17-05-2023

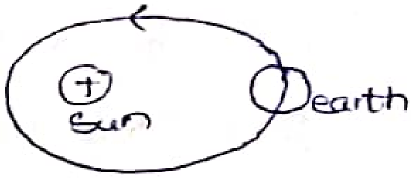
5. QUANTUM MECHANICS

* **Quantum Mechanics :-**

→ It is a branch of science which describes the dynamics of 'atomic' & 'subatomic particles'.

Dynamics :- controlling the flow.

Macroscopic



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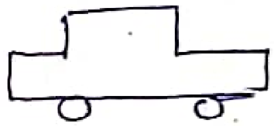


→ x

Robot → cup

$s = ut + \frac{1}{2}at^2$ ← [We use maths to understand dynamics]

Applications :-

1. From 'polymers' to 'semiconductors'.
2. From 'superfluids' to 'super conductors'.
3. From 'photonics' to 'Lasers'.
4. From 'developing drugs' to 'design of DNA'.

1. Semiconductors → 'Flow of e^-'
2. Magnetic materials → 'dynamics of e^-'
3. 'Lasers' ($h\nu$) & 'photonics'
4. Developing drugs to DNA.
5. Quantum computers [quantum computation & information].
   - → superposition of quantum states.

* **classical computers :-**

→ Bits (0 and 1).

→ Logic gates. [Transistors PNP & NPN].

→ Transistor acts as a switch → ON – '1', → OFF – '0'

* Quantum computers :-

→ Here we use 'Qbits'.

Ex:- ($|0\rangle$ and $|1\rangle$) ket vectors.

$$|01\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle\right].$$

$2^n = 2^4 = 16$ Tasks at a time.

→ If we have a code like 'XEMDP34X'.

→ To solve that code a 'classical computer' will takes 'a lot of time' by doing permutations & combinations.

→ But a 'quantum computer' can solve this code 'within minutes' [Takes less time].

Demerits of Quantum Mechanics:-

① It is very difficult to understand.

② The facts/postulates in it are not based on experimental facts.

Benefits:-

① We can make perfect security.

② We can prepare drugs.

③ We can use it to scan.

④ We can make extraordinary graphics.

⑤ We can design lot of technical games.

* → There were two independent formulations of Quantum mechanics.

(1925)

① 'First formulation' [Matrix mechanics] → Heisen-berg

② 'Second formulation' [Wave Mechanics] → Schrodinger (1926)

① Heisenberg [Matrix mechanics]

② Schrodinger [Wave Mechanics].

Dirac [bras kets]

$\boxed{\langle | \rangle}$

→ classical mechanics is useful for Macroscopic particles like car, planet etc—

→ It is not enough to explain the photo-electric effect and other phenomenon.

→ It is used to predict the dynamics of Macroscopic bodies.

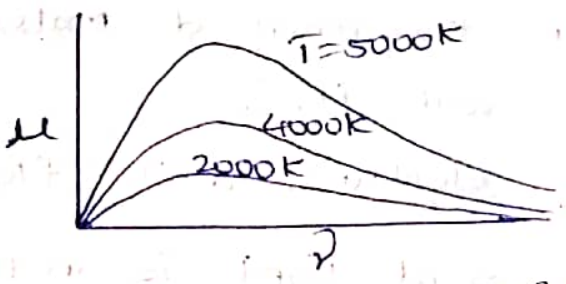
→ Failure of classical Mechanics:

① Photoelectric Effect.

② Black Body radiation.

① Black Body radiation:

→ It is an experimental fact.



→ The above shown is experimental spectrum.

① Wien's $\boxed{u(\nu,T) = A\,\nu^3 e^{-\beta\nu/T}}$

② Rayleigh's $\boxed{u(\nu,T) = \frac{8\pi\nu^2}{c^3} KT}$

③ Max planck said energy is b/w Matter & radiation is Discrete.

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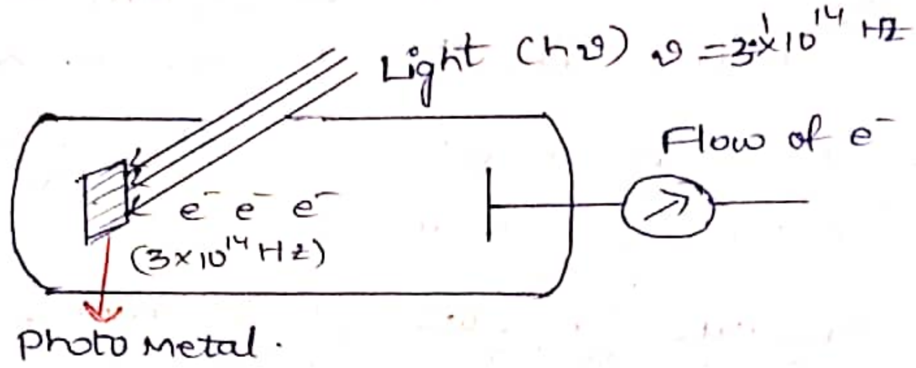
Planck, 'E = nhν'

$$\boxed{u(\nu, T) = \frac{8\pi\nu^2}{c^3} \times \frac{h\nu}{e^{h\nu/KT} - 1}}$$

→ He said the exchange of 'energy' between 'Matter' and 'radiation' is not in continuous manner but it is in 'Discrete manner'.

② Photo electric effect :-

→ It is also an experimental fact.



→ when light rays falls on a photo metal then electrons will flow.

Threshold frequency (ν)

→ If the frequency of light is more than threshold frequency of material then only electrons will flow.

→ otherwise electrons don't flow.

→ Einstein said light is in the form of quantum packets and each packet is called 'photon'

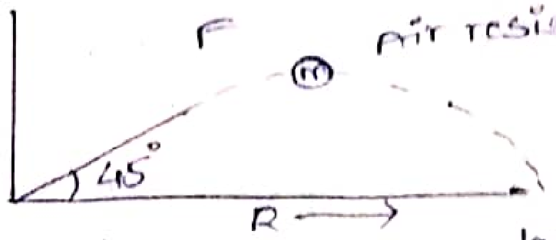
→ violet colour – High frequency – More electrons flow

Red colour – Low frequency – Electrons not flow

e^- ← from photometal ← Light.

① If energy of light > workfunction of metal.

②



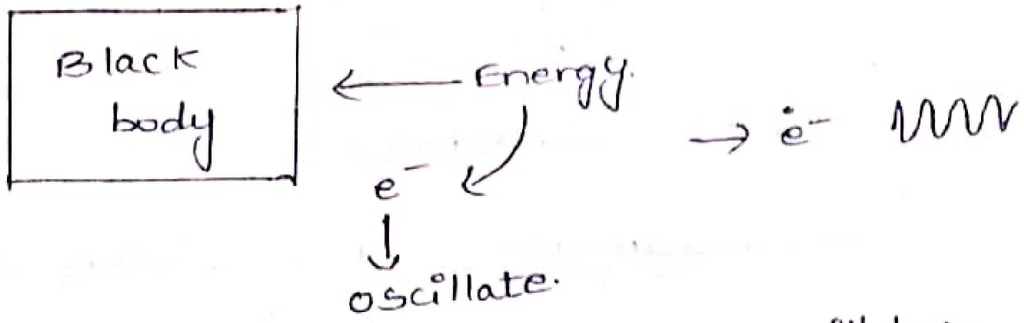
Newtonic Mechanics
↓
by Newton.

→ equations based on classical mechanism.

→ Projectile motion equations are theoretical equations.

③ Interaction of 'matter' and 'radiation' (Light)

ⓐ 'Blackbody radiation.'



→ Electron takes energy and oscillates.

→ oscillating e^- → radiates. [Rayleigh]

→ Rayleigh couldnot explain about entire spectrum.

$$\boxed{u(\nu,T) = \frac{8\pi\nu^2}{c^3} kT}$$

→ Planck - exchange of energy b/w radiation and matter must be discrete.

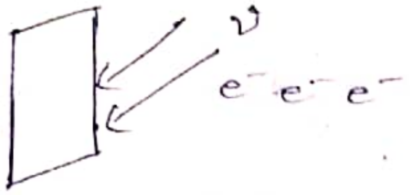
$$\boxed{E = n(h\nu)}$$

quantum

ν → frequency of oscillating charges.

$$\boxed{u(\nu,T) = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{h\nu/k_BT} - 1}}$$

* Observations of photoelectric effect :



→ Light is a wave $\psi(x,t) = A \cdot e^{i(kx-\omega t)}$

$= A \cdot \cos(kx - \omega t)$.

→ Minimum energy required to eject a electron is called workfunction:

photo metal.

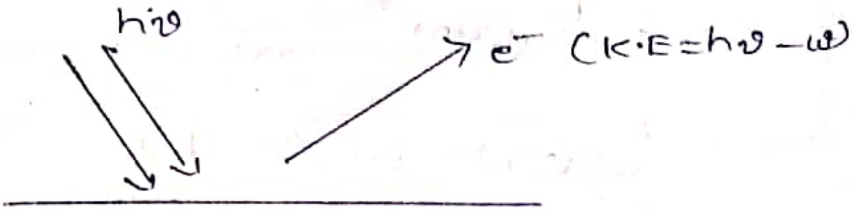
→ Work function → $E \propto \nu_0$ [Threshold frequency]

→ ν_R → No e^-

ν_V → e^- flows

→ Einstein inspired by planck's quantization and corpuscles concept. [corpuscles means particle].

→ Einstein assumed that Light is made of corpuscles, each carry energy $h\nu$ called photons.



$\omega = h\nu_0 \Rightarrow \nu_0 = \frac{\omega}{h}$.

$$\boxed{h\nu = W + K.E \text{ of } e^-}$$

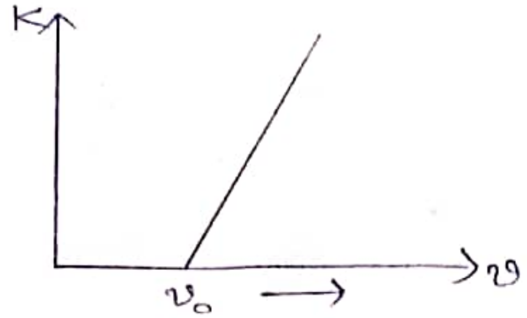
W = work function

K.E = kinetic energy

K.E of $e^- = h\nu - W$.

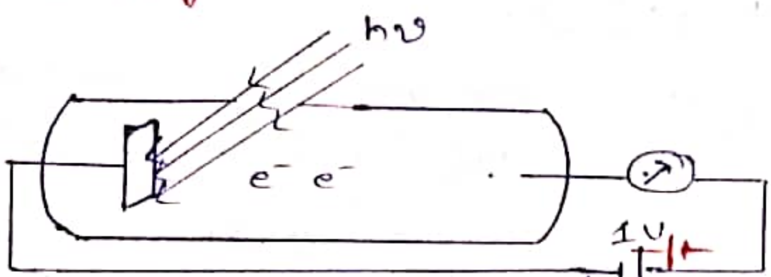
$\Rightarrow$ K.E of $e^- = h\nu - h\nu_0$ $\quad [W = h\nu_0]$

$\therefore \boxed{\text{K.E of } e^- = h(\nu - \nu_0)}$



$\therefore$ Eeinstein concluded that Light is a particle [corpuscles nature].

Experimentally:-



$\rightarrow$ Let us take a tube along a photometal and ammeter and give some potential energy.

$\rightarrow$ when '$h\nu > W$' then 'e^-' will eject from metal.

$$h\nu = W + \frac{1}{2} m v_e^2$$

$$\Rightarrow \frac{1}{2} m v_e^2 = h\nu - h\nu_0.$$

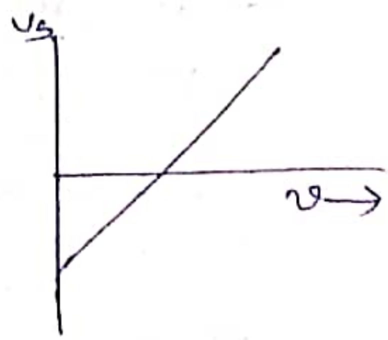
changing potential,
V_S - stopping potential.
current becomes zero
'$eV_S = \frac{1}{2} m v_e^2$'

Red- $\nu_R \Rightarrow h\nu_R > W \Rightarrow V_S = ?$

Blue- $\nu_B \Rightarrow h\nu_B > W \Rightarrow V_S = ?$

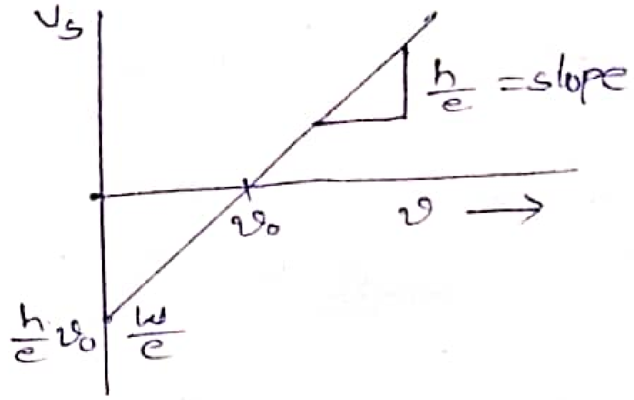
Green- $\nu_G \Rightarrow h\nu_G > W \Rightarrow V_S = ?$

Violet- $\nu_V \Rightarrow h\nu_V > W \Rightarrow V_S = ?$



$$eV_s = h\nu - h\nu_0$$

$$\Rightarrow V_s = \left(\frac{h}{e}\right)\nu - \left(\frac{h}{e}\right)\nu_0 \qquad \Rightarrow y = mx + c.$$



when $V_s = 0$.

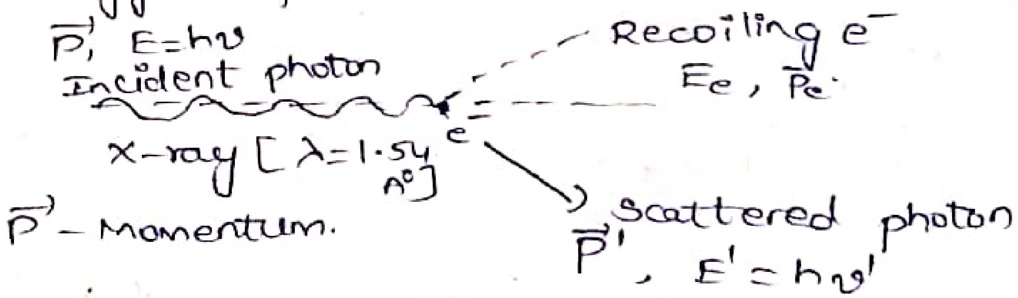
$\Rightarrow \nu = \nu_0$.

$$\Rightarrow \frac{h}{e}\nu_0 = \frac{W}{e}.$$

* compton effect :-

→ compton is the one, who confirms the particle nature of radiation [Light].

→ He considered an electron at rest and sends x-ray [photon] on this e^-. the energy of photon is $E = h\nu$.



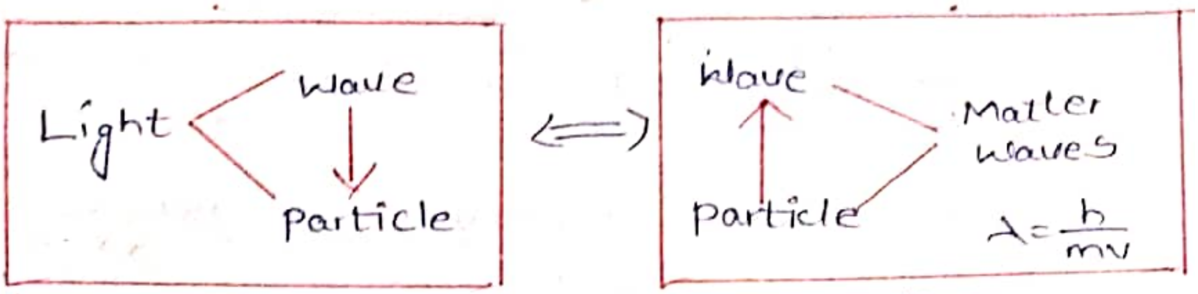
→ He found that "the scattered photon has more energy than Incident photon."

→ As the wave length of x-ray is small, its energy is Large.

→ This is explained by compton.

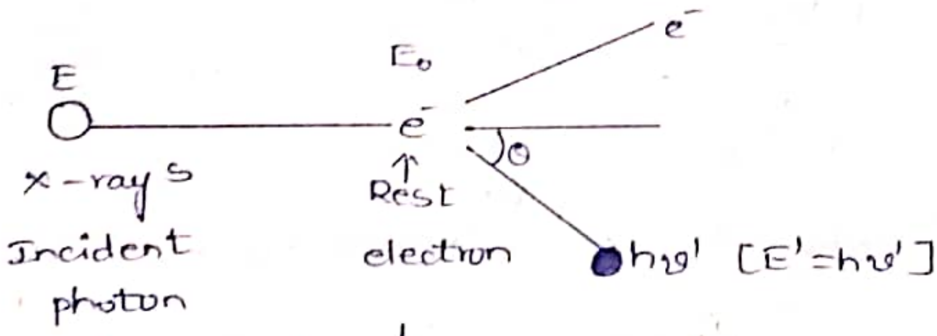
→ compton considered / treated the incident rays [incident radiation] as a stream of particles [photons].

→ They are colliding elastically with individual electrons.



compton | DeBroglie

→ As per compton assumptions,



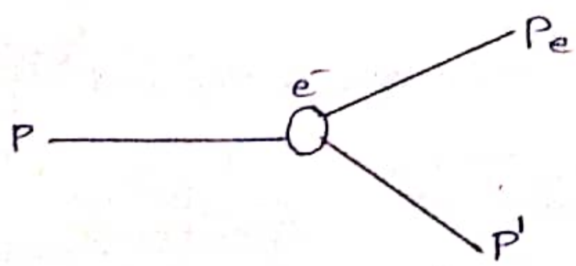
← Before collision → | ← After collision →

① Energy of incident photon $E = h\nu$.
Momentum of incident photon $p = \frac{h\nu}{c}$ } colliding with $e^\ominus$ which is at rest

② conservation of linear momentum :-

$$\boxed{\vec{P} = \vec{P}_e + \vec{P}'}$$

Here $\vec{P}'$ → momentum of photon
$\vec{P}_e$ → momentum of recoil electron.



$$P_e = \bar{P} - \bar{P}'$$

$$\Rightarrow P_e^2 = (\bar{P} - \bar{P}')^2$$

$$\Rightarrow P_e^2 = \bar{P}^2 + \bar{P}'^2 - 2PP'\cos\theta.$$

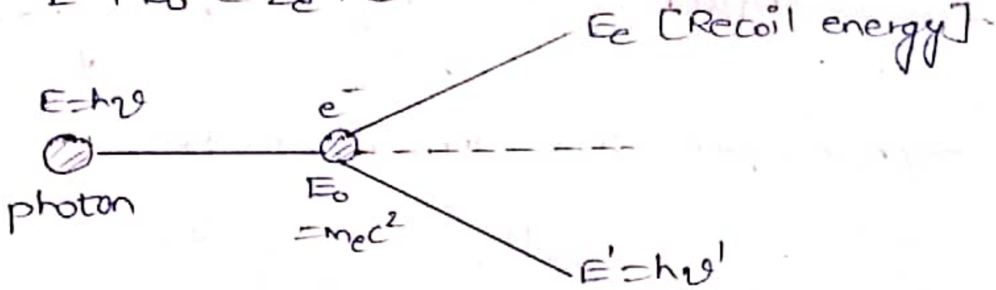
We know,

Momentum $P = \frac{h\nu}{c}$ $\quad P' = \frac{h\nu'}{c}$

$$\Rightarrow \boxed{P_e^2 = \frac{h^2}{c^2}(\nu^2 + \nu'^2 - 2\nu\nu'\cos\theta)} \longrightarrow (1)$$

(3) Let consider conservation of energy.

$$E + E_0 = E_e + E'$$



E_0 = Rest Energy of e^-

$\Rightarrow E_0 = m_e c^2 \longrightarrow$ Before collision

$E_e = \sqrt{P_e^2 c^2 + m_e^2 c^4} \longrightarrow$ After collision.

$$\downarrow$$

P = mass x velocity $= mc$

$$\Rightarrow E = mc^2 = (mc)c$$

$$\Rightarrow P = \frac{E}{c} \text{ (or) } E = Pc.$$

Now, $E_e^2 = P_e^2 c^2 + m_e^2 c^4$

$$\Rightarrow E_e = \sqrt{P_e^2 c^2 + m_e^2 c^4}.$$

Now,

$$E_e = h[\nu^2 + \nu'^2 - 2\nu\nu'\cos\theta + m_e^2 c^4]^{1/2}.$$

Substitute E_e value in $E + E_0 = E_e + E'$.

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$$h\nu + m_e c^2 = h\nu' + h[\nu^2 + \nu'^2 - 2\nu\nu'\cos\theta + m_e^2 c^4]^{1/2}$$

$$\Rightarrow \frac{h\nu - h\nu' + m_e c^2}{h} = [\nu^2 + \nu'^2 - 2\nu\nu'\cos\theta + m_e^2 c^4]^{1/2}$$

$$\Rightarrow (\nu - \nu')^2 + \cancel{m_e^2 c^4} + 2(\nu - \nu') \cdot m_e c^2 = \nu^2 + \nu'^2 - 2\nu\nu'\cos\theta + \cancel{m_e^2 c^4}$$

$$\Rightarrow \boxed{\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_e c^2}(1 - \cos\theta)} \quad \text{[By simplifying]}$$

$$\Rightarrow \frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_e c^2} 2\sin^2\frac{\theta}{2}$$

$$\Rightarrow \frac{c}{\nu'} - \frac{c}{\nu} = \frac{2h}{m_e c}\sin^2\frac{\theta}{2}$$

We have, $\frac{c}{\nu'} = \lambda'$ and $\frac{c}{\nu} = \lambda$.

$$\Rightarrow \lambda' - \lambda = \frac{2h}{m_e c}\sin^2\frac{\theta}{2}$$

$$\therefore \boxed{\Delta\lambda = \lambda' - \lambda = \frac{2h}{m_e c}\sin^2\frac{\theta}{2}} \quad - \text{compton shift}$$

This is the compton shifting.

Here, $\frac{2h}{m_e c} = 2.426 \times 10^{-12} m$ — compton wave length of electron e^-.

$$\therefore \boxed{\Delta\lambda = \lambda' - \lambda = 2\lambda_c \sin^2\frac{\theta}{2}}$$

conclusions :-

① From Planck,

Discrete Nature [Quantum Nature] of light

② From compton,

Particle Nature [corpuscles] of Light

wave-particle Duality [complementarity].

* De-broglie's Hypothesis :-

→ He assumed "Nature is Like symmetrically."

→ He said that wave-particle [dual behaviour] is not only for radiation but universely.

→ He said that "all material particles should also display a dual wave-particle behaviour"

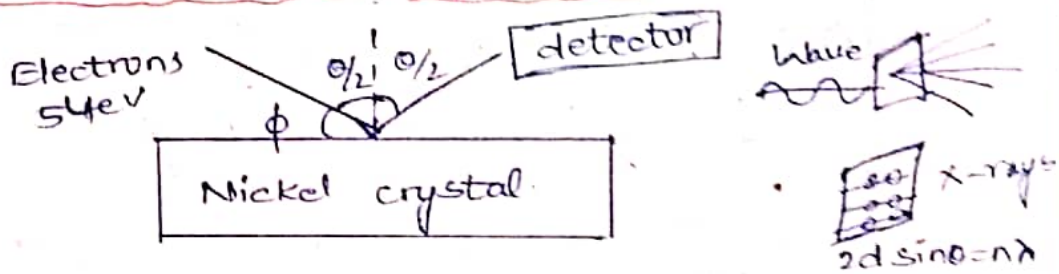
$$\boxed{\lambda = \frac{h}{p}}$$ De-broglie's wavelength.

We have, $p = \frac{h\nu}{c}$

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

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

① Davisson - Germer Experiment :-



→ They incidented electrons [54 ev] onto the Ni-crystal at θ = 35° [approx] it scatters.. [diffracts].

→ They observed "diffraction pattern" when they incident "electrons".

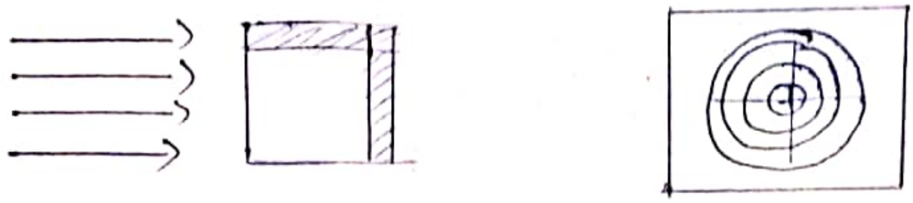
→ Actually, we observe diffraction due to waves, x-rays etc—

→ But here due to electrons, diffraction pattern occured.

→ They concluded that "particle has wave Nature"

(2) Thomson Experiment :-

→ He took a thin film and passed electron beam and he observed 'rings'.



→ From this also, he concluded "particle has wave nature."

Observing the Trajectory of e^- :-

→ consider an e^- to find its trajectory [nature].

→ To know its information Like 'momentum', 'energy of particle' and 'where it is located', we need a wave function.

Wave function:- It describes the behaviour/ Information of particle.

$$\boxed{\psi(r,t) = A \cdot e^{i(k \cdot r - \omega t)}}$$

Here, '$k = \frac{2\pi}{\lambda}$' → contains information of 'wave length' of e^-(particle)

r = 'contains information of position'.

ω = 'Angular frequency' = '$2\pi\nu$'.

We have, '$p = \frac{h}{\lambda} = \frac{h}{2\pi} k \cdot \hbar k$.'

'$E = h\nu = \hbar\omega$'

* Advantages of De-broglie's Hypothesis :-

① Electron microscopy ⟶ modern Technology.

⟶ 'Electron microscopy' is based on this De-broglie's Matterwaves.

② De-broglie explained all the bohr postulates with matter waves.

* Plane wave function [wave function] :-

⟶ We need to observe the sub-atomic particles [$\bar{e}$, n, p] behaviour, to identify the behaviour we need the wave function.

⟶ These 'plane waves' are represented as

It extends to the Infinity.

$$\boxed{\psi(r,t) = A \cdot e^{i(\bar{k}\cdot\bar{r} - \omega t)}}$$

⟶ This wave function describes the motion of particle [All the information of particle].

Here, $\vec{k} = \frac{2\pi}{\lambda}$ = wave vector.

$\lambda = \frac{h}{p}$ (or) $\frac{h}{mv}$. and $\hbar = \frac{h}{2\pi}$.

$\Rightarrow \vec{k} = \frac{2\pi}{h} \times p$. $\Rightarrow \boxed{\bar{p} = \hbar k}$

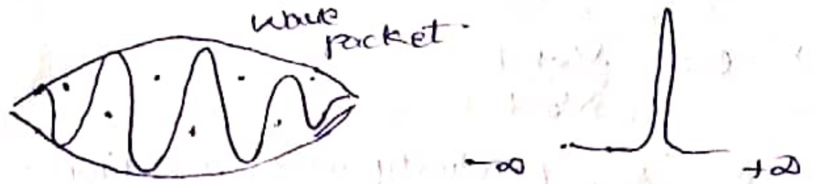
$E = h\nu = \hbar\omega$ [$\because \omega = 2\pi\nu$ & $\nu = \frac{\omega}{2\pi}$]

⟶ In 1-D,

$$\boxed{\psi(x,t) = A\, e^{i(k\cdot x - \omega t)}}$$

* Note: Heisenberg Uncertainity:

→ Let us consider a wave packet like this



↓ Here we cannot find the position of particle

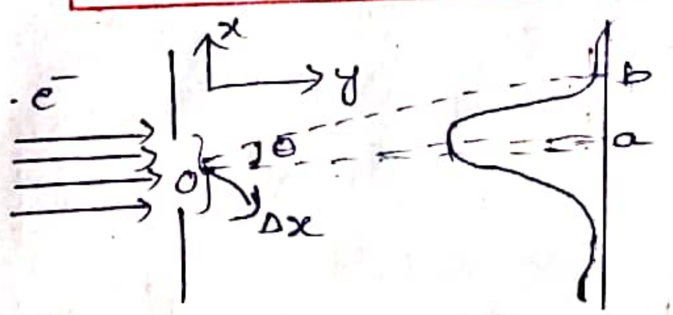
↓ Here we cannot find the velocity of particle

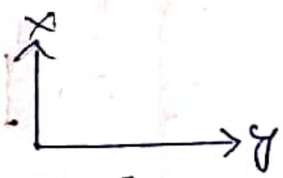
→ Heisenberg said for any canonical conjugates it is impossible to find the position & momentum of the body simultaneously at arbitrary precision.

Ex: x and P_x } canonically conjugate variables.
t and E
θ and L

→ He gave uncertainity principle as

$$\boxed{\Delta x \cdot \Delta P_x = \frac{h}{2\pi} = \hbar}$$





v=0 in x-direction at slit width

$\Delta x \sin\theta = \lambda$ [Δx = slit width]

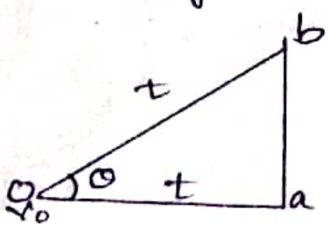
[$b\sin\theta = n\lambda$]

$\Rightarrow \sin\theta = \frac{\lambda}{\Delta x}$

If θ is small

$\Rightarrow \theta = \frac{\lambda}{\Delta x}$ [$\sin\theta \approx \theta$] $\longrightarrow$ (i)

From figure, $\tan\theta = \frac{ab}{oa}$



$\Rightarrow oa = v_0 t$

Let $v_{xb} = \frac{ab}{t}$

$\Rightarrow ab = v_{xb} t$

Now, $\tan\theta = \frac{ab}{oa} = \frac{V_{xb}t}{V_0 t}$

If θ is small

$\Rightarrow \theta = \frac{V_{xb}\cancel{t}}{V_0 \cancel{t}}$

$\Rightarrow \theta = \frac{V_{xb}}{V_0}$ [velocity in x'-direction]. → ②

From ① & ② equations

$\Rightarrow \frac{\lambda}{\Delta x} = \frac{V_{xb}}{V_0}$.

We can write $\frac{\lambda}{\Delta x} = \frac{h}{p\Delta x} = \frac{h}{mV_0 \Delta x}$

$\Rightarrow \frac{h}{mV_0\Delta x} = \frac{V_{xb}}{V_0}$.

We can write $V_{xb} = \Delta V$

$\Rightarrow \frac{h}{m\cancel{V_0}\Delta x} = \frac{\Delta V}{\cancel{V_0}}$

$\Rightarrow \Delta x(\Delta V \cdot m) = h$

$\therefore \boxed{\Delta x \cdot \Delta P = h}$

Note :-

① $\Delta x \, \Delta P_x \geq \hbar$

$\Delta y \, \Delta P_y \geq \hbar$

$\Delta z \, \Delta P_z \geq \hbar$

② $\Delta t \, \Delta E \geq \hbar$

③ $\Delta \theta \, \Delta L \geq \hbar$.

Uncertainities.

Advantages of Heisenberg uncertainity:-

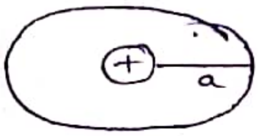
(or)

Applications:-

① "Groundstate energy and radius of Hydrogen atom":-

We know that $E = K.E + P.E.$

$$\Rightarrow E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 a} \quad \left[\begin{array}{l}\text{where } a = \text{radius} \\ \text{of } 1^{st} \text{ orbital}\end{array}\right]$$



Here uncertainity in the position [a].

$$\Rightarrow \Delta x \cdot \Delta P_x \cong \hbar \qquad [\hbar \rightarrow h \text{ ket}].$$

$$\Rightarrow a \cdot \Delta P = \hbar$$

$\therefore$ uncertainity in momentum, $\boxed{\Delta P = \frac{\hbar}{a}}$

$$\therefore E = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\varepsilon_0 a}.$$

For 'ground state', the energy 'e' has to be 'minimum'.

$$\Rightarrow \frac{dE}{da} = 0 \cdot = \frac{-\hbar^2}{ma_0^3} + \frac{e^2}{4\pi\varepsilon_0 a_0^2}.$$

$$\therefore \boxed{a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \simeq 0.5\,A^\circ.}$$

$a_0 \downarrow$ Radius of Groundstate of Hydrogen atom.

$$\text{Now, } E = \frac{-me^4}{(4\pi\varepsilon_0)^2 2\hbar^2} = \frac{-me^4}{8\varepsilon_0^2\hbar^2\pi^2}.$$

$$\therefore \boxed{E_G = \frac{-me^4}{8\varepsilon_0^2\hbar^2}}$$

② Width of spectral lines:

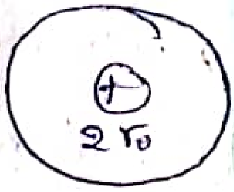
$$\Delta t \cdot \Delta E = \hbar \Rightarrow \Delta \nu = \frac{1}{2\pi\Delta t}$$

Since Life time, $\Delta t \simeq 10^{-8}$

$$\therefore \boxed{\Delta\nu = 10^8 \text{ Hz}}$$

(3) Non-existance of electron in the Nucleus:

$$\Delta p = \frac{\hbar}{2r_0}, \quad r_0 = 10^{-14}\ m$$



$$\Delta p = 5.28 \times 10^{-21}\ kg\ m/sec.$$

$$K.E = \frac{\Delta p^2}{2m} = \frac{(5.28 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31}}\ J \cong 95.7\ MeV$$

(4) Mass of meson..

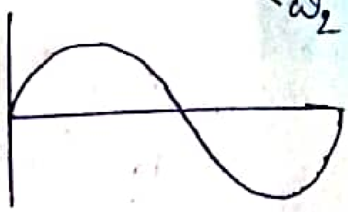
* Schrodinger Equation :-

$$\Psi(x,t) = A_0 e^{i(k \cdot x - \omega t)}. \quad [\text{plane wave}]$$

It is the wave function of particle which exhibits wave nature.

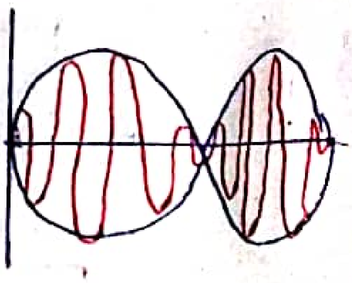
$e^- < \omega_1, \omega_2$

→ We will get the wave like this.



→ If we take two waves with different 'k' values, then we will get a wave packet.

→ Wave packet is superposition of an infinite number of plane waves with slightly different $k = \frac{2\pi}{\lambda}$



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

* Time Dependent Schrodinger Equation :-

(1) 1-D equation for a free particle [No force]

Energy, $E = K.E + P.E$

$$\Rightarrow E = \frac{1}{2}mv^2 + V \qquad \left[\begin{array}{l} F = -\nabla V \\ \text{if } F=0,\ V=0 \end{array}\right].$$

For a free particle, potential is zero then

$$E = \frac{1}{2}mu^2 = \frac{p^2}{2m}$$

Now,

$$E = \frac{\hbar^2 k^2}{2m} \qquad [\because p = \hbar k] \longrightarrow (1)$$

$$E = \hbar\omega. \longrightarrow (2)$$

From (1) & (2) equations

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

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

Substitute 'ω' value in equation (A).

$$\therefore \boxed{\psi(x,t) = \int_{-\infty}^{\infty} A(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk}$$

Differentiating '$\psi(x,t)$' with respect to 't'.

$$\Rightarrow \frac{\partial\psi}{\partial t} = \frac{-i\hbar}{2m}\int_{-\infty}^{\infty} k^2 A(k)\, e^{i\left(kx - \frac{\hbar^2 k^2}{2m}t\right)}\, dk \longrightarrow (3)$$

Differentiating $\psi(x,t)$ w.r.to 'x' twice.

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = -\int_{-\infty}^{\infty} k^2 A(k)\, e^{i\left(k.x - \frac{\hbar^2 k^2}{2m}t\right)}\, dk. \longrightarrow (4)$$

comparing (3) & (4) equations.

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

Multiply both sides with $i\hbar$.

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

$\therefore \boxed{i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2}}$ is the one-dimensional schrodinger equation. without any force.

→ It is in the form of

$$\boxed{E \cdot \psi(x,t) = \frac{P_x^2}{2m} \psi(x,t)}$$

Note :-

→ In Quantum mechanics, the particle is exhibiting in wave nature [wave packets]. and the entire information is in plane wave functions. so, we need to use operators to extract Information.

- Now, Rewriting the schrodinger equation as

$$\left(i\hbar \frac{\partial}{\partial t}\right) \Psi(x,t) = \frac{1}{2m} \underbrace{\left(-i\hbar \frac{\partial}{\partial x}\right)}_{P_x} \underbrace{\left(-i\hbar \frac{\partial}{\partial x}\right)}_{P_x} \psi(x,t)$$

* Operators for Momentum and Energy :-

→ Let us consider a ~~wave~~ particle exhibits wave nature and its wave function is

$$\psi(x,t) = A \cdot e^{ikx}.$$

Now, operator for Momentum is, $\left[P_x = -i\hbar \frac{\partial}{\partial x}\right]$

$$\hat{p}\, \psi(x,t) = -i\hbar \frac{\partial}{\partial x} A \cdot e^{ikx}$$

$$= -i\hbar\, (ik) \left[A \cdot e^{ikx}\right]$$

$\therefore \hat{p}\, \psi(x,t) = \hbar k \, \psi(x,t)$ — eigen value.

Now, Energy operator is '$E = i\hbar \frac{\partial}{\partial t}$'

Let us take a plane wave,

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

Then we will get energy.

* 3-Dimension :-

Dell operator:-

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

Here, $\nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}$

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

operators in 3-D:-

$$\boxed{P = -i\hbar \nabla.}$$

* Inclusion of Force :- [$F \neq 0$] i.e [$V \neq 0$]

→ The equation is as follows

$$\boxed{i\hbar \frac{\partial}{\partial t} \psi(r,t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(r)\right] \psi(r,t)}$$

This is "Time dependent schrodinger equation for a particle of mass m moving in a potential V(r)."

* Time Independent Schrodinger equation :-

→ Here we will ~~use~~ separate the spacial part and time.

→ we know the time dependent equation,

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(r)\right] \psi(r,t).$$

H = Hamiltonian operator $= \left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]$.

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

From the above two, $\boxed{\hat{E}\psi = \hat{H}\psi.}$

→ Here we will use "separation of variables" concept to separate 'spacial part' and 'time part.' [r and t].

"$\psi(r,t) = \psi(r)\,\phi(t)$."

Because both are independent. [$r(x,y,z)$]

Now, substitute this in time dependent equation. and we divide throughout by $\psi(r)\phi(t)$.

$$\Rightarrow \frac{1}{\psi(r)\phi(t)}\left[i\hbar\frac{\partial}{\partial t}\psi(r)\cdot\phi(t)\right] = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]$$

$$\frac{1}{\psi(r)\cdot\phi(t)}$$

$$\Rightarrow \frac{1}{\phi(t)}\left[i\hbar\frac{\partial}{\partial t}\phi(t)\right] = \frac{1}{\psi(r)}\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r).$$

$$\therefore \boxed{\underbrace{\frac{1}{\phi(t)}\left[i\hbar\frac{\partial}{\partial t}\phi(t)\right]}_{\text{Time part}} = \underbrace{\frac{1}{\psi(r)}\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r)}_{\text{Spacial part}}}$$

This is possible if and only if both are independent.

Let us consider the constant as 'E' for spacial part.

$$\Rightarrow \frac{1}{\psi(r)}\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E.$$

$$\Rightarrow \boxed{\frac{-\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\cdot\psi(r).}$$

This is time Independent schrodinger equation.

Note:-

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + u(r)\right]\psi(r) = E\psi(r)$$

$\Rightarrow \boxed{\hat{H}\psi = E\psi} \longrightarrow$ Eigen value.

Here H = 'Hamilton operator' [Total energy],

E = 'Energy eigen value of the particle.

→ For Time Independent → Hamilton operator.

For Time Dependent → Energy operator.

Now, Let us consider 'Time part = E'

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

Divide both sides with $i\hbar$.

$$\Rightarrow \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \frac{E}{i\hbar} = \frac{-iE}{\hbar}$$

$$\Rightarrow \boxed{\frac{\partial \phi(t)}{\partial t} = \frac{-iE}{\hbar}\phi(t).}$$

$$\Rightarrow \phi(t) = c \cdot e^{-iEt/\hbar}.$$

It is obtained as follows.

$$\Rightarrow \int \frac{\partial \phi(t)}{\phi(t)} = \int \frac{-iE}{\hbar}\partial t$$

$$\Rightarrow \ln \phi(t) = \frac{-iEt}{\hbar} + c.$$

$$\Rightarrow \phi(t) = e^{-iEt/\hbar} \cdot c$$

$\therefore \boxed{\phi(t) = c \cdot e^{-\frac{iEt}{\hbar}}.}$ – stationary state.

* calculate the Eigen values and Eigen functions of particle of mass 'm' confined in one dimensional potential well with conditions V=0 for region $-a<x<+a$ and V = infinite other than $-a<x<+a$ region. Draw symmetric & anti-symmetric wave function and explain them with the help of wave function.

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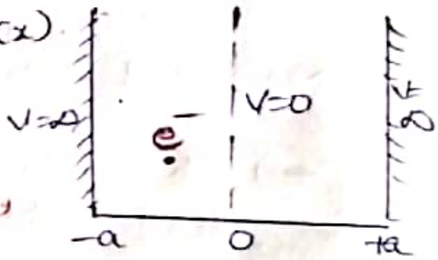
A) ① [ψ is complex, single value, finite function]

consider Time Independent Schrodinger equation

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

$$\Rightarrow H\psi = E\psi$$

where 'E → energy eigenvalue',
'ψ(x) → eigen function.'



① Let consider region '-a' to '+a', 'V(x)=0'.

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

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - E\psi(x) = 0.$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} - \frac{2mE}{\hbar^2}\psi(x) = 0.$$

Let put $\frac{2mE}{\hbar^2} = k^2$

$$\Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} - k^2\psi(x) = 0}$$

This is second order differential equation

The solution for this equation will be

$$\psi(x) = A\sin(kx) + B\cos(kx) \longrightarrow (1)$$

At $V(x) = \infty$, at $x = \pm a$.

$\Rightarrow \psi(\pm a) = 0$.

By applying this boundary condition.

① $\psi(+a) = 0 = A \cdot \sin ka + B \cos ka \longrightarrow$ (i)

② $\psi(-a) = 0 = -A \sin ka + B \cos ka \longrightarrow$ (ii)

Add the above equations and substract them.

$\Rightarrow 2B \cos ka = 0$ and $2A \sin ka = 0$

The solution $A=0$ and $B=0$ Leads to physically unacceptable solution $\psi = 0$.

case-I :-

(i) Let consider $A=0$ and $B \neq 0$.

$\therefore \cos ka = 0. \Rightarrow ka = \frac{n\pi}{2}$ where $n = 1, 3, 5 -$

$\Rightarrow k = \frac{n\pi}{2a} \Rightarrow k^2 = \frac{n^2\pi^2}{4a^2} \longrightarrow$ (1)

We have $k^2 = \frac{2mE}{\hbar^2} \longrightarrow$ (2)

From (1) & (2)

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

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

$\therefore$ Eigen energy value, $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}}$ $n = 1, 3, 5, \_\_$

Now, Eigen function,

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

Here we considered $A=0$ in this case

$\Rightarrow \psi(x) = B \cos kx.$

$\Rightarrow \boxed{\psi_{odd}(x) = B \cos \frac{n\pi x}{2a}}$ [where n is odd number]

[$\because k = \frac{n\pi}{2a}$] [from (1)]

$\therefore$ This is the corresponding eigen function.

Case-ii:-

B = 0, but A ≠ 0 so that $\sin ka = 0$.

$$\Rightarrow ka = \frac{n\pi}{2}, \quad n = 2, 4, 6, \ldots$$

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

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

compare it with $k^2 = \frac{2mE}{\hbar^2}$

$$\therefore \boxed{E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}} \quad \text{where } n = 2, 4, 6, \ldots$$

This is the Eigen value.

Now, wave function,

$$\boxed{\psi_{even}(x) = A \sin \frac{n\pi x}{2a}} \quad \text{where } n \text{ is even}.$$

Therefore, from 2 cases:-
The eigen values of particle in the region $-a < x < +a$ is given by.

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

Eigen functions from 2 cases are

$$\psi_{odd} = B \cos \frac{n\pi}{2a} x. \quad n = odd$$

$$\psi_{even} = A \sin \frac{n\pi}{2a} x. \quad n = even.$$

By using "probability interpretation",

$$\boxed{\int_{-\infty}^{\infty} \psi^* \psi \, d\tau = \int_{-\infty}^{\infty} |\psi(r,t)|^2 d\tau = 1}$$

Probability will need to be '1' – 'Normalization' one can multiply '$\psi(x,t)$' by a constant 'N', so that '$N\psi$' satisfies the above condition.

$$\int_{-\infty}^{+\infty} B^2 \cos^2 \frac{n\pi x}{2a} \, dx = 1$$

$$\Rightarrow B = \frac{1}{\sqrt{a}} \quad [\text{By solving}].$$

Similarly, By solving

$$\int_{-\infty}^{+\infty} A^2 \sin^2 \frac{n\pi x}{2a} \, dx = 1$$

we will get $A = \frac{1}{\sqrt{a}}$

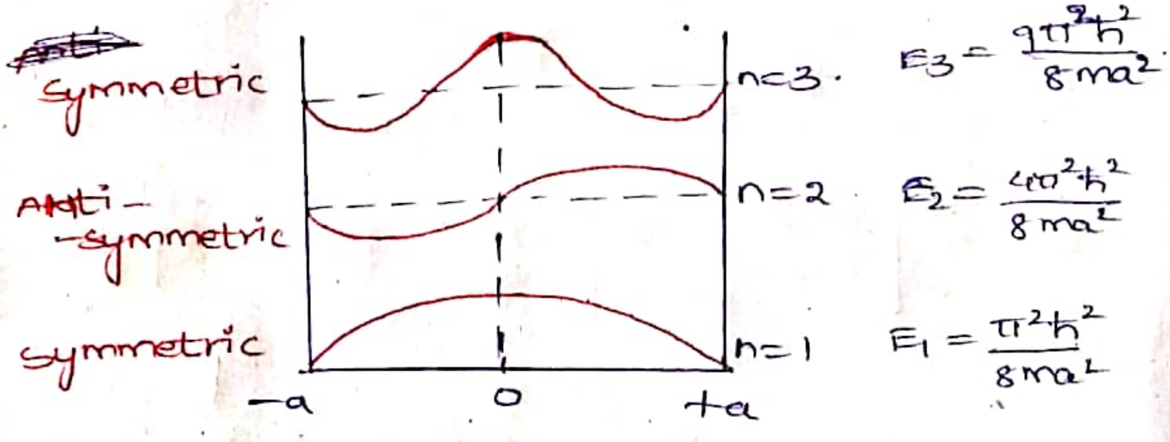
Born approximation (or) Normalization.

Now, $\psi_{even} = \frac{1}{\sqrt{a}} \sin \frac{n\pi x}{2a}$ $\quad [\because A = \frac{1}{\sqrt{a}}, B = \frac{1}{\sqrt{a}}]$.

$\psi_{odd} = \frac{1}{\sqrt{a}} \cos \frac{n\pi x}{2a}$.

These are "eigen functions" required.

Graph:-



ψ_{even} $n=2 \Rightarrow \frac{1}{\sqrt{a}} \sin \frac{2\pi x}{2a} \Rightarrow \frac{1}{\sqrt{a}} \sin \frac{\pi x}{a} = 0$

ψ_{even} functions are 'Anti-symmetric'

ψ_{odd} functions are 'symmetric'.