

Quantum Mechanics:—

Quantum Mechanics is a physical science dealing with the behavior of matter and energy on the scale of atoms & subatomic particles/waves.

In other ways we can say that the exchange of energy b/w the radiation & the matter takes place in discrete set of values.

PHOTON :— photon is an elementary particle, that is massless & has no charge.

It is a bundle of energy or packet of energy emitted by a source of radiation.

It moves with velocity of light. It can carry energy & momentum.

We know the relation b/w velocity of light & mass of particle is

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

$$\text{If } v = c, m = \infty$$

$$\text{If } \begin{matrix} m_0 = 0 \\ \& v = c \end{matrix} \quad m = \frac{0}{0}$$

So photons are never at rest & always keep moving with velocity of light.

Energy of photon $\Rightarrow$

$$E = h\nu$$

$\downarrow$
planck constant

$$\& E = mc^2$$

$$mc^2 = \frac{h\nu}{c} \Rightarrow m = \frac{h\nu}{c^2}$$

Since energy relation = $E^2 = p^2c^2 + m_0^2c^4$

since $m_0 = 0$ & $E = pc$ & momentum of photon is given by

$$p = \frac{E}{c} = \frac{mc^2}{c} = mc$$

$$p = \frac{h\nu}{c^2} \times c$$

$$p = \frac{h\nu}{c}$$

So the characteristic of the photon are

$$m_0 = 0, \quad E = h\nu, \quad m = \frac{h\nu}{c^2} \quad \& \quad p = \frac{h\nu}{c}$$

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Wave - Particle Duality $\Rightarrow$

→ Wave-particle duality is the concept in quantum mechanics that energy-carrying waves can also behave like particles & that particles can also display a wave aspect.

→ Light, for example, demonstrates the wave phenomena of diffraction & interference but, under other circumstances, appears to be a stream of tiny particles called photons.

Electrons, on other hand, which normally behave like particles, can be made to diffraction & interference as if they consisted of waves. Thus scientists began to conclude that light has both wave & particle nature.

→ The concept that matter behaves like a wave is also referred to as the de-Broglie hypothesis.

So According to De-Broglie hypothesis, particles like electron, proton & neutron etc show wavelike properties associated with them.

All material particles in motion possess a wave character. These wave are called Matter-waves or 'De-Broglie Waves'.

$$E = h\nu$$

$$E = mc^2 \Rightarrow m = \frac{E}{c^2} = \frac{h\nu}{c^2}$$

momentum

of photon

$$p = mc = \frac{h\nu}{c^2} \times c$$

$$\star \boxed{p = \frac{h\nu}{c}}$$

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

$$\text{So } p = \frac{h}{\lambda} \Rightarrow \star \boxed{\lambda = \frac{h}{p}}$$

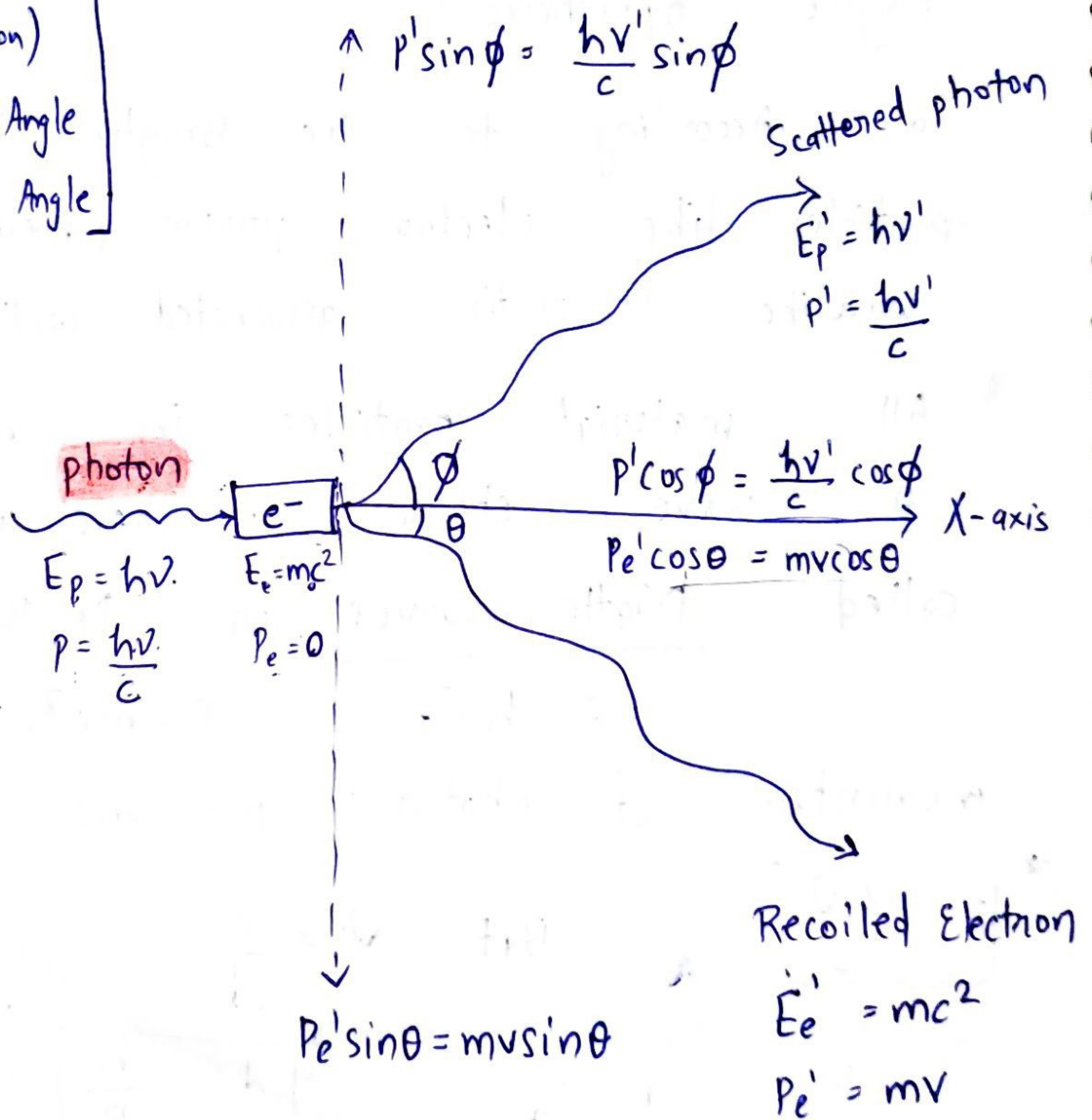
$$\text{if } m = m, \quad c = \nu \quad \text{then } \star \boxed{\lambda = \frac{h}{mv}} \star$$

However, the wave nature of light fails to explain the phenomena of Compton effect, photoelectric effect, continuous X-ray spectrum & blackbody radiation.

COMPTON Effect

(When a beam of monochromatic X-ray is incident on graphite block, it gets scattered)

(1 photon interact with 1 electron)
 ϕ = Scattering Angle
 θ = Recoiling Angle



→ A photon which is incident on Graphite block emits two types of photon wavelengths (λ and λ')

Compton shift: $\Delta \lambda = \lambda' - \lambda$, $\lambda' > \lambda$

Law of conservation of energy:-

$$\begin{aligned} \text{Energy Before Collision} &= \text{Energy After Collision} \\ E_p + E_e &= E_p' + E_e' \end{aligned}$$

$$h\nu + m_0c^2 = h\nu' + mc^2$$

$$h(\nu - \nu') = mc^2 - m_0c^2$$

$$h(\nu - \nu') = (m - m_0)c^2 \quad \text{--- (1)}$$

Law of momentum's conservation:-

$$'p' \text{ before Collision} = 'p' \text{ after Collision}$$

On X-axis

$$p + p_e = p' \cos \phi + p_e' \cos \theta$$

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos \phi + mv \cos \theta$$

$$h\nu = h\nu' \cos \phi + mvc \cos \theta$$

$$mvc \cos \theta = h\nu - h\nu' \cos \phi \quad \text{--- (2)}$$

On Y-axis

$$0 = p' \sin \phi - p_e' \sin \theta$$

$$0 = \frac{h\nu'}{c} \sin \phi - mv \sin \theta$$

$$mvc \sin \theta = h\nu' \sin \phi \quad \text{--- (3)}$$

→ Squaring & Adding eqⁿ - (2) + (3)

$$\therefore mv^2c^2(\cos^2\theta + \sin^2\theta) = (h\nu - h\nu'\cos\phi)^2 + h^2\nu'^2\sin^2\phi$$

$$\therefore mv^2c^2 = h^2\nu^2 - 2h^2\nu\nu'\cos\phi + h^2\nu'^2(\cos^2\phi + \sin^2\phi)$$

$$\therefore m^2v^2c^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu'\cos\phi \quad \text{--- (4)}$$

Now from eqⁿ - (1)

$$mc^2 = h(\nu - \nu') + m_0c^2$$

→ on squaring

$$\therefore m^2c^4 = (h(\nu - \nu') + m_0c^2)^2$$

$$\therefore m^2c^4 = h^2(\nu - \nu')^2 + m_0^2c^4 + 2h(\nu - \nu')m_0c^2$$

$$\therefore m^2c^4 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu' + m_0^2c^4 + 2h(\nu - \nu')m_0c^2$$

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$$\rightarrow \text{eqⁿ (5) - eqⁿ (4)}$$

$$m^2c^4 - m^2v^2c^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu' + m_0^2c^4 + 2h(\nu - \nu')m_0c^2 - h^2\nu^2 - h^2\nu'^2 + 2h^2\nu\nu'\cos\phi$$

$$m^2c^4 \left[1 - \frac{v^2}{c^2} \right] = -2h^2\nu\nu'(1 - \cos\phi) + m_0^2c^4 + 2h(\nu - \nu')m_0c^2 \quad \text{--- (6)}$$

Now Relativistic Mass formula

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

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

→ Eqn - (6) becomes

$$\cancel{m_0^2 c^4} = -2h^2 v v' (1 - \cos \phi) + \cancel{m_0^2 c^4} + 2h(v - v') m_0 c^2$$

$$2h^2 v v' (1 - \cos \phi) = 2h(v - v') m_0 c^2$$

$$\frac{v - v'}{v v'} = \frac{h}{m_0 c^2} (1 - \cos \phi) \quad \text{--- (7)}$$

We know that

$$\lambda = \frac{c}{v} \quad , \quad \lambda' = \frac{c}{v'}$$

$$\Delta \lambda = \lambda' - \lambda = \frac{c}{v'} - \frac{c}{v} = c \left[\frac{1}{v'} - \frac{1}{v} \right]$$

$$\frac{\lambda' - \lambda}{c} = \frac{v - v'}{v v'} \quad \text{--- (8)}$$

from eqn - (7) & (8)

$$\frac{\lambda' - \lambda}{c} = \frac{h}{m_0 c^2} (1 - \cos \phi)$$

$\Delta \lambda = \lambda' - \lambda = \left(\frac{h}{m_0 c} \right) (1 - \cos \phi)$

Compton Shift

↓
Compton constant 0.0242

$\rightarrow \Delta \lambda = \lambda_c (1 - \cos \phi)$
Compton's wavelength = $\frac{h}{m_0 c}$

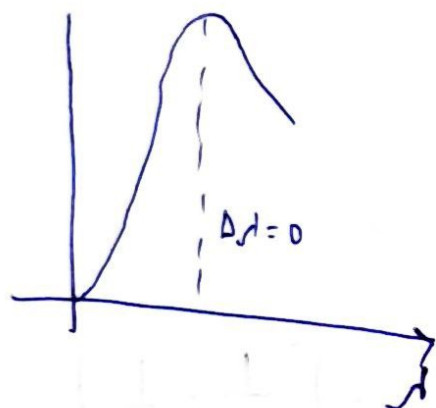
$\therefore \Delta \lambda = 0.0242 (1 - \cos \phi)$

(1)

$\phi = 0^\circ, \cos \phi = 1$

$\Delta \lambda = \lambda' - \lambda = 0$

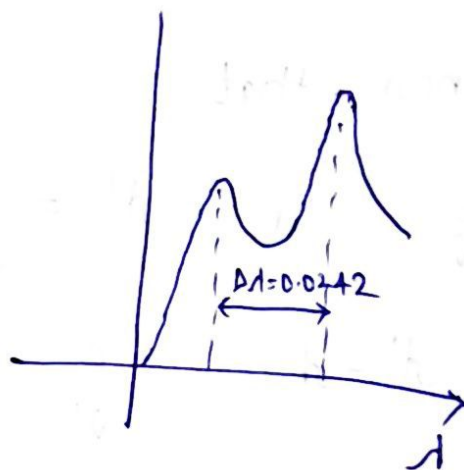
$\lambda' = \lambda$



(2)

$\phi = \frac{\pi}{2}, \cos \phi = 0$

$\Delta \lambda = 0.0242$

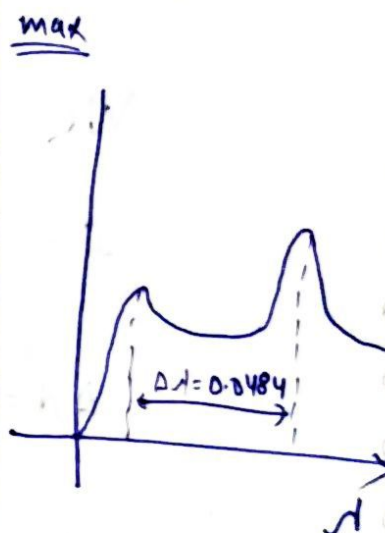


(3)

$\phi = \pi, \cos \pi = -1$

$\Delta \lambda = 2\lambda_c$

$\Delta \lambda = 0.0484$



WAVE function : —

The varying quantity characterising the matter wave is denoted by $\psi(x, y, z)$ at a point i.e. the quantity whose variation makes up the matter wave is known as wave function or wave amplitude.

The value of the wave function of a particle at a given point of space & time is related to likelihood of the particle's being there at the time.

Each particle is represented by a wavefunction Ψ (position, time)



Basic postulates of Wave-function :-

Postulate - I [Essential Boundary Conditions]

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Basic postulates of Quantum Mechanics :-

The relationship b/w quantum mechanics & operators has helped to present the concepts in form of some postulates. These are :-

Postulate - **I**

1. The state of a system is completely specified by the wavefunction $\Psi(x, y, z, t)$

wavefunction must satisfy the following conditions

(i) $\Psi(x)$ & $\frac{d\Psi(x)}{dx}$ must be finite for all values of x .

(ii) $\Psi(x)$ & $\frac{d\Psi(x)}{dx}$ must be continuous for all values of x .

(iii) $\Psi(x)$ as well as $\frac{d\Psi(x)}{dx}$ must be single valued for all x .

Wave fn also has 2 properties: -

(a) $\int \Psi \Psi^* dv = 1 \rightarrow$ Normalization condition

(b) $\int \Psi_i \Psi_j^* dv = 0$ or $\int \Psi_j \Psi_i^* dv = 0$

This is the orthogonal condition.

Postulate - (II)

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Every Observable quantity can be expressed by an operator in QM.

Variable	Classical Quantity	Operator Symbol	Quantum Mechanical Operator
1. Components of momentum	P_x, P_y, P_z	$\hat{P}_x, \hat{P}_y, \hat{P}_z$	$-\frac{i\hbar}{2\pi} \frac{\partial}{\partial x}, -\frac{i\hbar}{2\pi} \frac{\partial}{\partial y}, -\frac{i\hbar}{2\pi} \frac{\partial}{\partial z}$
2. Linear momentum	$\vec{P}$	$\hat{\vec{P}}$	$-\frac{i\hbar}{2\pi} \vec{\nabla}$
3. Total energy	$E = \frac{P^2}{2m} + V$	$\hat{E}$	$i\hbar \frac{\partial}{\partial t}$
4. Hamiltonian	$H = \frac{P^2}{2m} + V$	$\hat{H}$	$-\frac{\hbar^2}{8\pi^2 m} \nabla^2 + V$

Postulate - (III)

When a measurement of an observable quantity 'f' is made on system for which the wave ψ is Ψ , we get different values of 'f' during different measurements. The most probable value of 'f' is given by

$$\langle f \rangle = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{F} \Psi dv}{\int_{-\infty}^{\infty} \Psi^* \Psi dv}$$

where $\hat{F}$ = operator associated with observable quantity 'f'

Ψ^* = complex conjugate of wave ψ Ψ

$\langle f \rangle$ = expectation value or average value of observable quantity (f)

Postulate - (IV)

A particle moving in space can be represented by following wave eqⁿ.

$$\frac{-h^2}{8\pi^2 m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi + V\Psi = \frac{ih}{2\pi} \frac{\partial \Psi}{\partial t}$$

This is called Schrodinger wave eqⁿ.

Schrodinger's Wave Equation :-

Time dependent one dimension Schrodinger's wave Equation [STDE] $\Rightarrow$



Let a particle of mass m is moving along x -direction in conservation-force field.

$$\Psi_{(x,t)} = A \cdot e^{-i(\omega t - kx)} \quad \text{--- (1)}$$

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

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

$\lambda = \frac{h}{p}$ matter wave
de-Broglie wave

where E = total Energy

p = momentum

Putting value of ω & k in eqn - (1)

$$\Psi = A \cdot e^{-i \frac{2\pi}{h} (Et - Px)}$$

$$\Psi = A \cdot e^{-i/\hbar (Et - Px)}, \text{ where } \hbar = \frac{h}{2\pi}$$

--- (2)

Now differentiating eqn - (2) twice w.r.t. ' x '

$$\frac{\partial^2 \Psi}{\partial x^2} = A \cdot \left(\frac{iP}{\hbar} \right)^2 \cdot e^{-i/\hbar (Et - Px)}$$

$$= -1 \cdot \left(\frac{P^2}{\hbar^2} \right) \cdot A \cdot e^{-i/\hbar (Et - Px)} \quad \text{where } (i^2 = -1)$$

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = -\frac{p^2}{\hbar^2} \cdot \Psi(x,t)$$

$$\boxed{p^2 \Psi(x,t) = -\hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2}} \quad (3)$$

Now, differentiating eqⁿ-(2) once w.r.t. 't'

$$\frac{\partial \Psi(x,t)}{\partial t} = \frac{-i}{\hbar} \cdot E \cdot A \cdot e^{-i/\hbar (Et - px)}$$

$$\frac{\partial \Psi(x,t)}{\partial t} = \frac{-i}{\hbar} E \cdot \Psi(x,t)$$

$$E \Psi(x,t) = -\frac{\hbar}{i} \cdot \frac{\partial \Psi(x,t)}{\partial t}$$

(where $\frac{-1}{i} = i$)

$$\boxed{E \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}} \quad (4)$$

By means of the principle of conservation of energy in non-relativistic mechanics, we have

Total Energy = Kinetic Energy + Potential Energy

$$E \Psi(x,t) = \frac{p_x^2}{2m} + V(x,t)$$

~~1/2 m v^2~~

Multiplying by Ψ

$$E \Psi(x,t) = \frac{p^2}{2m} \cdot \Psi(x,t) + V(x,t) \cdot \Psi(x,t)$$

from eqⁿ - (3) & (4)

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

For free particle $V=0$ (the potential energy is considered to be zero)

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

→ Now for Hamiltonian form of SE

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(x,t) + V \Psi(x,t)$$

$$\text{Here } \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2 \quad \text{--- (5)}$$

(Laplacian Operator)

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi(x,t) + V \Psi(x,t) \quad \text{--- (6)}$$

This is Schrodinger 3D time dependent wave equation.

for free particle $V=0$

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi(n,t)$$

from eqⁿ - (6)

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V \right) \Psi(n,t) = i\hbar \frac{\partial \Psi}{\partial t} \quad \text{--- (7)}$$

↓
Hamiltonian
Operator

$$H = \frac{-\hbar^2}{2m} \nabla^2 + V \quad \text{--- (8)}$$

from eqⁿ - (7) & (8)

$$H \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \left(E\Psi \rightarrow i\hbar \frac{\partial \Psi}{\partial t} \right)$$

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

This eqⁿ is called Hamiltonian form of the Schrodinger wave eqⁿ.

Schrodinger Time Independent Wave Eqn

When the potential energy is constant in time we can simplify the wave equation

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

$$\Psi = A \cdot e^{-i/\hbar (Et - Px)}$$

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

$$\Psi = A \cdot e^{-i/\hbar (Px - Et)} = A \cdot e^{\frac{2\pi i}{h} (Px - Et)} \quad \text{--- (1)}$$

~~different~~

~~$$\Psi = A \cdot e^{\frac{2\pi i Px}{h}}$$~~

$$\Psi = A \cdot e^{\frac{2\pi i Px}{h}} \cdot e^{\frac{-2\pi i Et}{h}}$$

$$\boxed{\Psi(x, t) = \Psi(x) e^{\frac{-2\pi i Et}{h}}} \quad \text{--- (2)}$$

Where $\Psi(x) = A \cdot e^{2\pi i Px/h}$

$$\Rightarrow i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \cdot \Psi \quad (\text{Time dependent SE})$$

$$\frac{-\hbar}{2\pi i} \frac{\partial \Psi}{\partial t} = \left(\frac{-\hbar^2}{8\pi^2 m} \right) \left(\frac{\partial^2 \Psi}{\partial x^2} \right) + V \cdot \Psi(x, t)$$

$$\frac{i\hbar}{2\pi} \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{8\pi^2 m} \frac{\partial^2 \Psi}{\partial x^2} + V \cdot \Psi(x, t) \quad \text{--- (3)}$$

Now differentiating eqn (2) w.r.t 'x'

$$\frac{\partial \Psi}{\partial x} = \frac{\partial \Psi}{\partial x} e^{-2\pi i Et/h}$$

$$\left(\frac{h}{2\pi}\right)^2$$

$$ie = -1$$

$$ixi = -1$$

$$i = \frac{-1}{i}$$

Now again differentiating w.r.t. 'x'

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{\partial^2 \Psi(x)}{\partial x^2} e^{-2\pi i E t / \hbar} \quad \text{--- (4)}$$

→ Now differentiating eqⁿ (1) w.r.t. 't'

$$\frac{\partial \Psi(x,t)}{\partial t} = \frac{\partial}{\partial t} [\Psi(x) \cdot e^{-2\pi i E t / \hbar}]$$

$$\frac{\partial \Psi}{\partial t} = \Psi(x) \cdot \left(\frac{-2\pi i E}{\hbar} \right) \cdot e^{-2\pi i E t / \hbar} \quad \text{--- (5)}$$

Now putting value of $\frac{\partial \Psi}{\partial t}$ & $\frac{\partial^2 \Psi}{\partial x^2}$ and $\Psi(x,t)$ in eqⁿ (3)

$$\Rightarrow \frac{i\hbar}{2\pi} \Psi(x) \left(\frac{-2\pi i E}{\hbar} \right) e^{-2\pi i E t / \hbar} = \frac{-\hbar^2}{8\pi^2 m} \frac{\partial^2 \Psi(x)}{\partial x^2} e^{-2\pi i E t / \hbar} + V \cdot \Psi(x) \cdot e^{-2\pi i E t / \hbar}$$

$$\Rightarrow E \cdot \Psi(x) = \frac{-\hbar^2}{8\pi^2 m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V \Psi(x)$$

$$\frac{\hbar^2}{8\pi^2 m} \cdot \frac{\partial^2 \Psi(x)}{\partial x^2} - V \Psi(x) + E \Psi(x) = 0$$

By multiplying above eqⁿ by $\frac{8\pi^2 m}{\hbar^2}$ on both sides

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{8\pi^2 m}{\hbar^2} (E \Psi(x) - V \Psi(x)) = 0$$

$$\boxed{\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{8\pi^2 m}{\hbar^2} (E - V) \Psi(x) = 0}$$

In 3D, STIE is

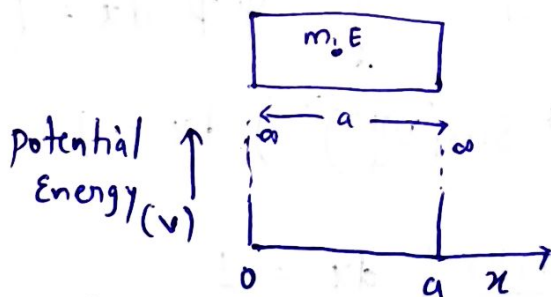
$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

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

Particle in a rigid One-Dimensional Box
(Infinite square well potential) $\Rightarrow$

Let us consider the motion of a particle of mass ' m ' along x -axis in one-dimensional potential box which has perfectly rigid walls of infinite potentials at $x=0$ & $x=a$



$$\begin{aligned} V(x) &= 0 & 0 < x < a \\ V(x) &= \infty & x \leq 0 \text{ \& \> } x \geq a \\ \psi(x) &= 0 & x > a, x \leq 0 \end{aligned}$$

Wave f^n is complex quantity, which itself has no physical significance

1-D STIE

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

$$\therefore V=0 \text{ and Let } \frac{8\pi^2 m E}{h^2} = k^2$$

$$\frac{d^2 \psi(x)}{dx^2} + k^2 \psi(x) = 0 \quad \text{--- (1)}$$

$$\psi = A \sin kx + B \cos kx \quad \text{--- (2)}$$

$$\text{at } x=0, \psi=0$$

$$x=a, \psi=0$$



$$\text{using } x=0, \psi=0 \text{ in eqn --- (2)}$$

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

$$\boxed{B=0} \quad \text{--- (3)}$$

$$\text{In eqn --- (2)} \quad \boxed{\psi = A \sin kx} \quad \text{--- (4)}$$

$$\text{Using boundary condition at } x=a, \psi(x)=0 \text{ in eqn --- (4)}$$

$$0 = A \sin ka$$

$$ka = n\pi, \quad n=1, 2, 3, \dots$$

$$\text{Using } k = \frac{n\pi}{a} \text{ in eqn --- (4)}$$

$$\boxed{\psi = A \sin \frac{n\pi x}{a}} \quad \text{--- (5)}$$

Normalization Condition

$$\int_0^a \psi \psi^* dx = 1$$

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

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

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

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

$$\Rightarrow \frac{A^2}{2} \int_0^a dx = \frac{A^2}{2} \cdot \frac{\sin(2n\pi x/a)}{2n\pi/a} \Big|_0^a = 1$$

$$\frac{A^2}{2} (a) - \frac{A^2}{2 \left(\frac{2\pi n}{a} \right)} \left[\sin \left(\frac{2n\pi a}{a} \right) - \sin(0) \right] = 1$$

$$A^2 = \frac{2}{a} \Rightarrow A = \sqrt{\frac{2}{a}} \quad \text{--- (6)}$$

Using eqⁿ - (6) in eqⁿ - (5)

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \left(\frac{n\pi x}{a} \right) \quad \text{Wave Function}$$

(where a = width of box)

$$\therefore k^2 = \frac{8\pi^2 m E}{h^2}, \quad k = \frac{n\pi}{a}$$

$$\frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 m E}{h^2} \Rightarrow E_n = \frac{n^2 \pi^2 h^2}{8\pi^2 m a^2}$$

$$E_n = \frac{n^2 \pi^2}{2m} \left(\frac{h^2}{4\pi^2} \right) \left(\frac{1}{a^2} \right)$$

$$E_n = \frac{n^2 \pi^2 h^2}{2m a^2}$$

Energy Eigen Value

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

Assume $E_1 = \frac{\pi^2 h^2}{2m a^2}$ ✓

$$E_n = n^2 E_1 \quad \text{--- (7)}$$

$$E_1, E_2 = 4E_1, E_3 = 9E_1, E_4 = 16E_1, \dots$$

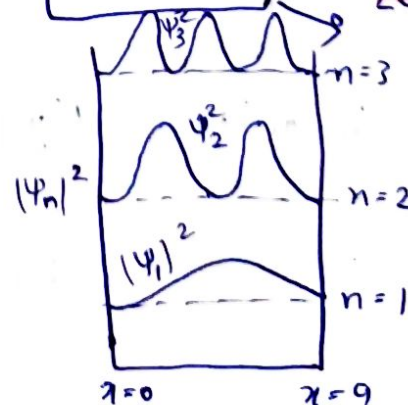
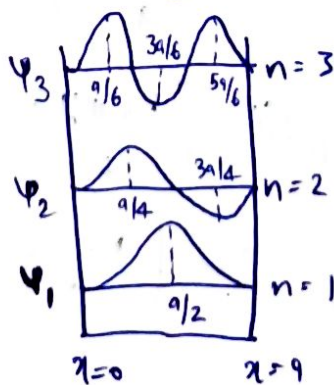
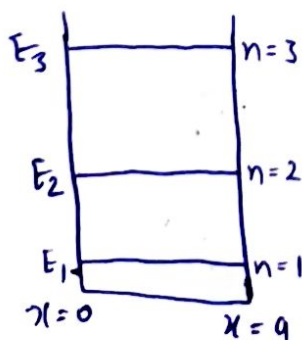
So Energy of particle is quantized & discrete.

min Energy $\neq 0$

it is

$$E_1 = \frac{\pi^2 h^2}{2m a^2}$$

zero point energy



Probability density in 1D Box

So wave function is a complex quantity,
which itself has no physical significance
But square of its magnitude gives the
probability of finding a particle in a given
volume of space at a given time.

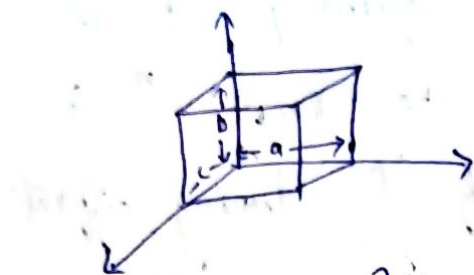
$$\Psi_a(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\right)x$$

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

$$P = \int_{x_1}^{x_2} |\Psi(x,t)|^2 dx$$

—————x—————

Free particle in a 3-D box



$$V(x, y, z) = 0 \quad , \quad 0 < x < a, 0 < y < b, 0 < z < c$$

$$V(x, y, z) = \infty \quad , \quad x \leq 0, x \geq a$$

$$y \leq 0, y \geq b$$

$$z \leq 0, z \geq c$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + \frac{8\pi^2 m}{h^2} (E \psi) = 0 \quad \text{--- (1)} \quad \text{where } V=0, V=\infty$$

$$\psi(x, y, z) = XYZ \quad \text{--- (2)}$$

$$\Rightarrow YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} = -\frac{8\pi^2 m E}{h^2} XYZ$$

$$\Rightarrow \frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = -\frac{8\pi^2 m E}{h^2}$$

These terms are independent so

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = -k_x^2 \Rightarrow \frac{\partial^2 X}{\partial x^2} + k_x^2 X = 0 \quad \text{--- (4)}$$

$$\frac{\partial^2 Y}{\partial y^2} + k_y^2 Y = 0 \quad \text{--- (5)}$$

$$\frac{\partial^2 Z}{\partial z^2} + k_z^2 Z = 0 \quad \text{--- (6)}$$

The solⁿ of eqⁿ - (4) can be written as

$$X(x) = A \sin k_x x + B \cos k_x x \quad \text{--- (8)}$$

$$\text{At } x=0, V(x)=\infty, X(x)=0 \checkmark$$

$$\text{At } x=a, V(a)=\infty, X(a)=0 \checkmark$$

$$\text{At } x=0, X(x)=0$$

$$0 = A \sin k_x(0) + B \cos k_x(0) \Rightarrow B=0$$

$$\text{In eqⁿ - (8)} \quad X(x) = A \sin k_x x \quad \text{--- (9)}$$

$$\text{At } x=a, X(a)=0$$

$$X(a) = A \sin k_x a = 0 \Rightarrow k_x a = n_1 \pi$$

$$k_x = \frac{n_1 \pi}{a} \quad \text{in eqn } \textcircled{9}$$

$$X(x) = A \sin\left(\frac{n_1 \pi}{a} x\right) \quad \textcircled{10}$$

$$\int_0^a X^*(x) X(x) dx = 1$$

$$\int_0^a A^2 \sin^2\left(\frac{n_1 \pi}{a} x\right) dx = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{a}}$$

$$\Rightarrow X(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_1 \pi x}{a}\right) \quad \textcircled{11}$$

Similarly $Y(y) = \sqrt{\frac{2}{b}} \sin\left(\frac{n_2 \pi y}{b}\right) \quad \textcircled{12}$

$$Z(z) = \sqrt{\frac{2}{c}} \sin\left(\frac{n_3 \pi z}{c}\right) \quad \textcircled{13}$$

Thus total Ψ of free particle in 3-D box

$$\Psi(x, y, z) = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi y}{b}\right) \sin\left(\frac{n_3 \pi z}{c}\right) \quad (14)$$

Substituting values of k_x, k_y & k_z in eqⁿ (7)

$$\left(\frac{n_1 \pi}{a}\right)^2 + \left(\frac{n_2 \pi}{b}\right)^2 + \left(\frac{n_3 \pi}{c}\right)^2 = \frac{8\pi^2 m E}{h^2}$$

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

$$E = \frac{h^2}{8m} \left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2 + \left(\frac{n_3}{c}\right)^2 \right]$$

Where box is cube $a=b=c$
the wave fⁿ is given by

$$\sqrt{\frac{8}{abc}} = \sqrt{\frac{(2)^3}{(a)^3}} = \left(\frac{2}{a}\right)^{3/2}$$

$$\Psi(x, y, z) = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi y}{a}\right) \sin\left(\frac{n_3 \pi z}{a}\right)$$

$$\text{Total energy } E_{n_1 n_2 n_3} = \frac{h^2}{8m a^2} (n_1^2 + n_2^2 + n_3^2)$$

$$E_{n_1 n_2 n_3} = E_0 (n_1^2 + n_2^2 + n_3^2) \quad , \quad E_0 = \frac{h^2}{8m a^2}$$