2} e^{-\frac{(E_c - E_f)}{k_B T}} \int_0^\infty \eta^{1/2} e^{-\eta} d\eta$$

$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}} \quad \left[\frac{\sqrt{\pi}}{2} \right]$$

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

$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$

$$n_0 = N_c e^{-\frac{(E_c - E_f)}{k_B T}}$$

$$N_c = 2 \left[\frac{2\pi m_e k_B T}{h^2} \right]^{3/2}$$

= Effective density
- of states for material
in conduction band

$$N_v = 2 \left[\frac{2\pi m_h k_B T}{h^2} \right]^{3/2}$$

$$p_0 = N_v e^{-\frac{(E_f - E_v)}{k_B T}}$$

$$p_0 = \int_{E_v}^{-\infty} g_v(E) [1 - f(E)] dE$$

$$g_v = \frac{4\pi (2m_h)^{3/2}}{h^3} (E_v - E)$$

$$p_0 = n_0 = n_i \text{ (Intrinsic carrier concentration)}$$

$$p_0 \cdot n_0 = n_i^2 \text{ (law of mass action in semi-conductor)}$$

$$n_i^2 = N_c N_v e^{-\frac{(E_c - E_f)}{k_B T}} e^{-\frac{(E_f - E_v)}{k_B T}}$$

$$= N_c N_v e^{-\frac{E_c + E_f - E_f + E_v}{k_B T}}$$

$$= N_c N_v e^{-\frac{(E_c - E_v)}{k_B T}}$$

$$= N_c N_v e^{-\frac{(E_g)}{k_B T}}$$

$$n_i^2 = N_c N_v e^{-\frac{E_g}{k_B T}}$$

$$n_i = (N_c N_v)^{1/2} e^{-\frac{E_g}{2k_B T}}$$

$$E_c - E_v = E_g$$

Location of the Fermi level in intrinsic semi-conductor:

$$n_0 = p_0 \quad E_F = E_{Fi}$$

$$n_0 = N_C e^{-(E - E_F)/k_B T} \quad p_0 = N_V e^{-(E_{Fi} - E_V)/k_B T}$$

$$n_0 = p_0 \Rightarrow N_C e^{-(E_C - E_{Fi})/k_B T} = N_V e^{-(E_{Fi} - E_V)/k_B T}$$

$$e^{-\frac{E_C + E_{Fi} + E_{Fi} - E_V}{k_B T}} = \frac{N_V}{N_C}$$

$$\Rightarrow e^{\frac{2E_{Fi} - (E_C + E_V)}{k_B T}} = \frac{N_V}{N_C}$$

$$\ln\left(\frac{N_V}{N_C}\right) = \frac{2E_{Fi} - (E_C + E_V)}{k_B T}$$

$$\Rightarrow E_{Fi} = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{N_V}{N_C}\right)$$

$$E_{Fi} = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{N_V}{N_C}\right)$$

$$E_{Fi} = E_{\text{midgap}} + \frac{3k_B T}{4} \ln\left(\frac{m_n^0}{m_p^0}\right)$$

$$\frac{N_V}{N_C} = \left(\frac{m_n^0}{m_p^0}\right)^{3/2}$$

$$\text{if } m_n^0 = m_p^0$$

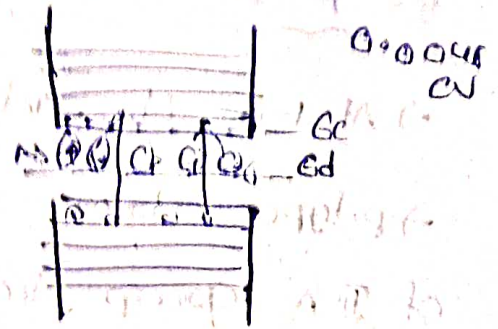
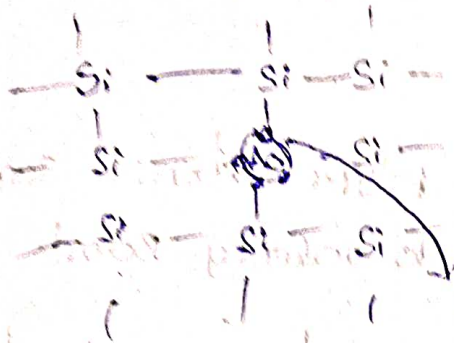
$$\Rightarrow E_{Fi} = E_{\text{midgap}}$$

Extrinsic Semiconductors

* IIIA - B, Al, Ga, In, Tl

p-type extrinsic semiconductor

Si + P, As (N-type) S.C.



N-type - extrinsic conductor:

* Extrinsic semiconductor is formed by the doping process

* N-type extrinsic semi-con formed by addition of 5th A

group ele (P, As, Sb, Bi, and Bi) to the intrinsic semiconductor

* The donor energy levels in n-type extrinsic semiconductor will be very close to the conduction band edge.

* If we increase the temperature donor atoms will get ionised and add elect the electrons to the conduction band without adding the holes in the V.C.

* As we further increase the temperature the covalent bonds starts breaking and form the electron hole pairs.

∴ The majority charge carriers in p-type semiconductor are electron and minority carriers are holes

2. p-type semi-conductor: (impure)

→ At $t=0$: it act as an insulator.

→ p-type extrinsic semiconductors are formed by addition of III A group impurities like B, Al to the intrinsic semi-conductor. (S)

→ The ~~energy~~^{Accepto} energy levels in p-type extrinsic semi-conductor will be very close to valency band and ready to accept an electron.

→ It creates large number of holes in valence band.

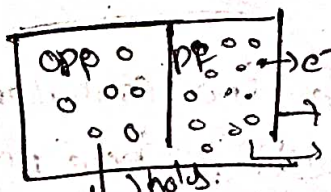
Carrier transport phenomena:

1. There are two process to transport the charge carriers.

1. Drift

2. Diffusion

Diffusion: In p-type semi-conductor.



it is diffusion current density for holes

$$J_p = -q D_p \frac{dp}{dx}$$

Diffusion constant

L) Magnitude of electric charge $= 1.6 \times 10^{-19}$

$$\frac{dp}{dx} = \frac{p_f - p_i}{L} = \frac{dp}{dx} \rightarrow \text{Hole concentration gradient.}$$

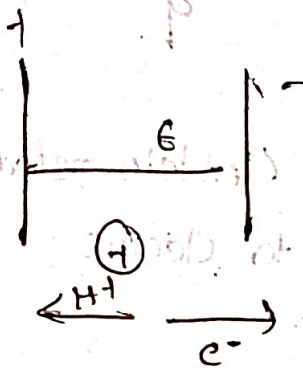
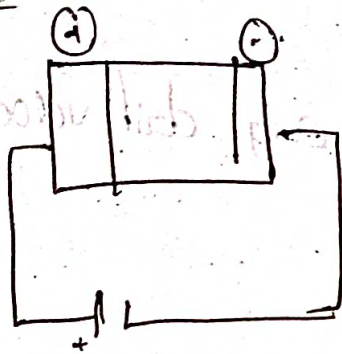
An n-type semiconductor

$$(J_n)_{diff} = q D_n \frac{dn}{dx}$$

D_n → diffusion co-efficient for electrons
 q → magnitude of the electron charge

$$J_{diff} = (J_p)_{diff} + (J_n)_{diff}$$

Drift



Drift velocity: The average velocity attained by charged particles such as electrons in a material due to an electric field.

Applying an electric field adds to this random motion a small net flow in one direction, thus is the drift.

$$V_{drift} \propto E$$

$$V_{drift} = \mu_p E \quad (\mu_p - \text{hole mobility})$$

V_{drift} - drift velocity

$$\mu_p = \frac{V_{drift}}{E}$$

avg drift velocity per unit electric field cm^2/V

$$(J_{drift}) \rightarrow J_d = \mu_e E$$

$$(J_p)_{drift} = \mu_p q_p E \quad \text{for } p$$

$$(J_n)_{drift} = q_n \mu_n E \quad \text{for } n$$

$$I_{\text{diff}} = (q_p \mu_p + q_n \mu_n) C_0 W L$$

2000 66

$$G = (q_{\text{pair}}, a_{\text{num}}) \in$$

6- conductivity of a semi-conductor.

$$\frac{p_p}{\mu_p} = \frac{D_n}{\mu_n} = V_T = \frac{k_B T}{q} \quad (\because V_T = \text{Thermal voltage})$$

$$V_T \approx 25 \mu V$$

$v_d = 25 \text{ cm/s}$
 This is called Einstein relation. avg. drift velocity
 is proportional to electric

