Black Body :-

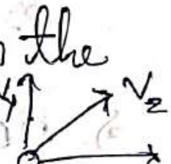
Ideal body, which emits and absorbs all frequency, is called a Black Body. The radiation emitted by such a body is called Black Body radiation.

The emissivity of a black body is 1.

eg - sun, iron ..etc.

Degree of Freedom :-

No of independent term in the expression of K.E.



for monoatomic particle D.O.F. is $(f) = 3$. $(\vec{x}, \vec{y}, \vec{z})$

Plank's radiation law (hypothesis) :-

light have particle nature.

$E = nh\nu$

$\lambda = \frac{h}{p}$, momentum of photon $p = \frac{h}{\lambda}$

hypothesis means → suggestion

De Broglie Hypothesis :-

Every microscopic moving particle is a wave, whose wavelength is given by

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

Compton Effect :-

The collision along x axis will be

$$\Rightarrow \frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + p\cos\theta \quad \text{(1)}$$

For Y axis collision will be

$$\Rightarrow 0 + 0 = \frac{h\nu'}{c}\sin\phi - p\sin\theta \quad \text{(2)}$$

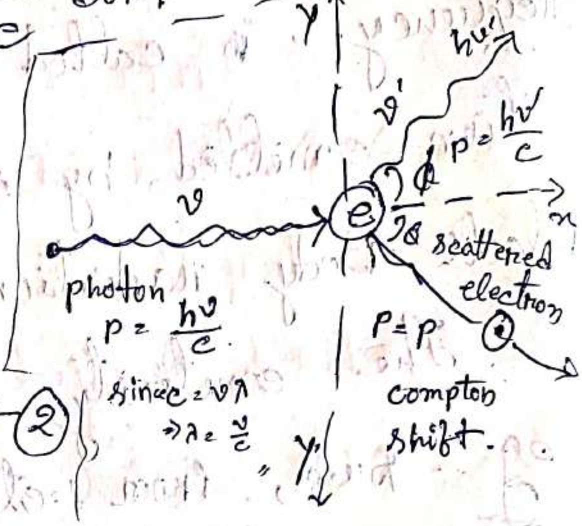


fig :-

multiply eqn (1) by c →

$$\Rightarrow \frac{h\nu c}{c} = \frac{h\nu' c}{c}\cos\phi + cp\cos\theta$$

$$\Rightarrow pc\cos\theta = h\nu - h\nu'\cos\phi \quad \text{(3)}$$

frequency $\nu \to \nu'$

wavelength $\lambda \to \lambda'$

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

Similarly multiplying eqn (2) by c, we get →

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

$$\Rightarrow pc\sin\theta = h\nu'\sin\phi \longrightarrow \text{(4)}$$

Squaring (3) and (4) and adding we get →

$$\Rightarrow p^2c^2\cos^2\theta + p^2c^2\sin^2\theta = h^2\nu^2 + h^2\nu'^2\cos^2\phi - 2h^2\nu\nu'\cos\phi + h^2\nu'^2\sin^2\phi$$

$$\Rightarrow p^2c^2\cdot 1 = h^2\nu^2 + h^2\nu'^2\cdot 1 - 2h^2\nu\nu'\cos\phi \longrightarrow \text{(5)}$$

Now total energy of a particle

$\Rightarrow E = K.E + mc^2$

We know that

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

$\Rightarrow K.E + mc^2 = \sqrt{m^2c^4 + p^2c^2}$

$\Rightarrow (K.E. + mc^2)^2 = (\sqrt{m^2c^4 + p^2c^2})^2$

$\Rightarrow K.E^2 + \cancel{m^2c^4} + 2K.E\,mc^2 = \cancel{m^2c^4} + p^2c^2$

$\Rightarrow p^2c^2 = K.E^2 + 2K.E\,mc^2$

here K.E of electron is $K.E = h\nu - h\nu'$

$\therefore p^2c^2 = (h\nu - h\nu')^2 + 2(h\nu - h\nu')mc^2$

Now putting the value of p^2c^2 in eq^n (b)

$\Rightarrow (h\nu - h\nu')^2 + 2(h\nu - h\nu')mc^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu'\cos\phi$.

$\Rightarrow \cancel{h^2\nu^2} + \cancel{h^2\nu'^2} - 2h^2\nu\nu' + 2h\nu mc^2 - 2h\nu' mc^2 = \cancel{h^2\nu^2} + \cancel{h^2\nu'^2} - 2h^2\nu\nu'(1-\cos\phi)$.

$\Rightarrow 2mc^2(h\nu - h\nu') = 2h^2\nu\nu'(1-\cos\phi)$

Putting $\nu = \frac{c}{\lambda}$, we get

$\Rightarrow 2mc^2\left(h\frac{c}{\lambda} - h\frac{c}{\lambda'}\right) = 2h^2\frac{c}{\lambda}\cdot\frac{c}{\lambda'}(1-\cos\phi)$

$\Rightarrow \cancel{2}m\cancel{c^2}\,ch\left(\frac{1}{\lambda - \lambda'}\right) = \cancel{2}h^2\frac{\cancel{c^2}}{\lambda\lambda'}(1-\cos\phi)$

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

$\Rightarrow \lambda' - \lambda = \frac{h}{mc}(1-\cos\phi)$ ($\lambda\lambda'$ is negligible)

$\Rightarrow \lambda' - \lambda = \lambda_c (1-\cos\phi)$ (where $\lambda_c = \frac{h}{mc}$ compton wavelength)

$\lambda' - \lambda$ will be maximum shift

if $\phi = 180°$

$\therefore \lambda' - \lambda = 2\lambda_c$ ($\lambda_c = 2.426$ pm)

④ Failure of Classical mechanics :-

Nature of Matter — ① Wave Nature
ⅱ Particle Nature

④ Origin of De Broglie's Concept of matter wave

① Nature prefers symmetry —
Matter and energy are two fundamental forms in which nature manifests itself. As energy possess both wave and particle nature, matter also must posses wave nature.

② Similarities betn mechanics and optics
From principle of least action

$\int_{P_1}^{P_2} P\,ds = \min$ then $\Delta \int_{P_1}^{P_2} P\,ds = 0$.

Again from Fermat's principle

$\int_{P_1}^{P_2} \mu\,ds = \min$. Therefore $\Delta \int_{P_1}^{P_2} \mu\,ds = 0$

here $\mu = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^2} + \dots$

This two principles show a close connection betn matter and wave.

(A) Phase velocity and Group velocity :-

defn :- Phase velocity (V_p) is the individual waves of a wave packet moves forward.

If dispersive medium V_p is different for different wavelength.

For non-dispersive medium V_p is same for different wavelength.

(A) Group velocity (V_g) is define as the velocity with which the maximum amplitude of the wave packet moves forward.

⇒ Expression for phase velocity and group velocity :-

A plane harmonic wave traveling along +ve x direction with amplitude 'A' and velocity 'v' is represented by

$$\psi(x,t) = A \sin \omega\left(t - \frac{x}{v}\right)$$

Now the phase ϕ of the wave of any time t is given by → $\phi(x,t) = \omega\left(t - \frac{x}{v}\right)$

differentiating w.r. to time 't' we get

$$\frac{\partial \phi}{\partial t} = \omega\left(1 - \frac{1}{v}\frac{dx}{dt}\right)$$

If the phase ϕ is independent of time

then $\frac{\partial \phi}{\partial t} = 0$

so $\omega\left[1 - \frac{1}{v}\frac{dx}{dt}\right] = 0$

here ω cannot be zero (0).

so $1 - \frac{1}{v}\frac{dx}{dt} = 0$

$$\Rightarrow \frac{1}{v}\left(\frac{dx}{dt}\right)_\phi = 1$$

$$\Rightarrow v = \left(\frac{dx}{dt}\right)_\phi$$

This represent the phase velocity with which a given phase moves forward.

so, $\psi(x,t) = A \sin \omega\left(t - \frac{x}{v_p}\right)$

$$= A \sin\left(\omega t - \frac{\omega x}{v_p}\right) \quad (1)$$

since $\psi(x,t) = A \sin(\omega t - Kx)$ — (2)

Comparing (1) and (2)

$$\Rightarrow \cancel{A \sin}\left(\cancel{\omega t} - \frac{\omega x}{v_p}\right) = \cancel{A \sin}\left(\cancel{\omega t} - Kx\right)$$

$$\Rightarrow \frac{\omega x}{v_p} = Kx$$

$$\Rightarrow \frac{\omega \cancel{x}}{K\cancel{x}} = v_p$$

$$\boxed{\Rightarrow v_p = \frac{\omega}{K}}$$

Expression for group velocity :-

Let the wave packet consist of two waves $\psi_1 = A \sin(\omega t - Kx)$

$$\psi_2 = A \sin\left[(\omega + \Delta\omega)t - (K+\Delta K)x\right]$$

Resultant displacement will be

$$\Rightarrow \psi = \psi_1 + \psi_2$$

$$= A \sin(\omega t + Kx) + A \sin\left[(\omega+\Delta\omega)t - (K+\Delta K)x\right]$$

$$\Rightarrow \psi = A\left\{\sin(\omega t - Kx) + \sin\left[(\omega+\Delta\omega)t - (K+\Delta K)x\right]\right\}$$

$$\Rightarrow \psi = 2A \cos\frac{\Delta\omega t - \Delta K x}{2} \sin\frac{1}{2}\left[(2\omega+\Delta\omega)t - (2K+\Delta K)x\right]$$

Since $\left.\begin{aligned} 2\omega + \Delta\omega &\simeq 2\omega \\ 2K + \Delta K &\simeq 2K \end{aligned}\right]$ $\Delta\omega, \Delta K$ are very very small compared to ω, K.

The amplitude of the resultant wave is

$$= 2A \cos(\Delta\omega t - \Delta K x)$$

maximum amplitude is $2A$.

If at $x = x'$ and $t = t'$ resultant amplitude is maximum

$$\therefore \frac{1}{2}(\Delta\omega t' - \Delta K x') = 0$$

$$\Rightarrow \Delta\omega t' = \Delta K x'$$

$$\Rightarrow \frac{x'}{t'} = \frac{\Delta\omega}{\Delta K}.$$

At $\Delta K \to 0$, $\lim\limits_{\Delta K \to 0} \frac{x'}{t'} = \lim\limits_{\Delta K \to 0} \frac{\Delta\omega}{\Delta K} = \frac{d\omega}{dk}$ is instantaneous velocity.

This is known as group velocity $\boxed{v_g = \frac{d\omega}{dK}}$

Relation between v_p and v_g :-

$$v_p = \frac{\omega}{K} \Rightarrow \omega = v_p K \quad \text{--- (1)}$$

$$v_g = \frac{d\omega}{dK}$$

Putting ~~$\frac{d}{dK}$~~ value we get

$$\Rightarrow \frac{d}{dK}(v_p K)$$

$$\Rightarrow v_g = v_p + K\frac{dv_p}{dK}$$

$$\Rightarrow v_g = v_p + \frac{K\,dv_p}{d\lambda}\frac{d\lambda}{dK}$$

$$\Rightarrow v_g = v_p + K\frac{dv_p}{d\lambda} \times \left(\frac{-2\pi}{K^2}\right)$$

$$\Rightarrow v_g = v_p - \lambda\frac{dv_p}{d\lambda}$$

since $K = \frac{2\pi}{\lambda}$

$\lambda = \frac{2\pi}{K}$

$\frac{d\lambda}{dK} = -\frac{2\pi}{K^2}$

since $\lambda = \frac{2\pi}{K}$

for non-dispersive medium v_p does not depend on λ.

i.e $\frac{dv_p}{d\lambda} = 0$

$\therefore v_g = v_p$

for dispersive medium $v_g < v_p$.

Matter wave :-

(i) De Broglie's relation for a photon :-

A photon with frequency ν has energy

$E = h\nu$,

Total relativistic energy of a particular of rest mass m and momentum p is equal.

i.e. $\Rightarrow E = \sqrt{m^2c^4 + p^2c^2}$

For a photon $m = 0$, so putting the value we get →

$\Rightarrow E = \sqrt{0 + p^2c^2}$

$\Rightarrow E = pc$

$\Rightarrow p = \frac{E}{c}$

$\therefore p = \frac{h\nu}{c}$ $\Rightarrow pc = h\nu$.

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

$\Rightarrow p = \frac{E}{c}$

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

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

[since $c = \nu\lambda$]

momentum $\Rightarrow p = \frac{h}{\lambda}$, or $\lambda = \frac{h}{p}$.

For a particle mass 'm' velocity 'v' the wavelength of the wave associated with the particle is $\lambda = \frac{h}{p}$

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

[$p = mv$ according to De Broglie].

Ex:- Suppose a cricket ball of mass 500 gm is flying with velocity 13.9 ms^{-1}.

Soln:- De Broglie wavelength is $\lambda = \frac{h}{mv}$

$\Rightarrow \lambda = \frac{6.62 \times 10^{-34}\ Js}{0.50\ kg \times 13.9\ ms^{-1}}$

$\Rightarrow \lambda \approx 10^{-24}$ m

i.e. for a macroscopic object $m \to \infty$
hence $\lambda \to 0$, which is why wave accosiated with macroscopic object is insignificent.

Let us calculate a wavelength for a electron →

Q.) Suppose the electron is moving with velocity 4.47×10^6 m/s.

Soln:- We know $\lambda = \frac{h}{mv}$

here $\lambda = \frac{6.62 \times 10^{-34} \text{ Js}}{9.1 \times 10^{-31} \text{ kg} \times 4.47 \times 10^6 \text{ m/s}}$

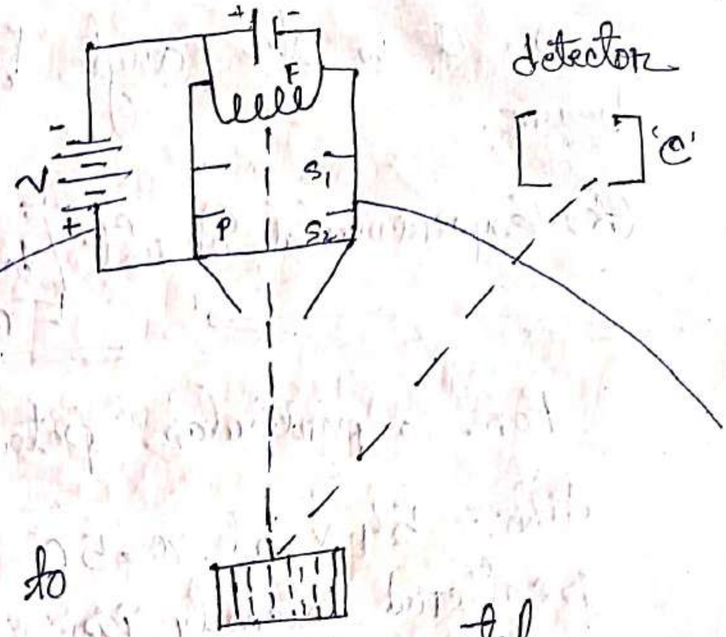
$\Rightarrow \lambda = 9.3 A^0$

The wavelength is comparable with the size of the electron. i.e. why the wave property of these sup atomic particles cannot be neglected.

(4) Division & Germer Experiment:-

The electron beam is produce by heating the filament 'F' and it is accelerated through a potential difference D- maintain betn filament F and plate P. The electron beam is colimated by passing through narrow slits S_1 and S_2.

The colimated beam is directed to fall normally on a large single crystal. fig:-



In different directions of the crystal, the electron beams are scattered and it collected by a Faradey Cup 'C'.

Consider the electron as electron wave, we can use Bragg's diffraction formula $2d\sin\theta = n\lambda$

∴ from fig

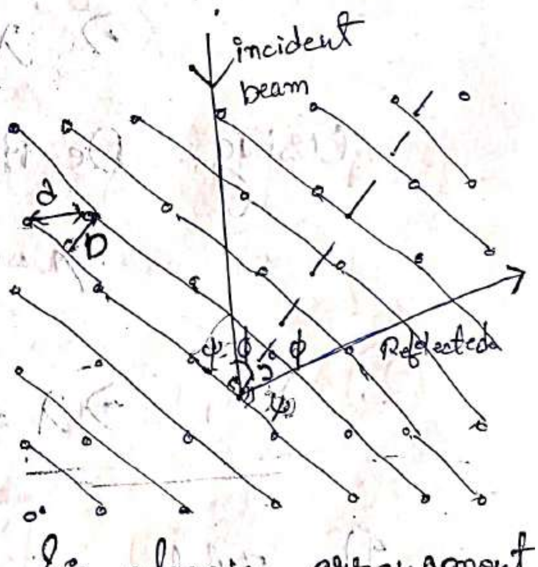


fig:- atomic arrangment in nickel crystal

$2D\sin\psi = n\lambda$

$\Rightarrow 2D\sin(90° - \phi) = n\lambda$

$\Rightarrow 2D\cos\phi = n\lambda$

$\Rightarrow 2d\sin\phi\cos\phi = n\lambda$

$\Rightarrow d\sin 2\phi = n\lambda$

$\Rightarrow d\sin\theta = n\lambda$

$\frac{D}{d} = \sin\phi$

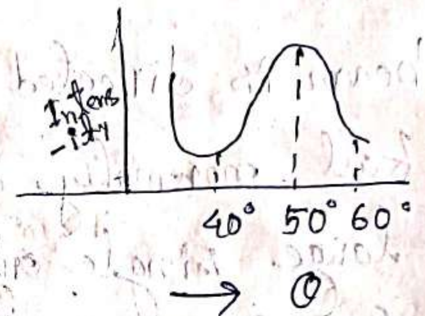
$\Rightarrow D = d\sin\phi$

$2\phi = \theta$

So, θ is the angle bet^n the reflected beam.

(A) Experimental Result [Varification of De Broglie hypothesis]

For a particular potential diff. 54 V at $\theta = 50^\circ$ scattered intensity is maximum. Considering $n = 1$ and using $d \sin\theta = \lambda$ for nickel atom. $d = 2.15\,A^\circ$



fig

Therefore $\Rightarrow 2.15\,A^\circ \times \sin 50^\circ = \lambda$

$\Rightarrow \lambda = 1.65\,A^\circ$

Using De Broglie hypothesis

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

$$\Rightarrow \lambda = \frac{h}{\sqrt{2mE}}$$

If K.E given

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

$\Rightarrow E = \frac{m^2v^2}{2m}$

since $p = mv$

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

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

If Total energy of electron is $E = eV$. K.E of e in a potential difference. then

$$\Rightarrow \lambda = \frac{h}{\sqrt{2meV}}$$

we can write directly →

P.T.O.

$$\Rightarrow \lambda = \frac{12.27}{\sqrt{V}} A^\circ$$

at 54 V $\Rightarrow \lambda = \frac{12.27}{\sqrt{54}} A^\circ$, $\Rightarrow \lambda = 1.67 A^\circ$

$$\Rightarrow \lambda = 1.67 A^\circ$$

(A) Non-Relativistic Speed:-

If electron 'e' is accelarated in a potential diff. V. The K.E. of the 'e' will be eV. The De Broglie wavelength of the electron $\Rightarrow \lambda = \frac{h}{\sqrt{2m eV}}$

$$\therefore \Rightarrow \lambda = \frac{12.27}{\sqrt{V}} A^\circ$$ (here V is vary)

(B) For Relativistic Speed:-

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

Again $E = E_{K.E} + m_0c^2$ (m_0c^2 is rest mass energy)

$$\Rightarrow E_{K.E} = E - m_0c^2$$

$$\therefore E_{K.E} = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2$$

$$\Rightarrow E_{K.E} + m_0c^2 = \sqrt{p^2c^2 + m_0^2c^4}$$

Squaring both sides

$$\Rightarrow (E_{K.E})^2 + \cancel{m_0^2c^4} + 2E_{K.E}m_0c^2 = p^2c^2 + \cancel{m_0^2c^4}$$

$$\Rightarrow P = \sqrt{\frac{E_{K.E}(E_K + 2m_0c^2)}{c^2}}$$

$$\Rightarrow p = \frac{\sqrt{E_K(E_K + 2m_0c^2)}}{c}$$

So ; $$\lambda = \frac{hc}{\sqrt{E_K(E_K + 2m_0c^2)}}$$

Most probable velocity at temparature T ; $\Rightarrow v = \sqrt{\frac{2KT}{m}}$

Therefore $$\lambda = \frac{h}{\sqrt{2mKT}}$$

Q. What is the De Broglie wavelength of an electron accelerated in a potential 100V.

Soln :- Given $V = 100\,v$

Therefore $$\lambda = \frac{12.27}{\sqrt{100}} \, A^\circ$$

$$= \frac{12.27}{10} \, A^\circ$$

$$= 1.227 \, A^\circ$$

(2) What is the De Broglie wavelength of an 'e^-' moving with velocity $v = \frac{3}{5}c$.

Soln :- We know that

$$m_0 = 9.1 \times 10^{-31} \, Kg$$

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

Therefore $\Rightarrow$ $$\lambda = \frac{h}{\frac{m_0}{\sqrt{1 - v^2/c^2}} \cdot v}$$

$$\Rightarrow \lambda = \frac{6.67}{\frac{9.1 \times 10^{-31}\ Kg}{\sqrt{1-\left(\frac{3}{5}\right)^2} \cdot \frac{3}{5}}}\ A^\circ$$

$$\Rightarrow \lambda = \frac{6.67}{\frac{9.1 \times 10^{-31} \times 5}{\sqrt{\frac{25-9}{25}} \cdot 3}}\ A^\circ$$

$$\Rightarrow \lambda = \frac{6.67}{\frac{45.5 \times 10^{-31}}{\sqrt{\frac{16}{25}} \cdot 3}}\ A^\circ = \frac{6.67}{\frac{45.5 \times 10^{-31}}{\frac{4}{5} \cdot 3}}\ A^\circ$$

$$\Rightarrow \lambda = \frac{6.67 \times 12}{45.5 \times 10^{-31} \times 5}\ A^\circ$$

$$\Rightarrow \lambda = 0.351824176 \times 10^{31}\ A^\circ$$

$$\Rightarrow \lambda = 3.52 \times 10^{30}\ A^\circ$$

③ What is the De Broglie wavelength of thermal neutron at $T = 27^\circ C$

__Soln__ here $T = 27^\circ + 273^\circ = 300\ K$

from De Broglie formula

$$\Rightarrow \lambda = \frac{h}{\sqrt{2mKT}}$$

Since $K = 1.376 \times 10^{-16}$ erg
$= 1.38 \times 10^{-23}\ J K^{-1}$

$$\Rightarrow \lambda = \frac{6.67}{\sqrt{2 \times 1.6 \times 10^{-27} \times 1.38 \times 10^{-23} \times 300}}$$

$m = 1.6 \times 10^{-24}$ gm
$= 1.6 \times 10^{-27}$ kg

$$\Rightarrow \lambda = \frac{6.67}{\sqrt{13248 \times 10^{-51}}}\ A^\circ$$

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(4) An electron and a proton have the same De Broglie wavelength. Which one will have the greater energy?

Solⁿ:- Given

$$\lambda_{e^-} = \lambda_{p^+}$$

$$\Rightarrow \lambda = \frac{h}{m_1 v_1} = \frac{h}{m_2 v_2}$$

$$\Rightarrow m_1 v_1 = m_2 v_2$$

Squaring both sides & divided by 2 we get

$$\frac{m_1^2 v_1^2}{2} = \frac{m_2^2 v_2^2}{2}$$

$$\Rightarrow m_1\left(\frac{1}{2} m_1 v^2\right) = m_2\left(\frac{1}{2} m_2 v^2\right)$$

$$= \frac{m_1}{m_2} = \frac{K.E \text{ of Proton}}{K.E\ e^-}$$

(A) Phase velocity of a De Broglie's wave has no significant.

We can write $v_p = \frac{\omega}{K} = \frac{E/\hbar}{P/\hbar} = \frac{E}{P}$

Using relativistic mass energy relation

$\Rightarrow E = mc^2$

here $v_p = \frac{mc^2}{mv} = \frac{c^2}{v}$

Thus $v_p >> c$

- This shows that phase velocity of a De Broglie wave is always greater than velocity of light. which cannot be true according to Einstain special theory of relativity.

Thus it is clear that a metarial particle can't be equivelent to a single wave i.e. a single wave can't describe the wave motion of a metarial particle. It was solved by schrodinger. According to him a metarial particle in motion is equivelent to a wave pocket rather than a single wave.

P.T.O.

Wave Packet :-

A wave packet is composed of a group of waves with slightly different velocities and wavelength. The phase and amplitudes of the wave are choosen, such that they interfer constructively in the region of space where the particle can be located. Outside the region the wave interfer destructively and the amplitude reduces to zero. i.e. There is no probability of finding the particle.

The wave packet moves with the group velocity and this group velocity is equal to the particle velocity.

Particle velocity for Relativistic and non-relativistic particle :-

We know $v_g = \frac{d\omega}{dK}$

total energy $E = \hbar\omega$

$\Rightarrow \omega = \frac{E}{\hbar}$

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

Since momentum $p = \hbar K$

$\therefore v_g = \frac{d\omega}{dK}$

$= \frac{d\,E/\hbar}{d\,P/\hbar}$

$\Rightarrow v_g = \frac{dE}{dP}$

$\Rightarrow K = \frac{P}{\hbar}$

$\Rightarrow dK = \frac{dP}{\hbar}$

(i) Now for non-relativistic particle $E = \frac{P^2}{2m}$

$\therefore \Rightarrow v_g = \frac{dE}{dP}$

$\Rightarrow v_g = \frac{1}{2m}\frac{d}{dP}P^2$

$\Rightarrow v_g = \frac{\cancel{2}P}{\cancel{2}m}$

$\Rightarrow v_g = \frac{P}{m} = \frac{mv}{m}$

$\Rightarrow v_g = v_{particle}$

(ii) For non relativistic particle

We know $E = \sqrt{P^2c^2 + m_0^2c^4}$

$\Rightarrow E^2 = P^2c^2 + m_0^2c^4$

differentiating w.r.to P we get

$\Rightarrow \cancel{2}E\frac{dE}{dP} = c^2 \cancel{2}P$

$\Rightarrow \frac{dE}{dP} = \frac{c^2P}{E}$ $\Rightarrow E = P.c^2$

Since $\Rightarrow P = mv$

for a particle of mass m_0

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

Therefore $\Rightarrow E = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}\cdot c^2$

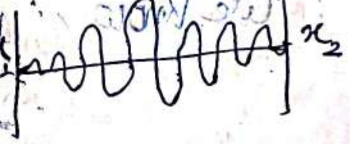
$$\therefore \Rightarrow \frac{dE}{dp} = \cancel{c^2} \frac{\cancel{m_0}}{\cancel{\sqrt{1-\frac{v^2}{c^2}}}} \cdot v \times \frac{\cancel{\sqrt{1-\frac{v^2}{c^2}}}}{\cancel{m_0}\,\cancel{c^2}}$$

$$\Rightarrow \frac{dE}{dp} = v_{\circ} \,//$$

④ Heisenburg Uncertainity Principle :-

According to De Broglie a wave is associated with a moving particle with wavelength $\lambda = \frac{h}{p}$. The wave associated with moving meterial particle is not a single wave, instead it is a wave packet moving with group velocity v_g. The group velocity of the wave packet is equal to the particle velocity.

fig 1:-



The wave packet has a linear extension Δx, in the region of space where there is a possibility of finding the particle. So there is a uncertainity of amount Δx associated with the position of the particle.

Wave packet is composed of large no of waves interfering constructively in the region where the particle is located and destructively interfering outside the region.

i.e. There is a uncertainity $\Delta\lambda$ associated with the wavelength of the wave packet.

According to De Broglie $P = \frac{h}{\lambda}$

~~i.e. if there is a un~~ $\Rightarrow \Delta P = -\frac{h}{\lambda^2}\Delta\lambda$ —— (1)

i.e. if there is an uncertainity in the wave-length according to eqn (1) there will be an uncertainity ΔP associated with the momentum of the particle.

For a free particle without facing any potential we can exactly tell the momentum. i.e. $\Delta P = 0$, and this particle can be located anywhere (from $-\infty$ to $+\infty$).

i.e. the uncertainity Δx in the position will be ∞.

If no. of interfering waves increases, $\Delta\lambda$ increases and hence ΔP also increases. In this case the waves interfere constructively in a particular region of space and therefore the linear spread of Δx decreases. If $\Delta P \to \infty$, then $\Delta x \to 0$

Mathematically -

$$\Delta x \times \Delta P_x \geq \hbar$$

(i) If $\Delta x = 0$, $\Delta P_x = \frac{\hbar}{\Delta x} = \infty$

(ii) If $\Delta P_x = 0$, $\Delta x = \frac{\hbar}{\Delta P_x} = \infty$

(iii) $\Delta x \times m \times \Delta V_x \geq \hbar$ $\Rightarrow \Delta V_x = \frac{\hbar}{m\Delta x}$. If $\Delta x = 0$, $\Delta V_x = \infty$

then $\Delta x \times \Delta v_x = \frac{\hbar}{m}$

It is impossible to measure the position and momentum simulteneously of a tiny particle.

For a macroscopic particle $m \longrightarrow \infty$, then $\Delta x \times \Delta v_x = 0$ i.e. for such particle we can accurately measure the momentum and position simultaneously.

4 Time and energy uncertainty Relⁿ:–

Elementary Proof:–

Suppose the wave packet having linear spread (width) Δx moves along 'x' axis with group velocity V_g. Therefore

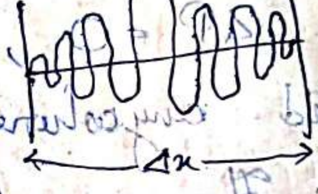


fig:–

$$V_g = \frac{\Delta x}{\Delta t}$$

$$\Rightarrow \Delta t = \frac{\Delta x}{V_g} \quad \text{--- (1)}$$

Let m is the mass of the particle, P_x is mome-ntum of the particle and E is the K.E of the particle.

Therefore – $E = \frac{P_x^2}{2m}$

differentiating $\Delta E = \frac{1}{2m} \cdot 2P_x \Delta P_x$

$$= \frac{P_x \Delta P_x}{m}.$$

$\Rightarrow \Delta E = \frac{m v_x . \Delta P_x}{m}$

$\Rightarrow \Delta E = v_x . \Delta P_x$ ——— (2)

multiplying eqn (1) × (2) we get

$\Rightarrow \Delta E \times \Delta t = v_x \Delta P_x \times \frac{\Delta x}{v_g}$

since $v_x = v_g$ (particle velocity v_x)

$\Rightarrow \Delta E \times \Delta t = v_x \Delta P_x \times \frac{\Delta x}{v_g} = \Delta P_x \times \Delta x$

i.e. $\Delta E \times \Delta t \geq \hbar$ $\quad \boxed{\because \Delta P_x \times \Delta x \geq \hbar}$

This is the uncertainity of time and K.E. Relation.

(*) Angular momentum and angular position uncertainty Reln.

(*) Illustration of heisenburg uncertainity Principle

(1) Electron diffraction through a single slite.

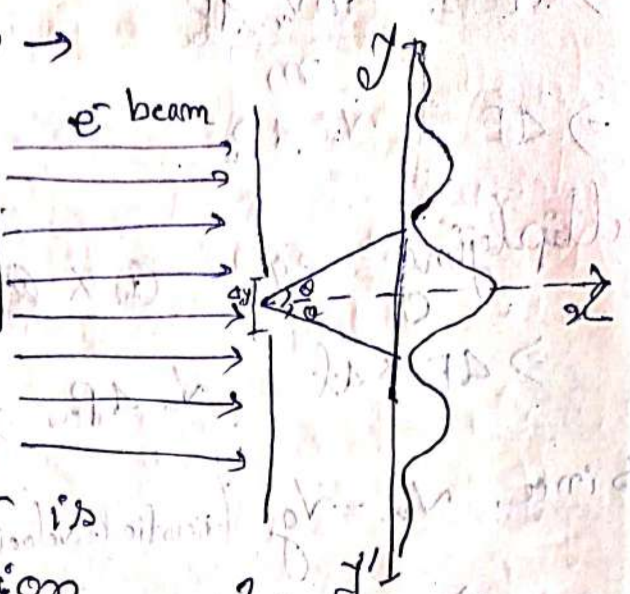
Let electron beams are incident on a single slite of width Δy. As according to De Broglie e⁻ in motion are associated with wave, the e⁻ after passing through the slite will form diffraction pattern on the screen.

The 1st minimum of the diffraction pattern satisfies the relation →

$$\Delta y \sin\theta = \lambda$$

$$\Rightarrow \Delta y = \frac{\lambda}{\sin\theta} \quad \text{—— (1)}$$

$\boxed{\begin{array}{l}\text{Bragg's law} \\ d\sin\theta = n\lambda \\ \downarrow \; \Delta y \quad \; \downarrow 1\end{array}}$



fig

Before incident the momentum of the e⁻ is along the x-direction and let it be P. After diffraction if the e⁻ moves along +ve y direction then the component of P is $P\sin\theta$. if e⁻ moves along -ve y direction then the component of P is $-P\sin\theta$. The uncertainity in the P in y-direction is ⇒

$$\Rightarrow \Delta P_y = P\sin\theta - (-P\sin\theta)$$

$$\Rightarrow \Delta P_y = 2P\sin\theta$$

$$\Rightarrow \Delta P_y = 2\frac{h}{\lambda}\sin\theta \quad \text{—— (2)}$$

$\boxed{\begin{array}{l}\text{De Broglie} \\ P = \frac{h}{\lambda}\end{array}}$

Now multiplying eq (1) × (2).

$$\Delta y \times \Delta P_y = \frac{\cancel{\lambda}}{\cancel{\sin\theta}} \times 2\frac{h}{\cancel{\lambda}}\cancel{\sin\theta}$$

$$\Rightarrow \Delta y \times \Delta P_y = 2\frac{h}{2\pi}$$

or it can be written as ⇒ $\Delta y \times \Delta P_y \geq \hbar$.

Application of uncertainity Principle:—

① **Non-existance of free e⁻ inside the nucleus:**—

If electron exist in the nucleus the

uncertainity in the position of e^- is equal to the diameter of the nucleus $\rightarrow$

$${}^{1}_{0}n = {}^{1}_{1}P + {}^{0}_{-1}e$$
$${}^{1}_{1}P = {}^{1}_{0}n + {}^{0}_{1}e$$

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

 10^{-14}

Uncertainity in the P of e^-

$$\Delta P_x = \frac{\hbar}{\Delta x} = \frac{6.67 \times 10^{-34}}{2 \times 3.14 \times 10^{-14} \times 2}$$

$$= 5.27\,8 \times 10^{-20}\, Kg\, m/s$$

So if the e^- exist in the nucleus so the minimum momentum must be

$$\Delta P_x = 5.278 \times 10^{-20}\, Kg\, m/s$$

The energy of the electron

$$\Rightarrow E_{min} = \sqrt{P_{min}^2 C^2 + m_0^2 C^4}$$

$$\Rightarrow E_{min} = 9.875\ MeV.$$

In order to exist in the nucleas it must have minimum energy of about 9.875 MeV. But experimentaly it's found that the e^-s during β-decay carry energy of about 2-3 MeV. Therefore free e^- don't exist in the nucleus. During β-decay electrons are created in the process of converting neutron into Proton.

Physical significent of Wave Function :-

Material Partical in motion are represented by wave packet. The wave packet is represented by $\psi(x,t)$, which is a f^n of

$\vec{r}$ and time t. $\psi(r,t)$ gives us the complete information about the particle at a particular time. $\psi(r,t)$ represents the probability of finding the particle at the position $\vec{r}$ in time t.

Form of wave function associated with De Broglie wave. We are considering a free particle moving in x-axis with a non relativistic speed. Let P is the momentum and E is the energy. De Broglie's wavelength associated with this particle is $\lambda = \frac{h}{p}$ — (1)

∴ Wave vector

$$K = \frac{2\pi}{\lambda} = \frac{2\pi P}{h} = \frac{P}{\hbar} \quad \text{— (2)}$$

Angular frequency $\omega = 2\pi\nu = \frac{E}{\hbar}$ — (3)

$$K.E.\ E = \frac{p^2}{2m} \Rightarrow P = \sqrt{2mE}$$

from eqn (1)

$$\Rightarrow K = \frac{\sqrt{2mE}}{\hbar} \quad \text{— (4)}$$

The possible wave representing a particle, travelling along x direction, are

$$\psi_1 = a_1 \sin(\omega t - Kx) \;/\; a_1 \cos(\omega t - Kx)$$

— (5)

and $\psi_2 = a_1 e^{-i(\omega t - kx)}$ / $a_1 e^{i(\omega t - kx)}$.

Let us consider the wave f^n associated with the wave packet is represented by

$\psi_1 = a_1 \sin(\omega t - kx)$; [along (+ve) x-direction]

The particle traveling along (-ve) x direction is represented by $\psi_1' = a_1 \sin(\omega t + kx)$.

According to the superposition principle "$\psi_1 + \psi_1'$" must represent the particle at a distance in time 't'.

$\Rightarrow \psi = \psi_1 + \psi_1' = a_1 \sin(\omega t - kx) + a_1 \sin(\omega t + kx)$

$\Rightarrow \psi = 2a_1 \sin\omega t \cos kx.$

Putting $t = 0$

$\Rightarrow \psi(x,t) = 0.$

$\therefore$ The probability of finding the particle is zero which can't be true.

i.e. $\psi = a_1 \sin(\omega t - kx)$ / $a_1 \cos(\omega t - kx)$ can't ~~repreit~~ represent a wave packet.

Let us consider the wave f^n ψ_2 is traveling along x (+ve) direction and $\psi_2' = a e^{-i(\omega t - kx)}$ is traveling along (-ve) x direction.

Now, according to superposition principle →

P.T.O.

$\psi = \psi_2 + \psi_2'$ must represente the particle

$\Rightarrow \psi = Ae^{-i(\omega t - kx)} + Ae^{-i(\omega t + kx)}$

$= A(\cos\theta - i\sin\theta) + A(\cos\theta - i\sin\theta)$

$\Rightarrow \psi = 2A\, e^{-i\omega t}\, \frac{e^{ikx} - e^{-ikx}}{2}$

$\Rightarrow \psi = 2A\, e^{-i\omega t} \cos kx$

at time $t=0$

$\Rightarrow \psi = \cos kx\, 2A$

$e^{-i\theta} = \cos\theta - i\sin\theta$

$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$

$\cos\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$

$\psi(x,t)$ doesnot vanish. Therefore $\psi_2 = Ae^{-i(\omega t - kx)}$ is an acceptable wave f^n for representing a moving particle.

$\psi_3 = Ae^{i(\omega t - kx)}$ can't represent a wave packet because the superposition $\psi = \psi_3 + \psi_3'$ is equal to $2A\cos(\omega t - kx)$. which is not acceptable wave. The acceptable wave f^n for a moving particle travelling along +ve x-direction is

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

$\Rightarrow \psi(x,t) = Ae^{-i\left(\frac{E}{\hbar}t - \frac{\sqrt{2mE}}{\hbar}x\right)}$

Partial differentiating w.r.to t we get

$\frac{\partial \psi}{\partial t} = Ae^{-i\left(\frac{E}{\hbar}t - \frac{\sqrt{2mE}}{\hbar}x\right)} \cdot -i\frac{E}{\hbar}$

$$\Rightarrow \frac{\partial \psi}{\partial t} = -i\frac{E}{\hbar}\psi(x,t) \quad \text{--- (6)}$$

similarly $\frac{\partial \psi}{\partial x} = Ae^{-i\left(\frac{E}{\hbar}t - \frac{\sqrt{2mE}}{\hbar}x\right)} \cdot +\frac{i\sqrt{2mE}}{\hbar}$

again diff ~~eqn 6~~ we get $= \psi \cdot i\frac{\sqrt{2mE}}{\hbar}$

$$\frac{\partial^2 \psi}{\partial x^2} = Ae^{-i\left(\frac{E}{\hbar}t - \frac{\sqrt{2mE}}{\hbar}x\right)} \cdot + i^2\left(\frac{\sqrt{2mE}}{\hbar}\right)^2$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = \psi(x,t) \cdot -\frac{2mE}{\hbar^2} \quad \text{--- (7)}$$

Now (6) $\times\, i\hbar = i\hbar\frac{\partial \psi(x,t)}{\partial t} = E\,\psi(x,t)$ --- (8)

and (7) $\times \frac{-\hbar^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = E\,\psi(x,t)$ --- (9)

from eqn (8) & (9)

$$\boxed{\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\frac{\partial \psi(x,t)}{\partial t}} \longrightarrow (10)$$

This eqn (10) is called schrodinger eqn for a free particle.

(A) Time dependent schrodinger eqn for 1. D. ~~&~~

$\Rightarrow$ for free particle

Let us consider a particle of mass 'm' moving with a velocity v in the +ve X-direc. The wave associated with the particle is $\rightarrow$

$$\psi(x,t) = Ae^{-i(\omega t - Kx)}$$
$$= Ae^{i(Kx - \omega t)}$$

since $\omega = \frac{E}{\hbar}$

and also $K = P_x/\hbar$

putting value of ω and k we get

$$\psi(x,t) = Ae^{i\left(\frac{P_x}{\hbar}x - \frac{E}{\hbar}t\right)}$$

$$\Rightarrow \psi(x,t) = Ae^{i/\hbar(P_x x - Et)} \quad \text{--- (1)}$$

Then $$\frac{\partial \psi(x,t)}{\partial t} = Ae^{i/\hbar(P_x x - Et)} \cdot -\frac{i}{\hbar}E$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = -i\frac{E}{\hbar}\psi(x,t).$$

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

$$\Rightarrow E\psi = \frac{-i^2\hbar}{-i}\frac{\partial \psi}{\partial t}$$

$$\Rightarrow E\psi = i\hbar\frac{\partial \psi(x,t)}{\partial t} \quad \text{--- (2)}$$

Now w.r.t. x

$$\Rightarrow \frac{\partial \psi}{\partial x} = Ae^{i/\hbar(P_x x - Et)} \cdot \frac{iP_x}{\hbar}$$

$$= \psi(x,t)\frac{iP_x}{\hbar}$$

differentiating again

$$\frac{\partial^2 \psi}{\partial x^2} = \psi(x,t) \cdot \frac{-P_x^2}{\hbar^2} \quad (\because i^2 = -1)$$

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

$$\Rightarrow P_x^2\psi(x,t) = -\hbar^2\frac{\partial^2 \psi}{\partial x^2} \quad \text{--- (3)}$$

From eqn ②

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

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

Now comparing eqn ③ & ④

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

It's the time dependent schrodinger eqn for 1. Dimension free particle.

● **When the particle is facing a potential :—**

Suppose the particle is acted upon by a potential V_x. The total energy of the particle,

$$E = \frac{P_x^2}{2m} + V_x$$

(K.E + P.E)

$$\Rightarrow E\psi = \frac{P_x^2}{2m}\psi + V_x\psi \quad \text{——— ①}$$

Since $\psi(x,t) = Ae^{i/\hbar(P_x x - Et)}$ ——— ②

here $\frac{\partial\psi}{\partial t} = Ae^{i/\hbar(P_x x - Et)}\cdot\frac{-iE}{\hbar} \Rightarrow E\psi = i\hbar\frac{\partial\psi}{\partial t}$

$$\Rightarrow \frac{\partial\psi}{\partial x} = Ae^{i/\hbar(P_x x - Et)}\cdot\frac{iP_x}{\hbar} \Rightarrow P_x\psi = -i\hbar\frac{\partial\psi}{\partial x}$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = \psi\cdot\frac{-P_x^2}{\hbar^2} \Rightarrow P_x^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}$$

Putting the value of $E\psi$, $P_x^2\psi$, in eqn ①

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

This is the eqn when particle facing a potential.

Time dependent and Time independent part of schrodinger eqn :-

Schrodinger eqn is

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

Let $\psi(x,t) = U(x)\, f(t)$

differentiating w.r. to x →

$$\frac{\partial \psi(x,t)}{\partial x} = f(t)\frac{dU(x)}{dx}$$

again differentiating it

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = f(t)\frac{d^2U(x)}{dx^2}$$

Now differentiating w.r. to t we get →

$$\frac{\partial \psi(x,t)}{\partial t} = U(x)\frac{df(t)}{dt}$$

Putting these values in eqn (1) we get

$$\Rightarrow -\frac{\hbar^2}{2m} f(t)\frac{d^2U(x)}{dx^2} + V(x)\, U(x) f(t) = i\hbar\, U(x)\frac{df(t)}{dt}$$

Deviding both sides by $\psi(x,t)$ we get

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{f(t)}{U(x) f(t)}\frac{d^2U(x)}{dx^2} + V(x)\frac{\cancel{U(x) f(t)}}{\cancel{U(x) f(t)}}$$

$$= i\hbar\frac{\cancel{U(x)}}{\cancel{U(x)} f(t)}\frac{df(t)}{dt}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{U(x)}\frac{d^2U(x)}{dx^2} + V(x) = i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = E \quad \text{--- (2)}$$

here E is the total energy of the particle.

from this eqn $\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + V(x) = E$ is called time independent part and

and $i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = E$ is called time dependent part.

Solution for time dependent part:—

Since $i\hbar\frac{1}{f(t)}\frac{d f(t)}{dt} = E$

$$\Rightarrow \frac{d f(t)}{dt} = \frac{E f(t)}{i\hbar}$$

$$\Rightarrow \frac{d f(t)}{dt} = \frac{-i E f(t)}{\hbar}.$$

Integrating both side w.r.t. time 't'

$$\Rightarrow \ln f(t) = \frac{-iE}{\hbar}t + \ln C$$

$$\Rightarrow \ln f(t) - \ln C = \frac{-iE}{\hbar}t$$

$$\Rightarrow \ln\left[\frac{f(t)}{C}\right] = \frac{-iEt}{\hbar}$$

$$\Rightarrow \frac{f(t)}{C} = e^{-\frac{iEt}{\hbar}}$$

$$\boxed{\Rightarrow f(t) = Ce^{-\frac{iEt}{\hbar}}} \quad \text{—— (2)}$$

This is the soln for time dependent part of schrodinger eqn.

④ Time independent part solⁿ :-

Schrodinger eqⁿ is $-\frac{\hbar^2}{2m}\frac{1}{u(x)}\frac{d^2u(x)}{dx^2}+V(x)=E$

multiplying above eqⁿ by $u(x)$ we get

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x) = Eu(x)$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = (E-V(x))u(x).$$

$$\Rightarrow \frac{d^2u}{dx^2} = \frac{-2m(E-V)u}{\hbar^2}.$$

$$\boxed{\Rightarrow \frac{d^2u}{dx^2}+\frac{2m}{\hbar^2}(E-V)u=0} \quad \text{——— ④}$$

This is the time independent schrodinger eqⁿ. For which $u(x)$ will be a solution.

So, the total solⁿ of eqⁿ ② is can be written as

$$\Rightarrow \psi(x,t) = u(x)\phi(t)$$

$$\Rightarrow \psi(x,t) = u(x)\,c\,e^{-\frac{iE}{\hbar}t}$$

$$\Rightarrow \psi(x,t) = c\,u(x)\,e^{-\frac{iE}{\hbar}t}$$

If $\psi_1(x,t)$, $\psi_2(x,t)$, ... $\psi_n(x,t)$ be a set of solⁿ corresponding to the energy $E_1, E_2 \ldots E_n$ then the most general solⁿ of eqⁿ ② will be ⟶

$$\psi(x,t) = \psi_1(x,t)+\psi_2(x,t)+\cdots+\psi_n(x,t)$$

$$\Rightarrow \psi(x,t) = C_1 u_1(x) e^{-\frac{iE_1}{\hbar}t} + C_2 u_2(x) e^{-\frac{iE_2 t}{\hbar}} + \cdots + C_n u_n e^{-\frac{iE_n t}{\hbar}}$$

$$\Rightarrow \psi(x,t) = \sum_{n=1}^{\infty} C_n u_n(x) e^{-\frac{iE_n t}{\hbar}}$$

Since $\omega = \frac{E}{\hbar}$. Therefore

$$\Rightarrow \psi(x,t) = \sum_{n=1}^{\infty} C_n u_n(x) e^{-i\omega_n t}$$

This is the most general soln of eqn ②.

④. 3. Dimension schrodinger eqn :-

In case of 3.D. the wave packet is represented by $\psi(\vec{r},t)$. i.e. $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

Therefore $\psi(x,t) = A e^{\frac{i}{\hbar}(P_x x - E t)}$

for 3.D $\Rightarrow \psi(\vec{r},t) = A e^{\frac{i}{\hbar}(\vec{P}\cdot\vec{r} - Et)}$

here $\vec{P} = \hat{i}P_x + \hat{j}P_y + \hat{k}P_z$

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

So. $\vec{P}\cdot\vec{r} = P_x x + P_y y + P_z z$

and total energy in 3. Dimension

$$E = \frac{P^2}{2m} + V(\vec{r})$$

$$\Rightarrow E = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + V(\vec{r}) \quad (1)$$

Now differentiating w.r.to t

~~the eqn~~ $\frac{\partial}{\partial t}[\psi(\vec{r},t)] = \frac{d}{dt}[A e^{i/\hbar(P_x x + P_y y + P_z z - Et)}]$

$\Rightarrow \frac{\partial \psi}{\partial t} = A e^{i/\hbar (P_x x + P_y y + P_z z - Et)}$

$\cdot \frac{-i}{\hbar} E$

$\Rightarrow \frac{\partial \psi}{\partial t} = \psi(\vec{r}, t) \cdot \frac{-iE}{\hbar} \Rightarrow E\psi = i\hbar \frac{\partial \psi}{\partial t}$

Now differentiating for x.

$\frac{\partial \psi}{\partial x} = A e^{i/\hbar (P_x x + P_y y + P_z z - Et)} \cdot \frac{iP_x}{\hbar}$

differentiating again w.r.t. x

$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = A e^{i/\hbar (P_x x + P_y y + P_z z - Et)} \cdot \frac{-P_x^2}{\hbar^2}$

$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = \frac{-P_x^2}{\hbar^2} \psi(\vec{r}, t)$

$\Rightarrow P_x^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2}$

Similarly $\Rightarrow P_y^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial y^2}$

and $\Rightarrow P_z^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial z^2}$

multiplying by ψ both sides of eqn (1)

we get $\Rightarrow E\psi = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2)\psi + V(\vec{r})\psi$.

Putting values

$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}\left[-\hbar^2 \frac{\partial^2 \psi}{\partial x^2} - \hbar^2 \frac{\partial^2 \psi}{\partial y^2} - \hbar^2 \frac{\partial^2 \psi}{\partial z^2}\right]$

$+ V(\vec{r})\psi$

$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi + V(\vec{r})\psi$

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

This is the schrodinger eqn of 3. Dimesion.

⊛ The time independent part in 3.D. will be $\nabla u^2 + \frac{2m}{\hbar^2}(E-V)u = 0$

⊛ Physical Interpritation of $\psi(\vec{r},t)$:-

$\psi(r,t)$ can be regarded as the probability of finding the particle at position $\vec{r}$ ~~and~~ in time t. As probability is a real no. therefore $\psi(\vec{r},t)$ can't represent the probability as it is a complex fn.

$\therefore \psi^*(\vec{r},t) \cdot \psi(\vec{r},t) = |\psi(\vec{r},t)|^2$

This represence the probability of finding the particle.

$|\psi(\vec{r},t)|^2 d^3r$ is the probability of finding the particle in the volm element d^3r oragin. The total probability of finding the particle anywhere is space is equal to 1.

i.e. $\int_{-\infty}^{\infty} |\psi(\vec{r},t)|^2 d^3r = 1.$

⊛ Normalization of wave function :—

P.T.O.

schrodinger eq^n and $\int_{-\infty}^{\infty} |\psi_1(r,t)|^2 d^3r = N^2$ —— (1)

Now let us consider $\psi(r,t) = \frac{1}{N}\psi_1(r,t)$ will be also be a sol^n of schrodinger eq^n.

$\psi_1(\vec{r},t) = N\psi(r,t)$; putting the vallue in (1) we get

$$\int_{-\infty}^{\infty} |N.\psi(r,t)|^2 d^3r = N^2$$

$$\Rightarrow \int_{-\infty}^{\infty} \cancel{N^2} |\psi(r,t)|^2 d^3r = \cancel{N^2}$$

$$\Rightarrow \int_{-\infty}^{\infty} |\psi(r,t)|^2 d^3r = 1 \quad \text{—— (2)}$$

$\psi(r,t)$ is said to be normalised and (2) is called normalisation condition. This can also be written as $\int_{-\infty}^{\infty} |\psi(r,t)|^2 \cdot d^3r = 1$,

because the probability doesnt include the time dependent part.

In 1-Dimension $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

$\left(|\psi(x)|^2 = \psi^*(x)\,\psi(x) \right)$

Q.) Normalised the wave f^n

$$\psi(x) = \begin{cases} A \sin\frac{\pi x}{a}, & 0 < x < l \\ 0, & \text{outside} \end{cases}$$

Sol^n:- Since condition is

$$\int_{-\infty}^{\infty} \psi^*(x)\, \psi(x)\, dx = 1$$

$$\Rightarrow \int_0^l \psi^*(x)\, \psi(x)\, dx = 1$$

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

$$\Rightarrow A^2 \int_0^l \frac{1}{2}\left(1 - \cos\frac{2\pi x}{l}\right) dx = 1 \quad \left[\because \sin^2\theta = \tfrac{1}{2}(1-\cos 2\theta)\right]$$

$$\Rightarrow \frac{A^2}{2}\left[\int_0^l dx - \int_0^l \cos\frac{2\pi x}{l}\, dx\right] = 1$$

$$\Rightarrow \frac{A^2}{2}\left[l - \underbrace{(\sin 2\pi - \sin 0)}_{\sin n\pi = 0}\right] = 0$$

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

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

$$\Rightarrow A = \sqrt{\frac{2}{l}}$$

This is the normalised constant.

(2) Find the probability of finding the particle bet^n $x = 1/a$ & $x = \frac{2}{a}$ if wave f^n is define by $\psi(x) = \sqrt{a} \cdot e^{-ax}$.

Sol^n:- Given $\psi(x) = \sqrt{a}\, e^{-ax}$.

$$\psi^*(x) = \sqrt{a}\, e^{-ax}.$$

So probability $\int_{1/a}^{2/a} \psi^*_{(x)} \psi_{(x)} \, dx = \int_{1/a}^{2/a} \sqrt{a} e^{-ax} \cdot \sqrt{a} e^{-ax} \, d$

$$= a \int_{1/a}^{2/a} e^{-2ax} \, dx$$

$$= a \left[\frac{e^{-2ax}}{-2a} \right]_{1/a}^{2/a}$$

$$= \frac{\cancel{a}}{-2\cancel{a}} \left[e^{-2\cancel{a} \cdot \frac{2}{\cancel{a}}} - e^{-\frac{2\cancel{a} \times 1}{\cancel{a}}} \right]$$

$$= -\frac{1}{2} \left[e^{-4} - e^{-2} \right]$$

$$= \frac{1}{2} \left[e^{-2} - e^{-4} \right]$$

(3) Find the normalised wave fn for

$$\psi_{(x)} = A e^{-a x^2}$$

Soln We know

$$\int_{-\infty}^{\infty} \psi^*_{(x)} \psi_{(x)} \, dx = 1, \quad \psi^*_{(x)} = A e^{-a x^2}$$

$$\Rightarrow \int_{-\infty}^{\infty} A^2 e^{-2ax^2} \, dx = 1$$

$$\Rightarrow A^2 \, 2 \int_{0}^{\infty} e^{-2ax^2} \, dx = 1 \quad \text{--- (1)}$$

since $\int_{-\infty}^{\infty} f(x) dx = 2 \int_{0}^{\infty} f(x) \, dx$ if $f(x)$ is even

Let $2ax^2 = t \Rightarrow x^2 = \frac{t}{2a}$

differentiating w.r. to t

$\Rightarrow 2a \cdot 2x\,dx = dt$

$\Rightarrow dx = \dfrac{dt}{4ax}$

Putting the values in eq^n ①

$\Rightarrow A^2\, 2\int_0^\infty e^{-t} \dfrac{dt}{4ax} = 1$

$x = \sqrt{\dfrac{t}{2a}}$

$\Rightarrow A^2\, 2\int_0^\infty e^{-t} \dfrac{dt}{4a}\left(\dfrac{2a}{t}\right)^{1/2} = 1$

$\Rightarrow \dfrac{A^2 \cancel{2} \sqrt{2a}}{\cancel{4}\, a\sqrt{a}}\int_0^\infty e^{-t}\, t^{-1/2}\, dt = 1$

$\Rightarrow \dfrac{A^2}{\sqrt{2a}}\int_0^\infty e^{-t}\, t^{\frac{1}{2}-1}\, dt = 1$

$\Gamma n = \int_0^\infty x^{n-1} e^{-x}\, dx$

$\Gamma \tfrac{1}{2} = \sqrt{\pi}$

here $\Gamma n = \Gamma \tfrac{1}{2}$

$\Rightarrow \dfrac{A^2}{\sqrt{2a}}\, \Gamma \tfrac{1}{2} = 1$

$\Rightarrow \dfrac{A^2}{\sqrt{2a}}\, \sqrt{\pi} = 1$

$\Rightarrow A = \sqrt{\dfrac{\sqrt{2a}}{\sqrt{\pi}}}$

$\Rightarrow A = \left(\dfrac{2a}{\pi}\right)^{1/4}$

Hence $\psi_{(x)} = \left(\dfrac{2a}{\pi}\right)^{1/4} e^{-ax^2}$ is the normelised eq^n.

(Q) $\psi_{(x)} = e^{-|x|} \sin ax$, Normelised the wave f^n?

Sol^n:- Given

$\psi_{(x)} = e^{-|x|} \sin ax$ where $|x| = \begin{cases} -x, & x<0 \\ x, & x>0 \end{cases}$

Here $\psi^*_{(x)} = e^{-|x|} \sin ax$

(5) $\psi_{(x)} = Ae^{-\frac{x^2}{a^2}+ibx}$ find the normalization constant ?

Soln:- Given $\psi_{(x)} = Ae^{-\frac{x^2}{a^2}+ibx}$

here $\psi^*_{(x)} = Ae^{-\frac{x^2}{a^2}-ibx}$.

Since we know $\int_{-\infty}^{\infty} \psi^*_{(x)} \psi_{(x)} dx = 1$

$$\Rightarrow \int_{-\infty}^{\infty} Ae^{-\frac{x^2}{a^2}+ibx} \cdot Ae^{-\frac{x^2}{a^2}+ibx} dx = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} A^2 e^{-2\frac{x^2}{a^2}} \cdot \cancel{e^{-ibx}} \cdot \cancel{e^{ibx}} dx = 1$$

$$\Rightarrow A^2 \int_{-\infty}^{\infty} e^{-2\frac{x^2}{a^2}} dx = 1$$

let $2\frac{x^2}{a^2} = t$

$x^2 = \frac{ta^2}{2} \Rightarrow x = \sqrt{\frac{ta^2}{2}}$

$\frac{2}{a^2} \cdot 2x\, dx = dt$

$\Rightarrow dx = \frac{a^2 dt}{4x}$

$$\Rightarrow A^2 \int_{-\infty}^{\infty} e^{-t} \frac{a^2 dt}{4x} = 1$$

$$\Rightarrow \frac{A^2}{4} \int_{-\infty}^{\infty} e^{-t} \left(\frac{2}{ta^2}\right)^{1/2} dt = 1$$

$$\Rightarrow \frac{A^2 a^{\cancel{2}} \sqrt{2}}{4\, \cancel{a}} \int_{-\infty}^{\infty} e^{-t}\, t^{1/2}\, dt = 1$$

$$\Rightarrow \frac{A^2 a \sqrt{2}}{4} \cdot 2 \int_{0}^{\infty} e^{-t}\, t^{\frac{1}{2}-1}\, dt = 1$$

$$\Rightarrow \frac{A^2 a}{\sqrt{2}} \Gamma\tfrac{1}{2} = 1$$

$$\Rightarrow \frac{A^2 a}{\sqrt{2}} \sqrt{\pi} = 1 \Rightarrow A = \left(\frac{\sqrt{2}}{a\sqrt{\pi}}\right)^{1/2}$$

(6) $\psi_{(x)} = \begin{cases} A\dfrac{x}{a}, & 0<x<a \\ A\dfrac{b-x}{b-a}, & a<x<b \\ 0 & \text{outside} \end{cases}$

Soln:- ~~Give~~ Since we know that

$$\int_{-\infty}^{\infty} \psi^*_{(x)}\, \psi_{(x)}\, dx = 1$$

here $\displaystyle\int_0^b \psi^*_{(x)}\, \psi_{(x)}\, dx = 1$

$$\Rightarrow \int_0^a \psi^*_{(x)}\, \psi_{(x)}\, dx + \int_a^b \psi^*_{(x)}\, \psi_{(x)}\, dx = 1$$

$$\Rightarrow \int_0^a A\frac{x}{a} \cdot A\frac{x}{a}\, dx + \int_a^b A\frac{b-x}{b-a} \cdot A\frac{b+x}{b+a}$$

$$\Rightarrow \frac{A^2}{a^2}\left[\frac{x^3}{3}\right]_0^a + \frac{A^2}{b^2-a^2}\int_a^b (b^2-x^2)\, dx = 1$$

$$\Rightarrow \frac{A^2}{3a^2} \cdot a^3 + \frac{A^2}{b^2-a^2}\left[b^2x - \frac{x^3}{3}\right]_a^b = 1$$

$$\Rightarrow \frac{A^2a}{3} + \frac{A^2}{b^2-a^2}\left(b^3 - ab^2 - \frac{b^3}{3} + \frac{a^3}{3}\right)$$

$$\Rightarrow \frac{A^2a}{3} + \frac{A^2}{b^2-a^2} \cdot \left(\frac{3b^3 - 3ab^2 - b^3 + a^3}{3}\right) = 1$$

$$\Rightarrow \frac{A^2a}{3} + \frac{A^2}{b^2-a^2}\left(\frac{2b^3 - 3ab^2 + a^3}{3}\right) = 1$$

$$\Rightarrow A^2\left(\frac{a(b^2-a^2)+3}{3(b^2-a^2)}\right)\left(\frac{2b^3 - 3ab^2 + a^3}{3}\right) = 1$$

$$\Rightarrow A = \sqrt{\left(\frac{3}{2b^3 - 3ab^2 + a^3}\right)\left(\frac{a(b^2-a^2)+3}{3(b^2-a^2)}\right)}$$

⑦ $\psi_{(x,t)} = A e^{-\lambda|x|} e^{-i\omega t}$ $\quad -\infty < x < \infty$

Sol^n $\psi_{(x,t)} = A e^{-\lambda|x|} e^{-i\omega t}$ $\quad$ here $|x| = -x, x<0$; $\quad x, x>0$

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

$$\int_{-\infty}^{\infty} \psi^*_{(x,t)} \psi_{(x,t)} dx = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} A e^{-\lambda|x|} \cancel{e^{i\omega t}} \cdot A e^{-\lambda|x|} \cancel{e^{-i\omega t}} dx = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} A^2 e^{-2\lambda|x|} dx = 1$$

$$\Rightarrow A^2 \left[\int_{-\infty}^{0} e^{-2\lambda|x|} dx + \int_{0}^{\infty} e^{-2\lambda|x|} dx\right] = 1$$

$$\Rightarrow A^2 \left[\int_{-\infty}^{0} e^{-2\lambda(-x)} dx + \int_{0}^{\infty} e^{-2\lambda x} dx\right] = 1$$

$$\Rightarrow A^2 \left[\left[\frac{e^{2\lambda x}}{2\lambda}\right]_{-\infty}^{0} + \left[\frac{e^{-2\lambda x}}{-2\lambda}\right]_{0}^{\infty}\right] = 1$$

$$\Rightarrow A^2 \left[\frac{1}{2\lambda}\left(e^{0} - e^{-\infty}\right) + \frac{-1}{2\lambda}\left(e^{-\infty} - e^{0}\right)\right] = 1$$

$$\Rightarrow A^2 \left[\frac{1}{2\lambda} + \frac{1}{2\lambda}\right] = 1$$

$$\Rightarrow A^2 \cdot \frac{2}{2\lambda} = 1$$

$$\Rightarrow A = \sqrt{\lambda}$$

Conservation of Probability :-

In case of normalised wave f^n the probability of finding the particle over all region of space is equal to 1.

i.e. $\int_{-\infty}^{\infty} |\psi(\vec{r}t)|^2 d^3r = 1$.

The total probability of finding the particle is independent of time.

i.e. $\frac{\partial}{\partial t} \int_{-\infty}^{\infty} |\psi(\vec{r}t)|^2 d^3r = 0$.

Probability current density :- (J) :-

The 3.D schrodinger eq^n is

$$i\hbar \frac{\partial \psi(\vec{r}t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}t) + V \psi(\vec{r}t) \quad (1)$$

here 'v' depend on position.

Taking the complex conjugate of eq^n (1)

$$\Rightarrow -i\hbar \frac{\partial \psi^*(\vec{r}t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi^*(\vec{r}t) + V \psi^*(\vec{r}t) \quad (2)$$

multiplying eq^n (1) by $\psi^*(\vec{r}t)$ & (2) by $\psi(\vec{r}t)$, we get

$$(1) \Rightarrow i\hbar \frac{\partial \psi(\vec{r}t)}{\partial t} \psi^*(\vec{r}t) = \frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + \psi^* V \psi \quad (3)$$

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

Now substituting eqn. (3) - (4)

$$\Rightarrow i\hbar\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) = \frac{-\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^* + \cancel{\nabla\psi^*\psi} - \cancel{\nabla\psi^*\psi}\right)$$

$$\Rightarrow i\hbar\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) = \frac{-\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$\Rightarrow \psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t} = \frac{-\hbar^2}{2m\,i\hbar}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$\Rightarrow \psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t} = \frac{i\hbar}{2m}\nabla\cdot\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

$$\Rightarrow \frac{\partial}{\partial t}(\psi^*\psi) = \frac{i\hbar}{2m}\nabla\cdot\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

for total probability

$$\Rightarrow \frac{\partial}{\partial t}\int_{-\infty}^{\infty}(\psi^*\psi)\,d\tau = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\nabla\cdot\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)d\tau$$

$$\Rightarrow \frac{\partial}{\partial t}\int_{-\infty}^{\infty}(\psi^*\psi)\,d\tau = \frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]_{-\infty}^{\infty}$$

for a localised wave packet

ψ & $\psi^* \longrightarrow 0$ as $x \to \pm\infty$. So in that case $\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\psi^*\psi\,d\tau = 0$. It's the conservation of probability. The term probability current density is define as

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}(\psi^*\psi)\,d\tau = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\nabla\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]d\tau$$

$\Rightarrow \int_{-\infty}^{\infty} \frac{\partial}{\partial t}(\psi^*\psi)\, d\tau + \nabla \cdot \frac{i\hbar}{2m}\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right] d\tau = 0$

here current density, $J = \frac{i\hbar}{2m}\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right]$ such that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 \quad \text{——— (5)} \quad \{\rho = \psi^*\psi\}$$

eqn (5) is eqn of continuity for probability.

Q1) Find the probability current density for the wave fn $\psi_{(r)} = \frac{A}{r} e^{ikr}$.

Soln Given $\psi_{(r)} = \frac{A}{r} e^{ikr}$

we know that

$$J = \frac{i\hbar}{2m}\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right] \quad \text{——— (1)}$$

here $\psi^* = \frac{A}{r} e^{-ikr}$

$$\frac{\partial \psi^*}{\partial r} = A \frac{\partial}{\partial r}\left(\frac{1}{r} e^{-ikr}\right)$$

$$= A\left(\frac{-1}{r^2} e^{-ikr} - \frac{1}{r} e^{-ikr} \cdot -ik\right)$$

$\Rightarrow \nabla\psi^* = \frac{-A}{r^2} e^{-ikr} + \frac{A}{r} e^{-ikr} \cdot ik$

$\Rightarrow \nabla\psi^* = \frac{A}{r} e^{-ikr} ik - \frac{A}{r^2} e^{-ikr}$

$\therefore$ Putting values in eqn (1) we get

$$J = \frac{i\hbar}{2m}\left[\frac{A}{r}e^{ikr} \cdot \frac{A}{r}e^{-ikr}\left(\frac{-1}{r} - ik\right) - \frac{A}{r}e^{-ikr} \cdot \frac{A}{r}e^{ikr}\left(ik - \frac{1}{r}\right)\right]$$

$$= \frac{i\hbar}{\cancel{2}m}\frac{\cancel{2}A^2}{r^2}\, im\,[ik]$$

$$= \frac{\hbar}{mr^2}\, i\, |A|^2 \cdot k$$

$$= \frac{\hbar k}{mr^2}|A|^2$$

$A + iB$

taking Imginary part

so there ik.

Q) Find the current probability density for the wave fn $\psi_{(x)} = Ae^{ikx}$.

Soln:- The formula of J is $= \frac{i\hbar}{2m}\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right]$

here $\psi_{(x)} = Ae^{ikx}$

$\nabla\psi_{(x)} = Ae^{ikx} \cdot ik$

$\psi^*_{(x)} = A^* e^{-ikx}$

$\nabla\psi^*_{(x)} = -A^* e^{-ikx} \cdot ik$

$$\therefore J = \frac{i\hbar}{2m}\left[Ae^{ikx} \cdot \left(-A e^{-ikx} \cdot ik\right) - Ae^{-ikx}\left(Ae^{ikx} \cdot ik\right)\right]$$

$$= \frac{i\hbar}{2m}\left[-2|A|^2 \cdot ik\, e^{ikx} e^{-ikx}\right]$$

We can write it as —

$$J = \frac{i\hbar}{m}\, im\left[\psi^* \nabla\psi\right]$$

$$= \frac{\hbar}{m}\, im\left[A^* e^{-ikx} \cdot Ae^{ikx}\, ik\right]$$

$$= \frac{\hbar}{m}\, im\left[|A|^2 e^{-ikx} e^{ikx}\, ik\right]$$

$$= |A|^2 \frac{\hbar^2}{2m}\, im[ik]$$

$$\Rightarrow J = |A|^2 \frac{\hbar}{m} K$$

$$= |A|^2 \frac{\hbar K}{m} = |A|^2 \frac{P}{m}$$

$$= |A|^2 \frac{mv}{m}$$

$$\Rightarrow J = |A|^2 v.$$

$\boxed{2}$ Find J for a wave fn $\psi(x) = A e^{-\frac{a^2x^2}{2}} e^{ikx}$.

Soln :- Given $\psi(x) = A e^{-\frac{a^2x^2}{2}} e^{ikx}$

$$\frac{\partial \psi(x)}{\partial x} = A e^{-\frac{a^2x^2}{2}} e^{ikx} (-a^2x + ik)$$

$$\psi^*(x) = A^* e^{-\frac{a^2x^2}{2}} e^{-ikx}$$

Therefore $J = \frac{\hbar}{m} \, im \left[\psi^* \nabla \psi\right]$

$$= \frac{\hbar}{m} \, im \left[A^* e^{-\frac{a^2x^2}{2}} e^{-ikx} A e^{-\frac{a^2x^2}{2}} e^{ikx} \cdot (-a^2x + ik)\right]$$

$$\Rightarrow J = \frac{\hbar}{m} \, im \left[|A|^2 ik\right]$$

$$\Rightarrow J = \frac{\hbar}{m} \cdot k |A|^2$$

$$= |A|^2 \frac{\hbar k}{m} = |A|^2 \frac{P}{m}$$

$$= |A|^2 \frac{mv}{m}$$

$$\Rightarrow J = |A|^2 v.$$

Operator :-

An operator is a mathematical rule or procedure while operating on one function transforms it into another function. Mathematically

$\hat{A}\psi(x) = \phi(x)$, where $\hat{A}$ is the operator, $\psi(x)$ is the f^n on which it operates and $\phi(x)$ is the transform f^n.

Operating Algebra (operator algebra) :-

① Addition and Substraction.

ⓐ $(\hat{A} \pm \hat{B})\psi(x) = \hat{A}\psi(x) \pm \hat{B}\psi(x)$

ⓑ $(\hat{A}+\hat{B})\psi(x) = (\hat{B}+\hat{A})\psi(x)$

② Multiplying of f^n with operator :-

If $\hat{B}\psi(x) = \phi(x)$

$\hat{A}\phi(x) = g(x)$ then we can write

as $\hat{A}.\hat{B}\psi(x) = g(x)$. [where $\hat{A}, \hat{B}$ are the multiplication operator.]

If $\hat{A} = \hat{B}$ then $\hat{A}.\hat{A}\psi(x) = g(x)$

$\Rightarrow \hat{A}^2\psi(x) = g(x)$

Commutators :-

The two operators $\hat{A}$ & $\hat{B}$ are said to commute, if $\hat{A}.\hat{B}\,\psi_{(x)} = \hat{B}\hat{A}\,\psi_{(x)}$

$[\hat{A},\hat{B}]$ is define as $\Rightarrow \hat{A}\hat{B} - \hat{B}\hat{A}$

If $[\hat{A},\hat{B}]$ commute then $\hat{A}\hat{B} = \hat{B}\hat{A}$

$$\hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

$$\Rightarrow [\hat{A},\hat{B}] = 0$$

If $\hat{A}$ & $\hat{B}$ don't commut then

$$[\hat{A},\hat{B}] \neq 0 \text{ or } \hat{A}\hat{B} \neq \hat{B}\hat{A}.$$

Q.1 Let $\hat{A} = \frac{\partial}{\partial x}$ and $\hat{B} = \frac{\partial^2}{\partial x^2}$

Let $\psi_{(x)}$ be the function.

Soln Given $\hat{A}\hat{B}\,\psi_{(x)}$

$$\Rightarrow \hat{A}\frac{\partial^2}{\partial x^2}\psi_{(x)} = \frac{\partial}{\partial x}\frac{\partial^2}{\partial x^2}\psi_{(x)}$$

$$= \frac{\partial^3}{\partial x^3}\psi_{(x)}$$

Now

$$\hat{B}\hat{A}\,\psi_{(x)} \Rightarrow \frac{\partial^2}{\partial x^2}\frac{\partial}{\partial x}\psi_{(x)}$$

$$= \frac{\partial^3}{\partial x^3}\psi_{(x)}$$

i.e. $\hat{A}\hat{B}\,\psi_{(x)} = \hat{B}\hat{A}\,\psi_{(x)} \Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A})\psi_{(x)} = 0$

$$\Rightarrow \hat{A}\hat{B} = \hat{B}\hat{A}$$

$$\Rightarrow [\hat{A},\hat{B}] = 0$$

Therefore $\frac{\partial}{\partial x}$ & $\frac{\partial^2}{\partial x^2}$ will commut

(Q) $\hat{A} = x$, $\hat{B} = \frac{d}{dx}$

Solⁿ Let $\psi(x)$ be the fⁿ

then $\hat{A}\hat{B}\psi(x) = x\frac{d}{dx}\psi(x)$

and $\hat{B}\hat{A}\psi(x) = \frac{d}{dx}\hat{x}\psi(x) = \frac{d}{dx}[x\psi(x)]$

$= \frac{xd}{dx}\psi(x) + \psi(x)$

$\therefore \hat{A}\hat{B}\psi(x) - \hat{B}\hat{A}\psi(x) = x\frac{d}{dx}\psi(x) - \frac{xd}{dx}\psi(x) - \psi(x)$

$= -\psi(x)$

$\Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A})\cancel{\psi(x)} = -\cancel{\psi(x)}$

$\Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A}) = -1$ $\qquad \left[\hat{x}, \frac{\partial}{\partial x}\right] = -1$

$\Rightarrow [\hat{A}, \hat{B}] = -1$.

— led

⊛ linear Operator :- Important

A operator 'A' is said to be linear operator if $\hat{A}[c\,\psi(x)] = c\,\hat{A}\,\psi(x)$ where c is constant.

*** Statement :-**

The operator $\hat{A}$ is said to be linear if it commutes with an arbitary constant

$$\hat{A}c\,\psi(x) = c\hat{A}\,\psi(x)$$

$$\Rightarrow \hat{A}c = c\hat{A}$$

$$\Rightarrow \hat{A}c - c\hat{A} = 0$$

$$\Rightarrow [\hat{A}, c] = 0$$

eg:- $\hat{A} = \frac{d}{dx}$

$$\hat{A}[c\,\psi(x)] = \frac{d}{dx}[c\,\psi(x)]$$

$$= c\frac{d}{dx}\psi(x)$$

$$= c\hat{A}\,\psi(x)$$ prove.

⊛ Properties of linear operators :-

① Linear operator commutes with an arbitary constant.

② Distributive law is followed by linear operator. i.e. $\hat{A}[\psi_1(x) + \psi_2(x)] = \hat{A}\psi_1(x) + \hat{A}\psi_2(x)$.

③ $[\hat{A} \pm \hat{B}]\hat{C} = \hat{A}\hat{C} \pm \hat{B}\hat{C}$

④ $(\hat{A}\hat{B})\hat{C} = \hat{A}[\hat{B}\hat{C}]$

⑤ $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

Operators corresponding to different dynamical variables :-

① Linear momentum operator :-

In quantum mechanics particle moving in x-direction is represented by wave

$$\psi_{(x,t)} = Ae^{i(kx-\omega t)}$$

$$\psi_{(x,t)} = Ae^{\frac{i}{\hbar}(P_x - Et)}$$

Now $\frac{\partial}{\partial x}\psi_{(x,t)} = Ae^{\frac{i}{\hbar}(P_x x - Et)} \cdot \frac{i}{\hbar}P_x$

$$= \frac{i}{\hbar}P_x\,\psi_{(x,t)}$$

$$\Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}\psi_{(x,t)} = P_x\,\psi_{(x,t)}$$

$$\Rightarrow -i\hbar\frac{\partial}{\partial x}\psi_{(x,t)} = P_x\,\psi_{(x,t)}$$

So here the linear momentum operator is

$$\boxed{\Rightarrow \hat{P}_x = -i\hbar\frac{\partial}{\partial x}},$$

in 3. Dimension $\hat{P} = -i\hbar\nabla$, $\left(\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right)$

Total Energy Operator :-

In quantum mechanics a moving particle along x-axis is represented by wave

$$\psi_{(x,t)} = Ae^{i/\hbar (P_x x - Et)}$$

So, $\frac{\partial \psi_{(x,t)}}{\partial t} = Ae^{\frac{i}{\hbar}(P_x x - Et)} \cdot -\frac{i}{\hbar}E$

$$\Rightarrow \frac{\partial \psi_{(x,t)}}{\partial t} = -\frac{iE}{\hbar} \psi_{(x,t)}$$

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

$$\Rightarrow i\hbar \frac{\partial \psi_{(x,t)}}{\partial t} = E\, \psi_{(x,t)}$$

So here $\boxed{\hat{E} = i\hbar \frac{\partial}{\partial t}}$ which is the total energy operator.

3) Kinetic Energy :-

Since $K.E = \frac{p^2}{2m}$

$$(K.E)\, \psi_{(x)} = \frac{\hat{p}_{x}^{2}}{2m} \psi_{(x)}$$

$$\Rightarrow (K.E)\, \psi_{(x)} = \frac{1}{2m} \left(i^2\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi_{(x)}$$

$$= \frac{1}{2m} \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi_{(x)}$$

$$\Rightarrow K.E\, \psi_{(x)} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{(x)}$$

$$\therefore \boxed{(\hat{K.E}) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}$$

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

$K.E.\psi = \frac{P_x^2}{2m}\psi$

$= \frac{1}{2m}\left(-i\hbar \frac{\partial}{\partial x}\right)^2$

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

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

for 3 Dimension $(K.\hat{E}) = \frac{-\hbar^2}{2m} \nabla^2$

Q 20) $[\hat{x}, \hat{P}_x]$

Soln:- Let $\psi_{(x)}$ is a function, $[A, B] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

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

here $\hat{A}.\hat{B} \Rightarrow \left[\hat{x}. \frac{\hbar}{i}\frac{\partial}{\partial x}\right]\psi_{(x)} = \hat{x}\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_{(x)}$

and $\hat{B}.\hat{A} \Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}\left[\hat{x}\psi_{(x)}\right] = \frac{\hbar}{i}\frac{\partial}{\partial x}\left[x\psi_{(x)}\right]$

$$= \frac{\hbar}{i}\left[\frac{x\partial\psi_{(x)}}{\partial x} + \psi_{(x)}\right]$$

Therefore $\hat{A}.\hat{B} - \hat{B}\hat{A} = \hat{x}\frac{\hbar}{i}\frac{\partial\psi_{(x)}}{\partial x} - \cancel{\frac{\hbar}{i}\frac{x\partial\psi_{(x)}}{\partial x}} - \frac{\hbar}{i}\psi_{(x)}$

$$(\hat{A}\hat{B} - \hat{B}\hat{A})\cancel{\psi_{(x)}} = -\frac{\hbar}{i}\cancel{\psi_{(x)}}$$

$$\boxed{\Rightarrow [\hat{x}, \hat{P}_x] = i\hbar}$$ So $\hat{x}$ & $\hat{P}_x$ don't commute.

$[\hat{x}, \hat{P}_x] = i\hbar$

Properties of Commutator :-

① $[\hat{A}, \hat{A}] = 0$

② $[\hat{A}, C] = 0$

③ $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

④ $[c\hat{A}, \hat{B}] = [\hat{A}, c\hat{B}] = c[\hat{A}, \hat{B}]$

⑤ $[\hat{A}, \hat{B} \pm \hat{C}] = [\hat{A}, \hat{B}] \pm [\hat{A}, \hat{C}]$

⑥ $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

⑦ $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$

Q.1) $\left[\hat{x}, \frac{\partial^2}{\partial x^2}\right]$

Soln we can write it as $\left[\hat{x}, \frac{\partial}{\partial x}\cdot\frac{\partial}{\partial x}\right]$

using formula ⑦ we get

$$= \frac{\partial}{\partial x}\left[\hat{x}, \frac{\partial}{\partial x}\right] + \left[\hat{x}, \frac{\partial}{\partial x}\right]\frac{\partial}{\partial x}$$

$$= \frac{\partial}{\partial x}(-1) + (-1)\frac{\partial}{\partial x}$$ [since we got before $\left[\hat{x}, \frac{\partial}{\partial x}\right] = -1$]

$$= -2\frac{\partial}{\partial x}$$

Prove of incompleted problem ~~before~~

④ Hemiltonian operator :-

Total energy of a particle in potential $V_{(x)}$ is $E = \frac{p_x^2}{2m} + V_{(x)}$

multiplying both the sides by ψ we get

$$E\psi = \frac{p_x^2\psi}{2m} + V_{(x)}\psi$$

$$\Rightarrow (E-V)\psi = \frac{p_x^2 \psi}{2m} \quad \left[\text{Since } p_x = -i\hbar \frac{\partial}{\partial x}\right]$$

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

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

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

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

$$= \hat{H}$$

Here $\hat{H}$ is called the Hamiltonian operator.

For 3D. it will be

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(x,y,z)$$

5 Angular momentum Operator :-

We know Angular momentum $\vec{L} = \vec{r} \times \vec{p}$

In terms of operator $\hat{L} = \hat{r} \times \hat{p}$

$$\Rightarrow \hat{L} = \hat{r} \times (-i\hbar \nabla)$$

$$\Rightarrow \hat{L} = -i\hbar (\hat{r} \times \nabla)$$

here $\hat{p} = -i\hbar\nabla$ for 3.D.

$$\therefore \hat{r} \times \nabla = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$\Rightarrow \hat{r} \times \nabla = \hat{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) + \hat{j}\left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right) + \hat{k}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

$\Rightarrow \vec{r} \times \nabla = \hat{i}\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right) + \hat{j}\left(z\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right)$

$+ \hat{k}\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$

$\Rightarrow \hat{L} = \left(\hat{i}\hat{L}_x + \hat{j}\hat{L}_y + \hat{k}\hat{L}_z\right) i\hbar$

where
$\Rightarrow \hat{L}_x = -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)$

$\Rightarrow \hat{L}_y = -i\hbar\left[z\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right)$

$\Rightarrow \hat{L}_z = -i\hbar\left[\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$ //.

Commutation relⁿ of angular momentum & position:-

Let the position & angular momentum along x-direction, and $\psi_{(x)}$ be a fⁿ.

Therefore
$[\hat{L}_x, \hat{x}]\psi_{(x)}$

$= \left(\hat{L}_x\hat{x} - \hat{x}\hat{L}_x\right)\psi_{(x)}$

$= \hat{L}_x\hat{x}\psi_{(x)} - \hat{x}\hat{L}_x\psi_{(x)}$

Now for, $\hat{L}_x\hat{x}\psi_{(x)}$

$= -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)x\,\psi_{(x)}$

$= -i\hbar\left[\left(\hat{y}\psi_{(x)}\frac{\partial x}{\partial z} + \hat{y}x\frac{\partial\psi_{(x)}}{\partial z}\right) - \left(\hat{z}\psi_{(x)}\frac{\partial x}{\partial y} + \hat{z}x\frac{\partial\psi_{(x)}}{\partial y}\right)\right]$

$= -i\hbar\left[\hat{y}\psi_{(x)}\frac{\partial x}{\partial z} + \frac{xy\,\partial\psi_{(x)}}{\partial z} - \hat{z}\psi_{(x)}\frac{\partial x}{\partial y} - xz\frac{\partial\psi_{(x)}}{\partial y}\right]$

Since it is along x-axis so $\frac{\partial x}{\partial z}$ & $\frac{\partial x}{\partial y}$ are zero.

$\therefore \Rightarrow \hat{L}_x \hat{x} \psi_{(x)} = -i\hbar \left[yx \frac{\partial \psi}{\partial z} - zx \frac{\partial \psi}{\partial y} \right]$ — ①

for $\hat{x} \hat{L}_x \psi_{(x)}$

$$= \hat{x} \cdot \left[-i\hbar \left(\hat{y} \frac{\partial}{\partial z} - \hat{z} \frac{\partial}{\partial y} \right) \psi_{(x)} \right]$$

$$= -i\hbar\, x \left(y \frac{\partial \psi_{(x)}}{\partial z} - \hat{z} \frac{\partial \psi_{(x)}}{\partial y} \right)$$

$\Rightarrow \hat{x} \hat{L}_x \psi_{(x)} = -i\hbar \left[xy \frac{\partial \psi}{\partial z} - xz \frac{\partial \psi}{\partial y} \right]$ — ②

From eqn ① & ②

$$\Rightarrow \hat{L}_x \hat{x} \psi_{(x)} - \hat{x} \hat{L}_x \psi_{(x)} = 0 \cdot \psi_{(x)}$$

$\therefore \hat{L}_x, \hat{x}$ are commutator.

② $[\hat{L}_y, \hat{y}] = 0$ prove that -

Soln Let $\psi_{(x)}$ is a function where $\hat{L}_y$ & $\hat{y}$ operator.

$[\hat{L}_y, \hat{y}] \psi_{(x)} = \hat{L}_y \hat{y} \psi_{(x)} - \hat{y} \hat{L}_y \psi_{(x)}$ — ①

here for $\hat{L}_y \hat{y} \psi_{(x)} = -i\hbar \left[\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right] \hat{y} \psi_{(x)}$

$$= -i\hbar \left[\left(\hat{z} y \frac{\partial \psi_{(x)}}{\partial x} + z \psi_{(x)} \frac{\partial y}{\partial x} \right) - \left(\hat{x} y \frac{\partial \psi}{\partial z} + \hat{x} \psi_{(x)} \frac{\partial y}{\partial z} \right) \right]$$

$$= -i\hbar \left[zy \frac{\partial \psi_{(x)}}{\partial x} + 0 - xy \frac{\partial \psi_{(x)}}{\partial z} + 0 \right]$$

$$= -i\hbar \left[zy \frac{\partial \psi_{(x)}}{\partial x} - xy \frac{\partial \psi_{(x)}}{\partial z} \right]$$ — ②

for $\hat{y} \hat{L}_y \psi_{(x)} = \hat{y} \left[i\hbar \left(\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right) \psi_{(x)} \right]$

$$= -i\hbar \left[y\hat{z} \frac{\partial \psi_{(x)}}{\partial x} - yx \frac{\partial \psi_{(x)}}{\partial z} \right]$$ — ③

Putting the values of ② & ③ in eqn ①

$\Rightarrow \hat{L}_y \hat{y} \psi_{(y)} - \hat{y} \hat{L}_y \psi_{(y)} = 0 . \psi_{(y)}$

$\Rightarrow [\hat{L}_y, \hat{y}] = 0$ i.e. $\hat{L}_y, \hat{y}$ commutator.

Proved

③ $[\hat{L}_z, \hat{z}] = 0$

Soln $[\hat{L}_z, \hat{z}] \psi_{(z)} = 0$

$\Rightarrow \hat{L}_z \hat{z} \psi_{(z)} - \hat{z} \hat{L}_z \psi_{(z)}$

$\Rightarrow -i\hbar \left[\left(\hat{x} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial \hat{x}} \right) \hat{z} \psi_{(z)} \right] - \hat{z} \left[-i\hbar \left(\hat{x} \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \psi_{(z)} \right]$

$= -i\hbar \left[\hat{x} z \frac{\partial \psi_{(z)}}{\partial y} + \hat{x} \psi_{(z)} \frac{\partial z}{\partial y} - \hat{y} \hat{z} \frac{\partial \psi}{\partial x} - \hat{y} \psi_{(z)} \frac{\partial z}{\partial x} \right]$

$+ i\hbar \left[z x \frac{\partial \psi_z}{\partial y} - z y \frac{\partial \psi}{\partial x} \right]$

$= -i\hbar \left[xz \frac{\partial \psi}{\partial y} - yz \frac{\partial \psi}{\partial x} \right] + i\hbar \left[zx \frac{\partial \psi}{\partial y} - yz \frac{\partial \psi}{\partial x} \right]$

$= 0$

$\Rightarrow [\hat{L}_z, \hat{z}] \psi_{(z)} = 0 . \psi_{(z)}$

$\therefore \hat{L}_z, \hat{z}$ are commutators.

④ $[\hat{L}_x, \hat{P}_x]$

$= (\hat{L}_x \hat{P}_x - \hat{P}_x \hat{L}_x) \psi_{(x)}$

$$= \hat{L}_x \hat{P}_x \psi - \hat{P}_x \hat{L}_x \psi$$

$$= -i\hbar\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(-i\hbar\frac{\partial \psi}{\partial x}\right)\right] - \left(-i\hbar\frac{\partial}{\partial x}\right)\hat{L}_x \psi$$

$$= -i\hbar\left(y\frac{\partial^2 \psi}{\partial x \partial z} - z\frac{\partial^2 \psi}{\partial y \partial x}\right) + i\hbar\left(y\frac{\partial^2 \psi}{\partial x \partial z} - z\frac{\partial^2 \psi}{\partial y \partial x}\right)$$

$$= 0$$

$$\Rightarrow \left[\hat{L}_x, \hat{P}_x\right] = 0$$

$\therefore$ $\hat{L}_x$, $\hat{P}_x$ are commutators.

Similarly $= \left[\hat{L}_y \hat{P}_y\right] = 0$

and $\left[\hat{L}_z \hat{P}_z\right] = 0$.

8. (i) $\left[\hat{L}_x, \hat{y}\right]$, (2) $\left[\hat{L}_z, \hat{z}\right]$

Soln (i) $\left[\hat{L}_x, \hat{y}\right] = \hat{L}_x \hat{y} - \hat{y}\hat{L}_x$

if $\psi(x,y)$ is the fn then

$$= \left[\hat{L}_x \hat{y}\psi - \hat{y}\hat{L}_x \psi\right]$$

$$= -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\hat{y}\psi - \hat{y}\left[-i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\psi\right]$$

$$= -i\hbar\left(y^2\frac{\partial \psi}{\partial z} + \cancel{z}\psi\frac{\partial y}{\partial z} - \hat{z}y\frac{\partial \psi}{\partial y} - \hat{z}\psi\frac{\partial y}{\partial y}\right)$$

$$+ i\hbar\left[y \cdot y\frac{\partial \psi}{\partial z} - yz\frac{\partial \psi}{\partial y}\right]$$

$$= -i\hbar\left(\cancel{y^2\frac{\partial \psi}{\partial z}} + 0 - zy\frac{\partial \psi}{\partial y} - z\psi\right) + i\hbar$$

$$+ i\hbar\left(\cancel{y^2\frac{\partial \psi}{\partial z}} - yz\frac{\partial \psi}{\partial y}\right)$$

$[\hat{L}_x, \hat{y}]\psi = +i\hbar z\psi$

$\Rightarrow \boxed{[\hat{L}_x, \hat{y}] = i\hbar \hat{z}}$

② $[\hat{L}_y, \hat{z}]$

Soln $\hat{L}_y \hat{z}\psi - \hat{z}\hat{L}_y\psi$

$= -i\hbar\left[\hat{z}\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right]z\psi - z\left[-i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\psi\right]$

$= -i\hbar\left[z^2\frac{\partial\psi}{\partial x} - xz\frac{\partial\psi}{\partial z} - x\psi\right] + i\hbar\left(z^2\frac{\partial\psi}{\partial x} - zx\frac{\partial\psi}{\partial z}\right)$

$= -i\hbar\, \cancel{z^2\frac{\partial\psi}{\partial x}} + \cancel{i\hbar\, xz\frac{\partial\psi}{\partial z}} + i\hbar x\psi + \cancel{i\hbar z^2\frac{\partial\psi}{\partial x}}$
$\cancel{- i\hbar zx\frac{\partial\psi}{\partial z}}$

$= i\hbar x\psi.$

$\Rightarrow [\hat{L}_y, \hat{z}]\psi = i\hbar x\psi$

$\boxed{\therefore [\hat{L}_y, \hat{z}] = i\hbar x}$

Similarly

$\boxed{③\ [\hat{L}_z, \hat{x}] = i\hbar \hat{y}}$

④ $[\hat{L}_x, \hat{P}_y]$

$\Rightarrow \hat{L}_x \hat{P}_y \psi - \hat{P}_y \hat{L}_x \psi$

$= -i\hbar\left(y\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right) - i\hbar\frac{\partial \psi}{\partial y} + i\hbar\frac{\partial \psi}{\partial y}\left(-i\hbar\left(y\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\psi\right)$

$= -\hbar^2\left(y\frac{\partial^2 \psi}{\partial z \partial y} - z\frac{\partial^2 \psi}{\partial y^2}\right) + \hbar^2\left(\frac{\partial^2 \psi}{\partial y \partial z} - z\frac{\partial^2 \psi}{\partial y^2}\right)$

$= -\hbar^2 y \cancel{\frac{\partial^2 \psi}{\partial z \partial y}} + \hbar^2 z \cancel{\frac{\partial^2 \psi}{\partial y^2}} + \hbar^2 \cancel{\frac{\partial^2 \psi}{\partial y \partial z}} - \hbar^2 z \cancel{\frac{\partial^2 \psi}{\partial y^2}}$

$= 0$

$\therefore \hat{L}_x \hat{P}_y \psi - \hat{P}_y \hat{L}_x \psi = 0$

$\Rightarrow [\hat{L}_x \hat{P}_y] = 0$ They are commutator.

Q. If $\hat{A}$ & $\hat{B}$ are two operators which commute with their commutator $[\hat{A},\hat{B}]$ then prove that

$$[\hat{A}^n \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}\ \hat{B}]$$

Soln:— Here

Given $[\hat{A}\hat{B}^n] = n\hat{B}^{n-1}[\hat{A}\hat{B}]$ ——— (1)

$\hat{A}[\hat{A},\hat{B}] = [\hat{A},\hat{B}]\hat{A}$ ——— (2)

$\hat{B}[\hat{A},\hat{B}] = [\hat{A},\hat{B}]\hat{B}$ ——— (3)

We got that reln (1) is true for $n=1$

for $n=2$ $[\hat{A}\hat{B}^2] = [\hat{A},\hat{B}\cdot\hat{B}]$

Using property we get

$\Rightarrow \hat{B}[\hat{A},\hat{B}] = [\hat{A},\hat{B}]\hat{B}$

Using condition $\rightarrow$

$2B,[\hat{A}\hat{B}^2] = 2B^{2-1}[\hat{A},\hat{B}]$

$= 2B[\hat{A},\hat{B}]$

This is true for $n=2$.

Let us consider it is valid for $n=K$

$\therefore [\hat{A}B^K] = K\hat{B}^{K-1}[\hat{A},\hat{B}]$ ——— (4)

Let's check for $n=K+1$

$[\hat{A}\ B^{K+1}] = [\hat{A}, B^K\cdot B] = [\hat{A},\hat{B}^K]\hat{B} + B^K[\hat{A},\hat{B}]$

from reln (4)

$[\hat{A},B^K] = K\hat{B}^{K-1}[\hat{A}\hat{B}]\hat{B} + B^K[\hat{A}\hat{B}]$

$= K B^{K-1} \hat{B} [\hat{A}, \hat{B}] + B^K [\hat{A}, \hat{B}]$

$= K B^K [\hat{A} \hat{B}] + B^K [\hat{A} \hat{B}]$

$\Rightarrow (K+1) B^K [\hat{A}, \hat{B}]$

$= (K+1) B^{K+1-1} [\hat{A}, \hat{B}]$

This formula is valid for $n = K+1$.
So this is valid for any value of "n".

Q] $[x^n P_x]$

Soln:- Here, we can write

$-[\hat{P}_x \hat{x}^n] = -n \hat{x}^{n-1} [\hat{P}_x, \hat{x}]$

$= -n x^{n-1} (-i\hbar)$

since $[\hat{x}, \hat{P}_x] = i\hbar$

$[\hat{P}_x \cdot x^n] = i\hbar n x^{n-1}$

Eigen function and Eigen values:-

If an operator $\hat{A}$ operating on a function $\psi_{(x)}$ results a constant (λ) times the wave f^n $\psi_{(x)}$ itself then $\psi_{(x)}$ is called eigen f^n $\hat{A}$ corresponding to the eigen value λ.

i.e. $\hat{A} \psi_{(x)} = \lambda \psi_{(x)}$.

Q 1) If Hamiltonian operator $\hat{H} = \frac{P^2}{2m} + V(x)$ then show that $[\hat{x}, [\hat{x}, \hat{H}]] = \frac{-\hbar^2}{m}$

Solⁿ :- $[\hat{x}, \hat{H}] = [\hat{x}, \frac{P^2}{2m} + V(x)]$

$= [\hat{x}, \frac{P^2}{2m}] + [\hat{x}, V(x)]$ $\left\{ [\hat{x}, V(x)] = 0 \text{ since } V(x) \text{ is constant} \right\}$

$= \frac{1}{2m} [\hat{x}, P^2]$

$= \frac{1}{2m} \times 2 \hat{p}^{2-1} [\hat{x}, \hat{p}]$ $\left[[\hat{A}, B^n] = n B^{n-1} [\hat{A}, \hat{B}] \right]$

$= \frac{\hat{P}}{m} \times i\hbar$

$= \frac{i\hbar}{m} \hat{P}$ $\left\{ \text{Since } [\hat{x}, \hat{P}_x] = i\hbar \right\}$

So $[\hat{x}, [\hat{x}, \hat{H}]] = [\hat{x}, \frac{i\hbar}{m} \hat{P}]$

$= \frac{i\hbar}{m} [\hat{x}, \hat{P}]$

$= \frac{i\hbar}{m} \times i\hbar = \frac{-\hbar^2}{m}$,,

Shown.

① ⇒ $\psi(x)$ is normalised if $\int_\tau |\psi(x)|^2 d\tau = 1$.

⇒ is not normalised if $\int_\tau |\psi(x)|^2 d\tau \neq 1$,

② Show that $[\hat{H}, \hat{P}] = 0$

Solⁿ since $\hat{H} = \frac{P^2}{2m} + V(x)$

$\therefore [\frac{P^2}{2m} + V(x), \hat{P}] = [\frac{P^2}{2m}, \hat{P}] + [V(x), \hat{P}]$,

$= \frac{1}{2m}[\hat{p}^2, \hat{p}] + 0$

$= \frac{1}{2m} \times 0$ [from commutator property]

$\Rightarrow [\hat{H}, \hat{P}] = 0$ showed

Properties of well behave f^n :-

① $\psi_{(x)}$ must be single valued and continuous everywhere.

eg:- (i) $f(x) = x$ or x^2 (single valued)

(ii) $f(x) = \sqrt{x}$ $\quad x = 4 = \sqrt{x} = \pm 2$ (two valued) donot satisfy

② $\int_{\tau} |\psi_{(x)}|^2 d\tau$ value must be finite.

③ $\psi_{(x)}$ must be finite as $x \to \pm\infty$.

④ $\psi_{(x)}, \frac{d\psi_{(x)}}{dx}$ must be continuous everywhere.

Eg: $A = \frac{d^2}{dx^2}$

$A\psi_{(x)} = \frac{d^2}{dx^2}\psi = -\lambda\psi$

Soln :- We can write

$\Rightarrow \hat{A}\psi_{(x)} = \frac{d^2\psi}{dx^2} + \lambda\psi = 0$ ——— ①

General soln of the eqn will be in the form

$\psi_{(x)} = Ae^{i\sqrt{\lambda}x} + Be^{-i\sqrt{\lambda}x}$ ——— ②

eqn ② may be expressed in the form of

$\psi_{(x)} = C\cos\sqrt{\lambda}x + D\sin\sqrt{\lambda}x$ ——— ③

(a) for $\lambda > 0$, [since $\cos(-\theta) = \cos\theta$]

$\psi_{(x)}$ is single valued function.

Again at $x \to \pm\infty$, $\psi_{(x)}$ is finite.

$\because -1 \leq \cos x \leq 1$

and $0 \leq \sin\theta \leq 1$

So, $\psi_{(x)}$ is then a well behaved f^n.

(b) if $\lambda = 0$, (i) will be

Then the soln of eqn

$$\frac{d^2\psi}{dx^2} + 0 = 0 \Rightarrow \frac{d^2\psi}{dx^2} = 0$$

here we can write

$$\psi_{(x)} = F_{(x)} + C_2$$

since as $x \to \pm\infty$, $\psi_{(x)} \to \pm\infty$ also.

So, it's not well behaved.

(c) For $\lambda < 0$, it will be

if, $\lambda = -4$, $\sqrt{\lambda} = 2i$,

Then soln will be

$$\psi_{(x)} = Ae^{-bx} + Be^{+bx}$$ [here $\sqrt{\lambda} = bi$]

The f^n is single valued and continuous.

at $x \to \pm\infty$

then $\psi_{(x)} \to \pm\infty$

[since $x \to -\infty$ & $x \to \infty$
$\underbrace{Ae^{+\infty}}_{\infty} + \underbrace{Be^{-\infty}}_{0}$ $\underbrace{Ae^{-\infty}}_{0} + \underbrace{Be^{+\infty}}_{\infty}$]

$\therefore \psi_{(x)}$ is not well behaved.

(A) Among the following wave f^{ns} which one is Physically acceptable.

(1) $3\sin \pi x$, (2) $4-|x|$ (3) $\sqrt{5x}$ (4) $e^{-\lambda x}$.

Solⁿ:-

(4) if $x \to \pm \infty$

for $x \to -\infty$, $e^{+\alpha x} = \psi_{(x)} \to \infty$, so its not an acceptable fⁿ.

(3) $\sqrt{5x}$ it is not single valued.

(2) $4-|x|$

The fⁿ is single valued.

if $x \to \pm\infty$, function $\psi_{(x)} \to \infty$, its not acceptable.

$|x| = -x \quad x<0, \quad |x| = x, \quad x>0$

$\psi^-_{(x)} = 4-|x| = 4+x$ but at $x=0$ its

$\psi^+_{(x)} = 4+|x| = 4-x$ $|\psi| <$

not contenceous $\frac{d\psi_{(x)}}{dx}$

(1) $3\sin\pi x$.

Its single valued. its finite because $0 \le x \le 1$.

at $x \to \pm\infty$, its finite & $\frac{d\psi}{dx}$ is also continuous. and its continuous &

here $\psi^*\psi = 9\sin^2\pi x$

$= 9\int_{-\infty}^{\infty} \sin^2 \pi x \, dx$

$= 9\int_{-\infty}^{\infty} \frac{1}{2}(1-\cos 2\pi x)\, dx$

$= 9\left[\frac{1}{2}x\right]_{-\infty}^{\infty} + \frac{9}{2}\left[\frac{-\sin 2\pi x}{2\pi}\right]_{-\infty}^{\infty}$

$= \infty$

This is an acceptable wave fⁿ for a limited range of x.

(8) Which of the following f^n is acceptable wave f^n?

(1) $\phi_{(x)} = A \tan x$, (II) $\phi_{(x)} = B \cos x$, B is real,

(3) $\phi_{(x)} = C \exp\left(\frac{-D}{x^2}\right) : C > 0,\ D < 0$.

(4) $\phi_{(x)} = E e^{-Fx^2}$ $E, F > 0$.

Sol^n (1) Since the value of $\tan(\pi/2)$ [at $x = \pi/2, 3\pi/2, 5\pi/2$] is infinite. and $x = 0 \leq x \leq \infty$. Therefore $\phi_{(x)}$ will also be infinite. i.e. $A \tan x$ is not acceptable.

(2) (1) Its single valued.

(2) It's finit & continuous and also differentiable

(3) $|\psi| = B^2 \int_{-\infty}^{\infty} \cos^2 x\, dx \Rightarrow |\psi| = B^2 \int_{-\infty}^{\infty} \frac{1}{2}(1 + \cos 2x)\, dx$

It will be acceptable, if we lower the range.

$\cos 2x = 2\cos^2 x - 1$
$\Rightarrow \cos^2 x = \frac{1 + \cos 2x}{2}$

(4) $\phi_{(x)} = E e^{-Fx^2}$ $E, F > 0$,

if $e^{-Fx^2} = e^{-\infty} = \frac{1}{e^{\infty}} = \frac{1}{\infty} \to 0$,

it's acceptable at $\frac{1}{\infty} \to 0$

Now, $= E \int_{-\infty}^{\infty} \phi^* \phi\, dx$

$= E^2 \int_{-\infty}^{\infty} e^{-2Fx^2}\, dx$

$= E^2\, 2 \int_{0}^{\infty} e^{-2Fx^2}\, dx$

let $2Fx^2 = t$, $x = \sqrt{\ }$
$\Rightarrow 4Fx\, dx = dt$
$\Rightarrow dx = \frac{dt}{4F} \left(\frac{2F}{t}\right)^{-1/2}$
$= \left(\frac{2F}{t}\right)^{-1/2} \frac{dt}{4F}$
$= \frac{t^{-1/2}\, dt}{2\sqrt{2}\sqrt{F}}$

putting value →

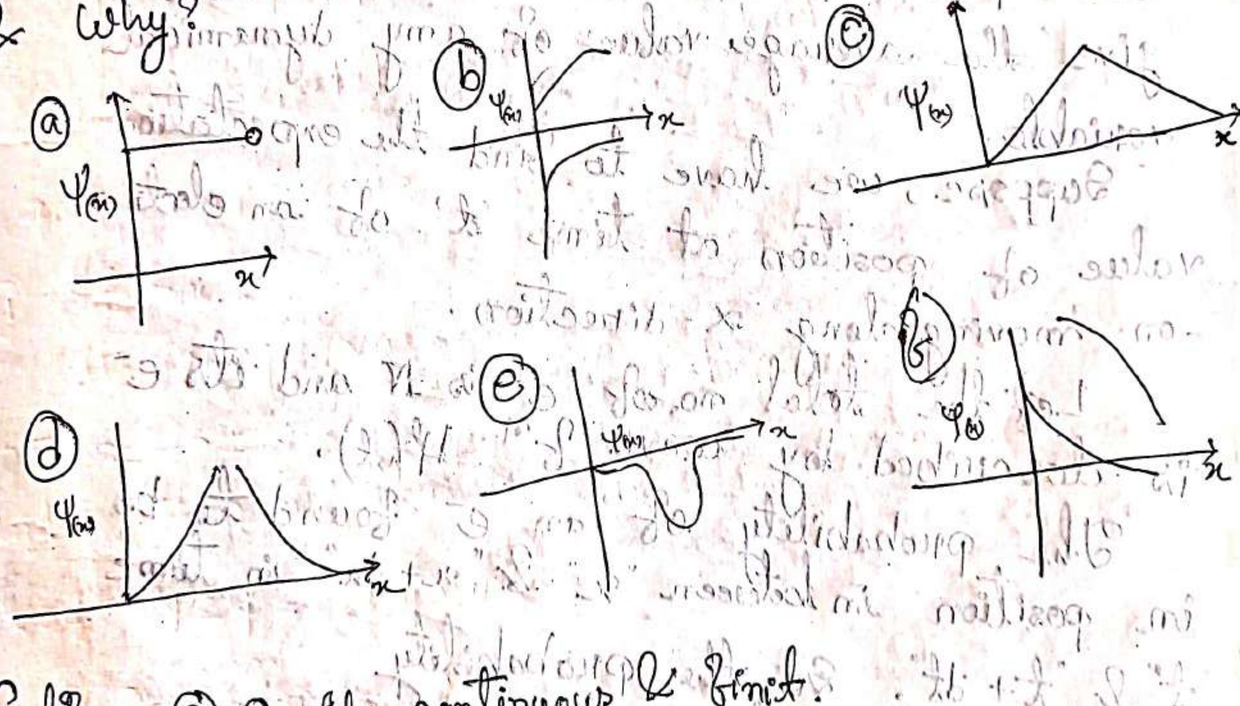
$$= E^2\, 2 \int_0^\infty e^{-t}\, \frac{t^{-1/2}}{2\sqrt{2}\sqrt{F}}\, dt$$

$$= \frac{E^2 \cancel{2}}{\cancel{2}\sqrt{2}\sqrt{F}} \int_0^\infty e^{-t}\, t^{\frac{1}{2}-1}\, dt$$

$$= \frac{E^2}{\sqrt{2}\sqrt{F}}\, \cancel{\int_0^\infty}\, \Gamma\tfrac{1}{2}$$

$$= \frac{E^2\sqrt{\pi}}{\sqrt{2F}}$$ It's an acceptable wave function.

② Which of the wave f^n shown in figure can have physical significance in the interval shown below & why?



<u>Sol^n:-</u> ⓐ ① It's continuous & finite.

② It's single valued.

③ $|\psi_{(x)}|^2$ is also finite.

It's acceptable.

ⓑ It's not single valued, it has not any significant not acceptable.

(c) not acceptable, $\frac{d\psi}{dx}$ discontinuous.

(d) not continuous.

(e) It's acceptable.

(f) not continuous.

(A) Expectation value :-

The wave fn $\psi_{(x,t)}$ is related to the probab interpretation and therefore it is essential to calculate the average value of any dynamical vari from the wave fn $\psi_{(x)}$. Dynamical variable means position momentum & energy of the system. The expectation value of a wave fn will give the average value of any dynamical variable.

Suppose, we have to find the expectation value of position at time 't' of an electron moving along x-direction.

Let the total no. of e^- is N and its e^- is described by wave fn $\psi(x,t)$.

The probability of an e^- found to be in position in between "x" & "x+dx" in time "t" & "t+dt". So the probability

$$P = \frac{\text{no of } e^- \text{ between } x \,\&\, x+dx}{N \text{ (total no. } e^-)}$$

Again in term of quantum wave mechanical the probability of finding e^- betn "x" & "x+dx".

So $\Rightarrow P(dx) = \psi^*_{(x,t)} \psi_{(x,t)}\, dx$.

The no electrons between "x" & "x + dx"

i.e. $dN = N \psi^*_{(x,t)} \psi_{(x,t)} \, dx$.

Now if $x_1, x_2, x_3, \ldots, x_N$ are the measured value of position of all the electrons then,

$$x_1 + x_2 + x_3 + \cdots + x_N = \int_{-\infty}^{\infty} x \left(N \psi^*_{(x,t)} \psi_{(x,t)} \right) dx$$

$$\Rightarrow \frac{x_1 + x_2 + x_3 + \cdots + x_N}{N} = \int_{-\infty}^{\infty} x \left(\psi^*_{(x,t)} \psi_{(x,t)} \right) dx$$

$$\Rightarrow \langle x \rangle = \int_{-\infty}^{\infty} \psi^*_{(x,t)} \hat{x} \, \psi_{(x,t)} \, dx$$, Where $\langle x \rangle$ is average of x, and $\hat{x} = x$

It's the expectation value of position.

⇒ The expectation value of position will be given by $\int_{-\infty}^{\infty} \psi^*_{(x,t)} \hat{x} \, \psi_{(x,t)} \, dx$, if the function $\psi_{(x,t)}$ is normalized.

If the f^n $\psi_{(x,t)}$ is not normalized then the expectation value of the position will be given by $\Rightarrow \langle x \rangle = \dfrac{\int_{-\infty}^{\infty} \psi^*_{(x,t)} \psi_{(x,t)} \, dx}{\int_{-\infty}^{\infty} \psi^*_{(x,t)} \psi_{(x,t)} \, dx}$

(A) Expectation value of momentum $(\hat{P}_x)$:-

$$\Rightarrow \langle P_x \rangle = \int_{-\infty}^{\infty} \psi^*_{(x,t)} \hat{P}_x \psi_{(x,t)} \, dx$$

$$= \int_{-\infty}^{\infty} \psi^*_{(x,t)} \left(-i\hbar \frac{\partial}{\partial x} \right) \psi_{(x,t)} \, dx$$

$$\Rightarrow \langle P_x \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*_{(x,t)} \frac{\partial}{\partial x} \psi_{(x,t)} \, dx.$$

This is the expectation value of momentum $\hat{P}_x$.

P.T.O.

(8) Calculate the expectation value of momentum for the wave f^n $\psi_{(x)} = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$, $0<x<L$

(2) $= 0$, otherwise.

Sol^n :- $\psi_{(x)} = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$

$$\psi^*_{(x)} = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$$

$$\Rightarrow \langle P_x \rangle = \int_0^L \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \cdot \hat{P}_x \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\, dx$$

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

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

$$= -i\hbar \frac{2}{L} \cdot \frac{\pi}{L} \int_0^L \sin\frac{\pi x}{L} \cos\frac{\pi x}{L}\, dx$$

$$= -i\hbar \frac{\pi}{L^2} \int_0^L 2\sin\frac{\pi x}{L} \cos\frac{\pi x}{L}\, dx$$

$$= -i\hbar \frac{\pi}{L^2} \int_0^L \sin\frac{2\pi x}{L}\, dx$$

$$= -i\hbar \frac{\pi}{L^2} \left[\frac{-\cos\frac{2\pi x}{L}}{\frac{2\pi}{L}}\right]_0^L$$

$$= -i\hbar \frac{\pi}{L^2} \times \frac{L}{2\pi} \cdot \left[-\cos 2\pi + \cos 0\right]$$

$$\Rightarrow \langle P_x \rangle = \frac{-i\hbar}{2} \left[-1+1\right]$$

$$\Rightarrow \langle P_x \rangle = 0$$

Sol:
(2) $\langle P_x^2 \rangle = \int_0^L \psi_{(x,t)}^* \hat{p}_x^2 \psi_{(x,t)} dx$

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

$$= -\frac{\hbar^2 2}{L} \int_0^L \sin\frac{\pi x}{L} \frac{\partial}{\partial x} \frac{\pi}{L} \cdot \cos\frac{\pi x}{L} \, dx$$

$$= -\hbar^2 \frac{2}{L} \cdot \frac{\pi}{L} \int_0^L \sin\frac{\pi x}{L} \left(-\sin\frac{\pi x}{L}\right) dx.$$

$$= -\hbar^2 \frac{2\pi}{L^2} \int_0^L -\sin^2\frac{\pi x}{L} \, dx$$

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

$$= \hbar^2 \frac{2\pi}{L^2} \left[\frac{1}{2} L - \left(\cos\frac{2\pi x}{L}\right)_0^L \cdot \frac{L}{2\pi}\right]$$

$$= \hbar^2 \frac{2\pi}{L^2} \times \frac{L}{2\pi} \left[\frac{L}{2} - (\cos 2\pi - \cos 0)\right]$$

$$= \frac{\hbar^2}{L}\left(\frac{L}{2} - (1-1)\right)$$

$$\Rightarrow \langle P_x^2 \rangle = 0$$

(4) Expectation value of K.E. :-

Since $\langle E_K \rangle = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$.

$$\Rightarrow \langle E_K \rangle = \int_{-\infty}^{\infty} \psi_{(x,t)}^* \hat{E} \psi_{(x,t)} dx.$$

$$= \int_{-\infty}^{\infty} \psi_{(x,t)}^* \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{(x,t)} dx.$$

$$= \frac{-\hbar^2}{2m} \int_{-\infty}^{\infty} \psi_{(x,t)}^* \frac{\partial^2 \psi_{(x,t)}}{\partial x^2} dx.$$

$$\Rightarrow \langle E_k \rangle = \frac{-\hbar^2}{2m}\left\{\left[\psi^*_{(x,t)} \frac{\partial \psi}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\frac{\partial \psi^*_{(x,t)}}{\partial x}\int\frac{\partial \psi}{\partial x}\right) dx\right\}$$

as $\psi^*_{(x,t)} \rightarrow 0$ at $x \rightarrow \pm\infty$

$$\langle E_K \rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}\, dx$$

$$\boxed{\Rightarrow \langle E_k \rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left|\frac{\partial \psi}{\partial x}\right|^2 dx}$$

Expectation value of Energy :-

$$\langle E \rangle = \int_{-\infty}^{\infty}\psi^*_{n(x,t)}\,\hat{E}\,\psi_{n(x,t)}\, d\tau$$

Schrodinger eqn of time dependent part

$$\psi_{(x,t)} = \psi_n(x,t)\, e^{-\frac{iE_n t}{\hbar}}$$

$$\Rightarrow \langle E \rangle = \int_{-\infty}^{\infty}\psi^*_{n(x,t)}\, -i\hbar\, e^{-\frac{iE_n t}{\hbar}}\, \psi_{(x,t)}\, d\tau$$

$$= \int_{-\infty}^{\infty}\psi^*_{n(x,t)}\, e^{i\frac{E_n}{\hbar}t}\, i\hbar\frac{\partial}{\partial t}\psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}\, d\tau$$

$$\Rightarrow \langle E \rangle = i\hbar\int_{-\infty}^{\infty}\psi_{n(x)}\, e^{i\frac{E_n}{\hbar}t}\, \psi_{n(x)}\, e^{-i\frac{E_n}{\hbar}t} \cdot -i\frac{E_n}{\hbar}t$$

$$\Rightarrow \langle E \rangle = i\hbar \times \frac{-iE_n}{\hbar}\int_{-\infty}^{\infty}\psi^*_{n(x)}\,\psi_{n(x)}\, d\tau = 1$$

If ψ_n is normalised then $\langle E \rangle = E_n$

Ehrenfest's theorem :-

This theorem gives the correspondence between the motion of a classical particle & the motion of a wave packet which is associated with the particle.

In the limit when the wave packet associated with the particle reduces to a point, the particle is expected to behave like classical one.

Expectation value of position $\langle x \rangle = -\infty$ to $+\infty$.

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx \quad \text{--- (1)}$$

$$\Rightarrow \frac{d\langle x \rangle}{dt} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx$$

$$= \int_{-\infty}^{\infty} \left(\psi^* x \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} x \psi \right) dx \quad \text{--- (2)}$$

Only for ψ

$$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{(x)} \right] \psi$$

from ψ^*

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{(x)} \right] \psi^*$$

Using this two eq^n we get and eq^n (1) become

$$\Rightarrow \frac{d\langle x \rangle}{dt} = \frac{-i\hbar}{2m} \int_{-\infty}^{\infty} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx \quad \text{--- (3)}$$

$$\Rightarrow \int_{-\infty}^{\infty} \psi \frac{\partial \psi^*}{\partial x} \, dx = -\int_{-\infty}^{\infty} \psi \frac{\partial \psi}{\partial x} + \int_{-\infty}^{\infty} \psi^* \psi \, dx.$$

Now Using property —

$$\frac{d}{dx}(fg) = g\frac{df}{dx} + f\frac{dg}{dx}$$

$$\Rightarrow f\frac{dg}{dx} = -g\frac{df}{dx} + \frac{d}{dx}(fg)$$

$$\Rightarrow \int_a^b f\frac{dg}{dx} = -\int_a^b g\frac{df}{dx} + fg\Big]_a^b$$

$$\therefore \Rightarrow \int_{-\infty}^{\infty} \psi \frac{\partial \psi^*}{\partial x} dx = -\int_{-\infty}^{\infty} \psi \frac{\partial \psi}{\partial x} + \int_{-\infty}^{\infty} \psi^* \psi \, dx$$

Since $x \to \pm\infty$, $\psi^*\psi \to 0$.

eq^n (3) Can be simplyfy using the above property as above eq^n and for localised wave packet. i.e. ψ & $\psi^* \to 0$ at $x \to \pm\infty$

$$\therefore \frac{d\langle x\rangle}{dt} = \frac{-i\hbar}{m}\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \frac{1}{m}\int_{-\infty}^{\infty} \psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\psi \, dx$$

$$\Rightarrow m\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} \psi^* \hat{P}_x \psi \, dx$$

Here the right hand part is nothing but expectation value of $\langle \hat{P}_x \rangle$. i.e. In the limit wave packet reduces to a point expectation value becomes $\langle x\rangle = x$ then $\langle P_x \rangle = P_x$ and the particle follows the classical eq^n —

$$m\frac{dx}{dt} = P_x$$