UNIT: 3 "Quantum Physics"

* **Wave-particle duality :-** According to Einstein, the energy of light is concentrated into small regions. This represents the smallest quantity of energy known as photon. This photon is an energy particle. Hence light shows itself as wave nature at one hand and particle nature on the other hand. This shows that light is having wave nature as well as particle nature. This nature of light is known as dual nature and the property is known as wave-particle duality.

* **Matter Waves or de-Broglie waves :-** Acc. to de-Broglie " a moving matter particle is surrounded by a wave whose wavelength depends upon the mass of the particle and its velocity. These waves associated with the matter particles are known as matter waves or de-Brglie waves.

* **Wavelength of de-Broglie waves :-**

Since energy of Photon is given by

$$E = h\nu = \frac{hc}{\lambda} \quad \text{——} (I) \qquad \because c = \nu\lambda,\ \nu = \frac{c}{\lambda}$$

and according to Einstein's mass-energy rel^n.

$$E = mc^2 \quad \text{——} (II)$$

from eq^n (I) & (II)

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

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

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

$$\boxed{\lambda = \frac{h}{p}} \quad \text{—— (III)}$$

where $p = mc$ momentum of particle

$h = 6.62 \times 10^{-34}$ J.S.

If in place of photon a particle of mass m, moving with vel. v then its momentum $p = mv$.

from eq^n (III)

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

* de-Broglie wavelength in terms of K.E. :-

$\because$ K.E $\quad E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m}$

$$E = \frac{p^2}{2m} \qquad \because p = mv$$

$$p^2 = 2mE$$

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

from eq^n (III) de-Broglie wavelength

$$\boxed{\lambda = \frac{h}{\sqrt{2mE}}} \text{—— (V)}$$

* de-Broglie wavelength for gas molecule :-

Acc. to kinetic theory of gases.

K.E $\quad E = \frac{3}{2}kT$

where $k = 1.38 \times 10^{-23}$ J/K Boltzmann const. & T – temp.

from eq^n (V)

$$\lambda = \frac{h}{\sqrt{\cancel{2}m.\frac{3}{\cancel{2}}kT}}$$

$\lambda = \quad h$

de-Broglie Wavelength of an electron :-

Suppose an electron accelerates through a potential diff^c of V volts then

Workdone by electric field = Gain in K.E

$$eV = \frac{1}{2} mv^2$$

$$eV = E$$

from eq^n (v) de-Broglie wavelength

$$\boxed{\lambda = \frac{h}{\sqrt{2meV}}} \quad \text{--- (vii)}$$

(i) for an electron $m = 9.1 \times 10^{-31}$ kg

$e = 1.6 \times 10^{-19}$ C

$h = 6.62 \times 10^{-34}$ J.s

$$\lambda = \frac{6.62 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \cdot V}}$$

$$\boxed{\lambda = \frac{12.27}{\sqrt{V}} \text{Å}} \quad \text{--- (viii)}$$

(ii) for a neutron, $m = 1.67 \times 10^{-27}$ kg

$$\boxed{\lambda = \frac{0.286}{\sqrt{V}} \text{Å}} \quad \text{--- (ix)}$$

Properties of Matter Waves:

from the expression of de-Broglie wavelength $\lambda = \frac{h}{mv}$ it is clear that:

① $\lambda \propto \frac{1}{m}$ i.e. de-Broglie wavelength of a wave associated with light particle is greater than the wavelength associated with heavier particle.

② The de-Broglie wavelength of a wave associated with a slow moving particle is greater than the wavelength associated with fast moving particle.

③ The matter waves generated only when the material particle are in motion.

④ the matter waves are generated by moving charged particle as well as moving neutral particle

⑤ The velocity of matter waves is not constant. like the radiations.

⑥ de-Broglie waves are not electromagnetic waves.

Phase Velocity (V_p):- When a monochromatic wave travels through a medium, its velocity of advancement in the medium is called phase velocity. It is represented by V_p.

Consider a wave whose displacement is y as.

$$y = a\sin(\omega t - kx) \quad \text{--- (1)}$$

where a - amplitude

$\omega = 2\pi\nu$. angular freq.

$k = \frac{2\pi}{\lambda}$. propagation const.

In eq^n (1) the phase term.

$$\omega t - kx = \text{const.}$$

diff. w.r.to 't' we get

$$\omega \cdot 1 - k\frac{dx}{dt} = 0$$

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

$$\frac{dx}{dt} = \frac{\omega}{K}$$

or Phase velocity $V_p = \frac{d\omega}{dk} = \frac{\omega}{K}$

$$\boxed{V_p = \frac{\omega}{K}}$$

Group Velocity (V_g) :- When two or more waves travels in a medium, when they superimpose on each other, then the velocity of resultant wave is called group velocity. and it is denoted by V_g.

Consider two waves having displacement y_1 & y_2 then

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

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

where a - amplitude

ω_1, ω_2 - angular frequencies

k_1, k_2 - propagation const.

According to the principle of superposition

$$y = y_1 + y_2$$

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

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

$$y = \quad \because \sin A + \sin B = 2\sin\left(\frac{A+B}{2}\right) \cdot \cos\left(\frac{A-B}{2}\right)$$

$$y = 2a \sin\left\{\frac{(\omega_1 t - k_1 x) + (\omega_1 t + k_2 x)}{2}\right\} \cdot \cos\left\{\frac{(\omega_1 t - k_1 x) - (\omega_2 t - k_2 x)}{2}\right\}$$

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

$$y = 2a \sin\left\{\frac{(\omega_1 + \omega_2)t - (k_1 + k_2)x}{2}\right\} \cdot \cos\left\{\frac{(\omega_1 - \omega_2)t - (k_1 - k_2)x}{2}\right\}$$

$$y = 2a \sin\left\{\frac{(\omega_1 + \omega_2)}{2}t - \frac{(k_1 + k_2)x}{2}\right\} \cdot \cos\left\{\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2}\right\}$$

let $\frac{\omega_1 + \omega_2}{2} = \omega$. $\frac{k_1 + k_2}{2} = k$ $\quad k_1 - k_2 = \Delta k$ & $\omega_1 - \omega_2 = \omega$

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

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

$$y = A \sin(\omega t - kx) \quad \text{--- (3)}$$

where $A = 2a\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)$ amplitude --- (4)

In eqn. (4) the term

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = \text{const.}$$

Diff. w.r. to 't' we get

$$\frac{\Delta\omega}{2} \cdot 1 - \frac{\Delta k}{2}\frac{dx}{dt} = 0$$

$$\frac{\Delta\omega}{\cancel{2}} = \frac{\Delta k}{\cancel{2}}\frac{dx}{dt}$$

$$\frac{dx}{dt} = \frac{\Delta\omega}{\Delta k} = \frac{\omega_1 - \omega_2}{k_1 - k_2}$$

But

$$\lim_{\substack{\Delta\omega \to 0 \\ \Delta k \to 0}} \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$$

$$\frac{dx}{dt} = \frac{d\omega}{dk}$$

or group velocity $V_g = \frac{dx}{dt} = \frac{d\omega}{dk}$

or $\boxed{V_g = \frac{d\omega}{dk}}$ --- (5)

Relation betn group vel. (V_g) and phase velocity (V_p):-

∵ phase velocity $V_p = \frac{\omega}{k}$

$$\omega = V_p \cdot k$$

& Group velocity $V_g = \frac{d\omega}{dk}$

$$V_g = \frac{d}{dk}(V_p \cdot k)$$

$$V_g = V_p \cdot 1 + k\frac{dV_p}{dk}$$

$$V_g = V_p + \frac{2\pi}{\lambda} \cdot \frac{dV_p}{d\left(\frac{2\pi}{\lambda}\right)}$$

$$V_g = V_p + \frac{\cancel{2\pi}}{\lambda} \cdot \frac{dV_p}{\cancel{2\pi}\, d\left(\frac{1}{\lambda}\right)}$$

$$V_g = V_p + \frac{1}{\lambda} \cdot \frac{dV_p}{-\lambda^{-2} d\lambda}$$

$$V_g = V_p - \frac{\lambda^{\cancel{2}}}{\cancel{\lambda}} \frac{dV_p}{d\lambda}$$

$$\boxed{V_g = V_p - \lambda \frac{dV_p}{d\lambda}} \quad \text{—— (1)}$$

this eqn (1) represents reln betn V_g & V_p in a dispersive medium ie here $\boxed{V_p > V_g}$

In non-dispersive medium $V_p = \text{const.}$

from eqn (1) $\frac{dV_p}{d\lambda} = 0$

$$V_g = V_p - 0$$

⊛ Relation betⁿ V_g, V_p & V for relativistic particle:-

☆ Relation betⁿ phase vel. (V_p) & Particle vel. (v):-

Since $\omega = 2\pi\nu = \frac{2\pi h\nu}{h}$ $\quad \left\{ \begin{array}{l} h\nu = E \\ h\nu = mc^2 \end{array} \right.$

$$\omega = \frac{2\pi mc^2}{h} \quad \text{—— (i)}$$

and $k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/mv}$ $\quad \because \lambda = \frac{h}{mv}$

$$k = \frac{2\pi mv}{h} \quad \text{—— (ii)}$$

phase velocity $V_p = \frac{\omega}{k}$

$$V_p = \frac{\cancel{2\pi}\cancel{m}c^2/\cancel{h}}{\cancel{2\pi}\cancel{m}v/\cancel{h}}$$

$$\boxed{V_p = \frac{c^2}{v}} \quad \text{—— (iii)}$$

☆ Relation betⁿ group vel. (V_g) and particle vel. (v):-

Since group velocity $V_g = \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{d\left(\frac{2\pi}{\lambda}\right)}$

$$V_g = \frac{d\nu}{d(1/\lambda)}$$

or

$$\frac{1}{V_g} = \frac{d}{d\nu}\left(\frac{1}{\lambda}\right) \quad \text{—— (i)}$$

$\because$ total energy of a particle

$$E = K.E + P.E$$

$$E = \frac{1}{2}mv^2 + V$$

$$\frac{1}{2}mv^2 = E - V$$

$$v^2 = \frac{2(E-V)}{m}$$

$$v = \left\{\frac{2(E-V)}{m}\right\}^{1/2} \quad \text{———— (2)}$$

∵ de-Broglie wavelength $\lambda = \frac{h}{mv}$

$$\frac{1}{\lambda} = \frac{mv}{h} = \frac{m}{h}\left\{\frac{2(E-V)}{m}\right\}^{1/2}$$

from eqn. (1)

$$\frac{1}{v_g} = \frac{d}{d\nu}\left[\frac{m}{h}\left\{\frac{2(E-V)}{m}\right\}^{1/2}\right]$$

$$\frac{1}{V_g} = \frac{m}{h}\left\{\frac{2(h\nu - V)}{m}\right\}^{1/2} \qquad \because E = h\nu$$

$$= \frac{\cancel{m}}{\cancel{h}} \cdot \frac{1}{\cancel{2}}\left\{\frac{2(h\nu-V)}{m}\right\}^{-1/2} \cdot \frac{\cancel{2}\cancel{h}}{\cancel{m}}$$

$$= \left\{\frac{2(h\nu - V)}{m}\right\}^{-1/2}$$

$$\frac{1}{V_g} = \left\{\frac{2(E-V)}{m}\right\}^{-1/2} \qquad \text{from eqn (2)}$$

$$\frac{1}{V_g} = \frac{1}{v}$$

or $\boxed{V_g = V}$

∴ $\boxed{\text{Group vel.} = \text{particle vel.}}$

Heisenberg's Uncertainty Principle :-

According to Heisenberg's uncertainty principle "It is impossible to determine exact position and momentum of a particle simultaneously with certainty."

If Δx and Δp be the uncertainties in position and momentum resp. then

$$\boxed{\Delta x \cdot \Delta p \approx h} \quad \text{or} \quad \boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}}$$

* **Proof :-** let us consider two waves having displacement y_1 & y_2 as

$$y_1 = a\sin(\omega_1 t - k_1 x) \quad \text{--- (1)}$$

$$y_2 = a\sin(\omega_2 t - k_2 x) \quad \text{--- (2)}$$

According to the principle of superposition -

$$y = y_1 + y_2$$

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

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

$$\because \sin A + \sin B = 2\sin\left(\frac{A+B}{2}\right) \cdot \cos\left(\frac{A-B}{2}\right)$$

$$y = 2a\sin\left\{\frac{(\omega_1 t - k_1 x) + (\omega_2 t - k_2 x)}{2}\right\} \cdot \cos\left\{\frac{(\omega_1 t - k_1 x) - (\omega_2 t - k_2 x)}{2}\right\}$$

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

$$y = 2a\sin\left\{\frac{(\omega_1 + \omega_2)t - (k_1 + k_2)x}{2}\right\} \cdot \cos\left\{\frac{(\omega_1 - \omega_2)t - (k_1 - k_2)x}{2}\right\}$$

$$y = 2a\sin\left\{\frac{(\omega_1 + \omega_2)}{2}t - \frac{(k_1 + k_2)}{2}x\right\} \cdot \cos\left\{\frac{(\omega_1 - \omega_2)}{2}t - \frac{(k_1 - k_2)}{2}x\right\}$$

let $\frac{\omega_1 + \omega_2}{2} = \omega$, $\frac{k_1 + k_2}{2} = k$, $\omega_1 - \omega_2 = \Delta\omega$ & $k_1 - k_2 = \Delta k$

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

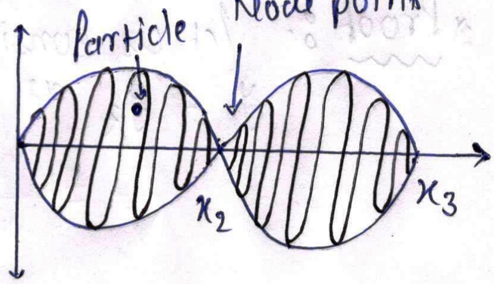
$$y = 2a \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\cdot \sin(\omega t - kx)$$

$$y = A \sin(\omega t - kx) \quad \text{——— (3)}$$

where $A = 2a\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)$ ——— (4)

is amplitude of wave packet.

At node points $x_1, x_2, x_3 \ldots$ the amplitude



$A = 0$ or

$$2a\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = 0$$

$$\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = 0$$

$$\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = \cos(2n+1)\frac{\pi}{2}$$

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = (2n+1)\frac{\pi}{2}$$

$n = 0, 1, 2, 3 \ldots$

at node point x_1

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1 = (2n+1)\frac{\pi}{2} \quad \text{——— (5)}$$

at x_2

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 = (2n+3)\frac{\pi}{2} \quad \text{——— (6)}$$

eqn (6) − (5)

$$\cancel{\frac{\Delta\omega}{2}t} - \frac{\Delta k}{2}x_2 - \cancel{\frac{\Delta\omega}{2}t} + \frac{\Delta k}{2}x_1 = (2n+3)\frac{\pi}{2} - (2n+1)\frac{\pi}{2}$$

$$\frac{\Delta k}{2}x_1 - \frac{\Delta k}{2}x_2 = \frac{\pi}{2}(\cancel{2n}+3-\cancel{2n}-1)$$

$$\frac{\Delta k}{2}(x_1 - x_2) = \frac{\pi}{\cancel{2}} \times \cancel{2}$$

$$\frac{\Delta k}{2}(x_1 - x_2) = \pi$$

$$x_1 - x_2 = \frac{2\pi}{\Delta k}$$

$\left\{ \because \Delta x = x_1 - x_2 \right.$

$\left(k = \frac{2\pi}{\lambda} \right.$

$\Rightarrow \quad \Delta x = \dfrac{2\pi}{\Delta\left(\frac{2\pi p}{h}\right)}$ $\left\{ k = \frac{2\pi p}{h} \right.$

$$\Delta x = \frac{2\pi}{\frac{2\pi}{h} \cdot \Delta p}$$

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

or

$$\boxed{\Delta x \cdot \Delta p \approx h} \quad --- (7)$$

for more accuracy

$$\boxed{\Delta x \cdot \Delta p \geq \frac{h}{4\pi} \left(\text{or } \frac{\hbar}{2}\right)} \quad \left\{ \hbar = \frac{h}{2\pi} \right\}$$

This is uncertainty principle.

✱ Energy and time uncertainty :-

Since K.E. $\quad E = \frac{1}{2} mv^2 = \frac{m^2 v^2}{2m}$

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

$\therefore$ uncertainty in energy

$$\Delta E = \frac{\Delta p^2}{2m} = \frac{2p \Delta p}{2m} = \frac{\cancel{m} v \Delta p}{\cancel{m}}$$

If Δt be the uncertainty in time then

$$\Delta t = \frac{\Delta x}{v} \quad \text{--- (ii)} \qquad \left\{ \text{time} = \frac{\text{dist.}}{\text{vel.}} \right.$$

eq^n (i) × (ii) we get

$$\Delta E \times \Delta t = \cancel{v}\, \Delta P \cdot \frac{\Delta x}{\cancel{v}}$$

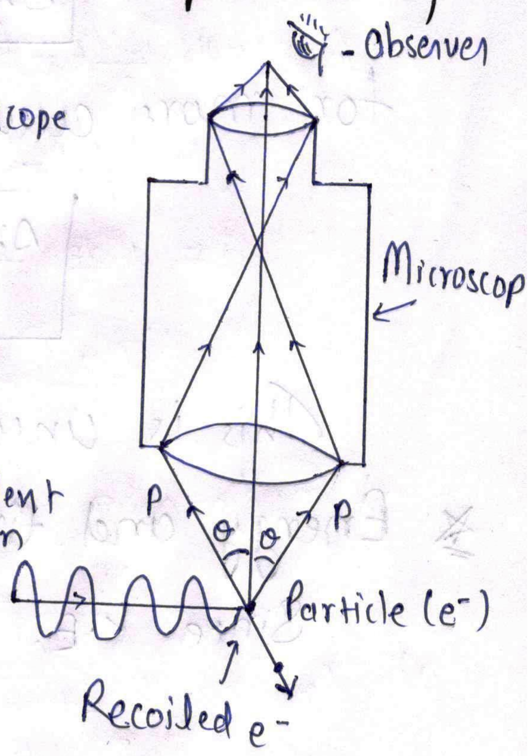
$$\Delta E \cdot \Delta t = \Delta x \cdot \Delta P$$

But $\Delta x \cdot \Delta P \approx h$ uncertainty principle

$$\Rightarrow \quad \boxed{\Delta E \cdot \Delta t \approx h} \quad \text{--- (iii)}$$

Applications of Uncertainty Principle :-

(1) Determination of the position of a particle by Microscope :-



Since the resolving limit of microscope is given by

$$\Delta x = \frac{\lambda}{2\sin\theta} \quad \text{--- (i)}$$

uncertainty in x-component of momentum

$$\Delta P_x = P\sin\theta - (-P\sin\theta)$$

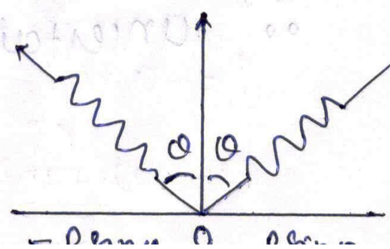
$$= P\sin\theta + P\sin\theta$$

$$= 2P\sin\theta$$

$$\Delta P_x = 2\frac{h}{\lambda}\sin\theta \quad \text{--- (ii)}$$

eq^n (i) × (ii)

$$\Delta x \cdot \Delta P_x = \frac{\lambda}{2\sin\theta} \cdot \frac{2h}{\lambda}\sin\theta$$



(ii) Non-existence of electrons in the nucleus :-

According to Bohr the size of nucleus $= 10^{-14}$ m. (radius)
If any type of particle is to exist in the nucleus, then the uncertainty in their position in a nucleus is

$$\Delta x = 2 \times 10^{-14} \, m$$

Acc. to uncertainty principle, uncertainty in momentum

$$\Delta P = \frac{h}{\Delta x} = \frac{6.62 \times 10^{-34}}{2 \times 10^{-14}} = 3.31 \times 10^{-20} \, kg\,m/sec$$

∴ The relativistic energy of an e^- in the nucleus is given by.

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

$$E = \sqrt{(9.1 \times 10^{-31})^2 (3 \times 10^8)^4 + (3.31 \times 10^{-20})^2 (3 \times 10^8)^2}$$

$$E = \sqrt{6.7 \times 10^{-27} + 98.6 \times 10^{-24}}$$

$$E = 99.3 \times 10^{-13} \text{ Joules}$$

$$E = \frac{99.3 \times 10^{-13}}{1.6 \times 10^{-19}} \, eV$$

$$E = 62 \times 10^6 \, eV$$

$$\boxed{E = 62 \, MeV}$$

Thus if the e^- resides in the nucleus it should have an energy of the order of 62 MeV. However electrons emitted during β-decay have energies of the order of 3 MeV. Hence e^- do not resides in the nucleus.

WAVE FUNCTION AND ITS PROPERTIES :-

In general, a wave is associated with quantities which vary periodically. In case of matter waves, the quantity that varies periodically is called a wave function. This is represented by ψ. This has no direct physical significance and is not an observable quantity. It is related to the probability of finding the particle at a given place at a given time.

Acc. to Max Born $\psi\psi^* = |\psi|^2$ gives the probability of finding the particle in the state ψ. ie. ψ^2 is a measure of probability density. The wave functions are generally complex.

The total probability of finding a particle in volume $dx\,dy\,dz$ is

$$\iiint_{-\infty}^{+\infty} |\psi|^2 \, dx\,dy\,dz = 1$$

ψ satisfying above requirement is said to be normalized.

(*) Properties of wave functions:-

Besides being normalized, the wave function ψ must be:

(i) Finite every where.

(ii) Single valued.

(iii) Continuous.

✱ Energy and momentum operators :-

The wave eq^n for a free particle is given by.

$$\psi = A e^{-\frac{i}{\hbar}(Et - px)} \quad \text{——} (1)$$

Partially Diff^t w.r.to t, we get

$$\frac{\partial \psi}{\partial t} = A e^{-\frac{i}{\hbar}(Et - px)} \cdot \left(-\frac{iE}{\hbar}\right)$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \cdot \psi$$

$$E\psi = -\frac{\hbar}{i} \cdot \frac{\partial \psi}{\partial t} \times \frac{i}{i}$$ multiply & divide by i

$$E\psi = \frac{-i\hbar}{i^2} \cdot \frac{\partial \psi}{\partial t}$$ $\because i^2 = -1$

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

$\therefore$ Energy operator $\boxed{E = i\hbar \frac{\partial}{\partial t}}$ —— (11)

Now partially diff^t eq^n (1) w.r.to x, we get

$$\frac{\partial \psi}{\partial x} = A e^{-\frac{i}{\hbar}(Et - px)} \cdot \frac{ip}{\hbar}$$

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar} \cdot \psi$$

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

$\therefore$ Momentum operator

$\hat{p} = \frac{\hbar}{i} \ldots \quad \hat{p} = \frac{\hbar}{i}\partial \ldots \quad \hat{p} = \frac{\hbar}{i} \cdot \partial \ldots$

SCHRODINGER'S WAVE EQUATION :

Schrodinger's time-independent wave eqⁿ :-

According to de-Broglie theory, a particle of mass m is always associated with a wave of wavelength $\lambda = h/mv$
If particle has wave properties, it then the behaviour of the particle described by Schrodinger eqⁿ.
Since the classical differential eqⁿ. of a wave motion is given by.

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right)$$

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \nabla^2 \psi \quad \text{———} \quad (1)$$

where - $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. Laplacian operator

v - vel. of wave

let the solⁿ. of eqⁿ (1) is given by

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

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

diffⁿ. w.r.to 't'

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

again $$\frac{\partial^2 \psi}{\partial t^2} = \psi_0\, e^{-i\omega t} (-i\omega).(-i\omega)$$

$$\frac{\partial^2 \psi}{\partial t^2} = \psi.\, i^2 \omega^2 \qquad i^2 = -1$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi$$

from eqⁿ.

$$-\omega^2 \psi = v^2 \nabla^2 \psi$$

$$-\frac{\omega^2}{v^2} \psi = \nabla^2 \psi$$

$$\nabla^2 \psi + \frac{\omega^2}{v^2} \psi = 0 \quad \text{——} \; (2)$$

$$\omega = 2\pi\nu \qquad \because \text{vel.} = \nu\lambda$$

$$\omega = \frac{2\pi v}{\lambda} \qquad \nu = \frac{v}{\lambda}$$

$$\frac{\omega}{v} = \frac{2\pi}{\lambda} = \frac{2\pi \, mv}{h}$$

$$\nabla^2 \psi + \left(\frac{2\pi mv}{h}\right)^2 \psi = 0$$

$$\nabla^2 \psi + \frac{m^2 v^2}{\hbar^2} \psi = 0 \qquad \because \hbar = \frac{h}{2\pi}$$

$\because$ total energy of particle

$$E = K.E + P.E$$

$$E = \frac{1}{2} mv^2 + V$$

$$\frac{1}{2} mv^2 = E - V$$

$$mv^2 = 2(E - V)$$

$$m^2 v^2 = 2m(E - V)$$

$$\therefore \boxed{\nabla^2 \psi + \frac{2m(E-V)}{\hbar^2} \psi = 0} \quad \text{——} \; (3)$$

for free particle P.E $\boxed{V = 0}$

$$\boxed{\nabla^2 \psi + \frac{2mE}{\hbar^2} \psi = 0} \quad \text{——} \; (4)$$

This is schrodinger time-independent eqⁿ.

★ Schrodinger's time dependent wave equation:-

The Schrodinger's time dependent wave eqⁿ. may be obtained from Schrodinger's time independent eqⁿ.

Since the differential eqⁿ. representing a one-dimensional wave function is

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \nabla^2 \psi \quad \text{——} (1)$$

The general solⁿ. of eqⁿ. (1) is

$$\psi_{(x,y,z,t)} = \psi_0 (x,y,z)\, e^{-i\omega t}$$

or

$$\psi = \psi_0 e^{-i\omega t} \quad \text{——} (2)$$

Diffⁿ. w.r.to 't'. we get

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

$$\frac{\partial \psi}{\partial t} = -i\omega . \psi \qquad \because \omega = 2\pi\nu$$

$$\frac{\partial \psi}{\partial t} = -i\, 2\pi\nu \psi$$

or

$$h\frac{\partial \psi}{\partial t} = -i\, 2\pi h\nu \psi \qquad E = h\nu$$

$$h\frac{\partial \psi}{\partial t} = -i\, 2\pi . E\psi$$

$$-\frac{h}{i 2\pi}\frac{\partial \psi}{\partial t} = E\psi \qquad \because i^2 = -1$$

$$E\psi = -\frac{i h}{i^2 . 2\pi}\frac{\partial \psi}{\partial t} \qquad \frac{h}{2\pi} = \hbar$$

$$\boxed{E\psi = i\hbar \frac{\partial \psi}{\partial t}} \quad \text{——} (3)$$

Substitute the value of $E\psi$ in Schrodinger time-independent eqn. ie

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

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

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

$$\nabla^2\psi = -\frac{2m}{\hbar^2}\left\{i\hbar\frac{\partial\psi}{\partial t} - V\psi\right\}$$

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

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}} \quad \text{———} (4)$$

This is time dependent wave eqn.

Eigen Values and Eigen functions: The values of E_n (Energy) for which Schrodinger steady state eqn. can be solved are called eigen values (proper values) and the corresponding wave function ψ_n are called eigen functions.

⁘ Application of Schrodinger eq^n. for particle in a one-dimensional potential box :-
(Eigen values of energy and wave function)

Let us consider the case of a particle of mass m moving along x-axis bet^n. two rigid walls A & B at $x=0$ and $x=l$. The particle is free to move bet^n. walls.

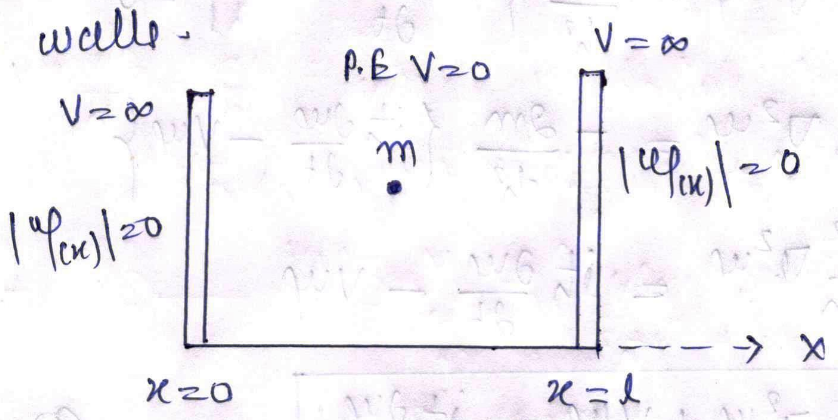


fig: one dimensional square well pot^l.

Potential energy $V = \infty$ for $x<0$ & $x>l$

$V = 0$ for $0 \leq x \leq l$

The schrodinger wave eq^n. for the particle is given by

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

As $V=0$ bet^n the walls, hence

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

or

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

where $K^2 = \frac{2mE}{\hbar^2} = \frac{8\pi^2 m}{h^2}E$ $\quad \because \hbar = \frac{h}{2\pi}$

The general solu^n of eq^n (3) is given by

$$\psi_{(x)} = A \sin kx + B \cos kx \quad \text{—— (4)}$$

taking boundary cond^n:

when $x=0$ & $|\psi_{(x)}|=0$ from eq^n (4)

$$0 = A \sin 0 + 0$$

$$\boxed{A=0}$$

and when $x=l$ and $|\psi_{(x)}|=0$ then from (4)

$$0 = A \sin kl$$

$$\sin kl = 0$$

$$kl = n\pi$$

$$\boxed{k = \frac{n\pi}{l}}$$

eq^n (4) Becomes

$$\psi_{(x)} = A \sin \frac{n\pi}{l} x \quad \text{—— (5)}$$

$\because$ $$k^2 = \frac{8\pi^2 mE}{h^2}$$

$$\frac{n^2\pi^2}{l^2} = \frac{8\pi^2 mE}{h^2}$$

$$E = \frac{n^2 h^2}{8ml^2}$$

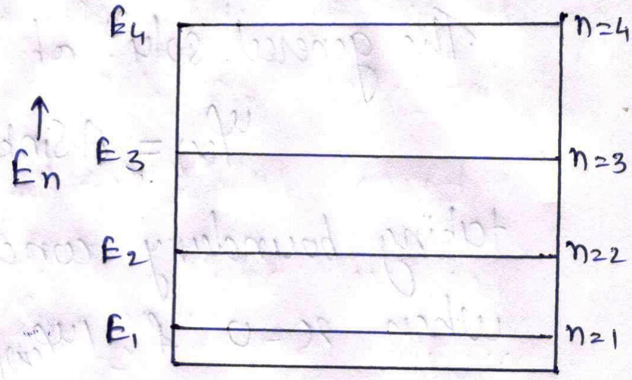
or

$$\boxed{E_n = \frac{n^2 h^2}{8ml^2}} \quad \text{—— (6)}$$

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

ie $$E_1 = \frac{h^2}{8ml^2}, \quad E_2 = \frac{4h^2}{8ml^2} = 4E_1, \quad E_3 = \frac{9h^2}{8ml^2} = 9E_1 \ldots\ldots$$

i.e. the energy levels are discrete



The constant A can be obtained by applying the normalization condition. ie

$$\int_0^l |\psi_{(x)}|^2 dx = 1$$

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

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

$$\frac{A^2}{2} \int_0^l \left\{ 1 - \cos \frac{2n\pi}{l} x \right\} dx = 1$$

$$\frac{A^2}{2} \left[x - \frac{\sin \frac{2n\pi}{l} x}{\frac{2n\pi}{l}} \right]_0^l = 1$$

$$\frac{A^2}{2} (l - 0) = 1$$

$$\frac{A^2}{2} l = 1$$

$$A^2 = \frac{2}{l} \quad \text{or} \quad \boxed{A = \sqrt{\frac{2}{l}}}$$

from eqn ⑤

$$\boxed{\psi_{(x)} = \sqrt{\frac{2}{l}} \cdot \sin\left(\frac{n\pi}{l} x\right)}$$

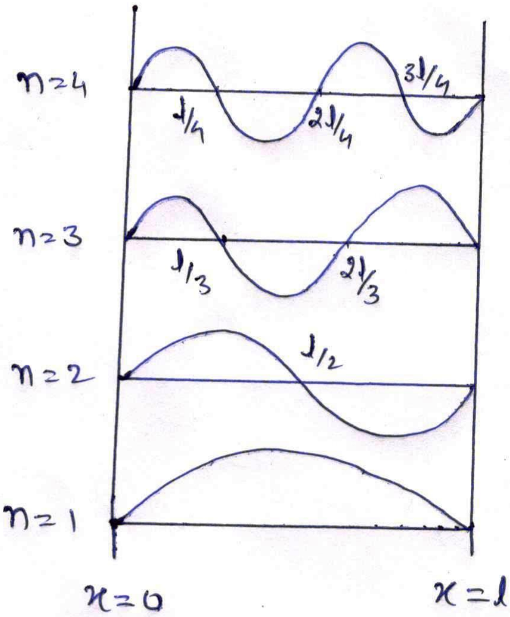
or

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{l}} \left(\frac{n\pi}{l} x\right)} \quad \text{—— ⑧}$$

when $n = 1$.

$$\psi_1(x) = \sqrt{\frac{2}{l}} \sin \frac{\pi}{l} x$$

$$\boxed{x = 0, l}$$



$n=2$

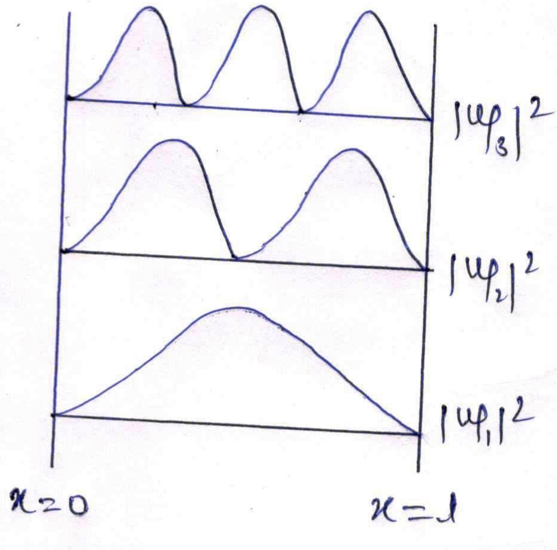
$$\psi_2(x) = \sqrt{\frac{2}{l}} \sin \frac{2\pi}{l} x$$

$$x = 0, \frac{l}{2}, l$$

$n = 3$

$$\psi_3(x) = \sqrt{\frac{2}{l}} \sin \frac{3\pi}{l} x$$

$$x = 0, \frac{l}{3}, \frac{2l}{3}, l \text{ ------}$$



$n = 4$

$$\psi_4(x) = \sqrt{\frac{2}{l}} \sin \frac{4\pi}{l} x$$

$$x = 0, \frac{l}{4}, \frac{2l}{4}, \frac{3l}{4}, l.$$