

QUANTUM MECHANICS

CHAPTER I

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Q.1 What is De-Broglie hypothesis? Prove it from the analogy of radiation. (4)

Ans (I) According to De-Broglie's hypothesis, if a material particle of mass m is moving with velocity v , then the wavelength (λ) associated with it is given by

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

where h , plank's constant

$f p = mv \rightarrow$ momentum of particle,

(II) Proof

① For radiation, energy of photon is given by

$$E = h\nu = hc \quad (\nu = c/\lambda) \rightarrow ①$$

h → plank's constant

ν → frequency of radiation

λ → wavelength of radiation

$f c$ → Velocity of light.

② According to Einstein's mass-energy relation, energy of photon is

$$E = mc^2$$

→ ②

m → mass of photon.

③ equating ① + ②

$$hc = mc^2$$

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

where $p = mv$ = momentum of particle

(2)

Q Using the analogy from radiation, De-Broglie proposed that if instead of photon, it is a material particle moving with velocity v , then the wavelength λ associated with it

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

where $p = mv$ = momentum of particle

Q. 2 What is De-Broglie's hypothesis? Express it in terms of kinetic energy ($K.E.$).

Ans (I) \rightarrow same.

$$(II) \quad \lambda = \frac{h}{mv} = \frac{h}{P} \quad (1)$$

K.E. of the particle is

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

$$= \frac{1}{2m}(m^2v^2)$$

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

$$P = \sqrt{2mE} \quad (2)$$

(III)

(2) in (1) gives

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

$$V \rightarrow \text{vel} \\ V \rightarrow \text{pot}$$

(3)

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(B)

Q. 3 → state De-Broglie's hypothesis of matter wave? (OR) Explain wave nature of matter. Show that the de-Broglie wavelength of a charged particle is inversely proportional to the square root of the accelerating potential. Comment on its significance.

Ans (I)

same

$$\lambda = \frac{h}{mv} = \frac{h}{p} \quad (1)$$

(II)

Let us consider a charged particle (e^-) of velocity v accelerated through a potential difference of V volts, then the K.E. gained by it is given by

$$\boxed{\frac{1}{2}mv^2 = eV} \quad (2)$$

$m \rightarrow$ mass of the particle

$v \rightarrow$ velocity

$e \rightarrow$ charge of the particle

$\therefore V \rightarrow$ accelerating voltage

From (2)

$$v = \sqrt{\frac{2eV}{m}}$$

$$\therefore \lambda = \frac{h}{mv} = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{m\sqrt{2eV}}$$

$$\therefore \lambda = \frac{h}{\sqrt{2meV}} \quad (3)$$

(III)

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

Hence proved.

(III)

Significance.

(W) varying accelerating potential V , have matter waves of various wave lengths. Higher the potential V , lower will be the De-Broglie wavelength.

Q.4 → Express De-Broglie wavelength of an electron in terms of accelerating potential V .

Ans. (II) → same. $\frac{1}{2}mv^2 = eV \quad \text{--- (1)}$

$$\gamma = \frac{h}{\sqrt{2meV}} \quad \text{--- (2)}$$

Taking $m = m_0$ (rest mass)

$$\gamma = \frac{h}{\sqrt{2m_0eV}} \quad \text{--- (2)}$$

h , m_0 and e are universal constants.

$$h = 6.625 \times 10^{-34} \text{ J-S}$$

$$m_0 = 9.1 \times 10^{-31} \text{ kg} \quad (\text{mass of } e^-)$$

$$e = 1.6 \times 10^{-19} \text{ C} \quad (\text{charge of } e^-)$$

(III) substituting in (2)

$$\gamma = 6.62 \times 10^{-34}$$

$$\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times V}$$

$$= 12.27 \times 10^{-10} \text{ meters}$$

$$\boxed{\gamma = \frac{12.27}{\sqrt{V}} \text{ A}^\circ}$$

Q. 5 What is the difference between group velocity and group velocity? Show that De-Broglie wave group associated with moving particle travels with the same velocity as the particle.

Ans (1) As per De-Broglie's hypothesis a material particle of mass m , moving with velocity v is associated with a monochromatic wave of wavelength λ moving with velocity v_p called phase velocity.

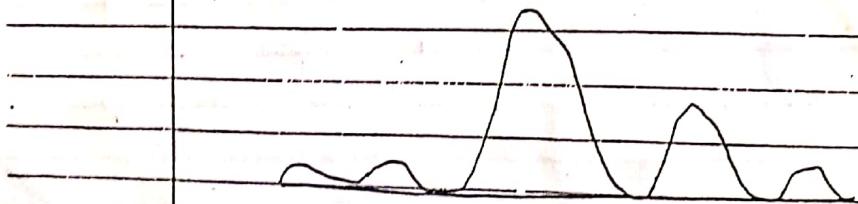
This creates two problems:

(2) How can a wave which spreads out over a large region of space represents particle?

(3) How velocity of the wave (phase velocity) v_p comes to be greater than velocity of light c .

(3) The above problem can be solved by considering wave packet or group of waves associated with the particle. The velocity with which of the wave group is called as group velocity (v_g)

(4) Wave group (or wave packet) can be obtained by interference of many waves of different frequencies and amplitudes so that resultant has a high value of amplitude near the vicinity of the particle. This wave packet moves with the velocity of the particle.



(5) To show, $v_g = v_p$.

Let the two waves of equal amplitudes and different angular frequencies w_1 & w_2 and propagation constant k_1 and k_2

are represented by

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

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

Resultant is

$$y = y_1 + y_2$$

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

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

$$+ \sin \left[\frac{(\omega_1 + \omega_2)t}{2} \right] - \frac{(k_1 + k_2)x}{2} \right\}$$

$$(\sin A + \sin B = 2 \sin \frac{A+B}{2} \cos \frac{A-B}{2})$$

comparing with

$$y = A \sin(\omega t - kx)$$

resultant amplitude

$$A = 2a \cos \left[\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2} \right]$$

Amplitude of wave group is modulated both in space (x) and time (t) and its velocity

$$\boxed{\frac{v_g}{v_p} = \frac{(\omega_1 - \omega_2)}{(k_1 - k_2)} = \frac{dw}{dk}} \quad (v = w/k)$$

→ To show $v_g = v_p$, consider K.E

$$V_g = \frac{dE}{dp} = \frac{dE}{dp} \cdot \frac{c^2}{E} = c^2 \cdot \frac{1}{E} \quad (E = p^2/c^2)$$

$$E = \frac{1}{2} mv^2 = \frac{1}{2m} (m^2 v^2) = \frac{p^2}{2m}$$

$$V_g = \frac{dE}{dp}$$

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

then
Hence

$$F = \frac{p^2}{2m} \quad (P \rightarrow \text{momentum of particle})$$

$$\frac{dE}{dp} = V$$

$$L = n \cdot \omega$$

$$= \frac{h \cdot \omega}{2\pi}$$

$$E = \hbar \omega$$

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

According to De-Broglie wavelength

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

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

$$= \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda}$$

$$P = \hbar \cdot k$$

(3)

(3) in (1) \Rightarrow

$$E = \frac{\hbar^2 k^2}{2m}$$

(4)

$$(2) \Rightarrow E = \hbar \omega$$

$$\text{i} i \quad \hbar \omega = \frac{\hbar^2 k^2}{2m}$$

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

$$\frac{d\omega}{dk} = \frac{\hbar}{2m} (2k)$$

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

$$\text{From (3)} \quad \frac{d\omega}{dk} = \frac{P}{m}$$

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

$$v_g = v$$

Hence proved.

- Q.6 Discuss the properties of matter waves. (4)
 Ans Matter waves are generated by a moving particle. The wavelength is

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

where $m \rightarrow$ mass of particle
 $v \rightarrow$ velocity of the particle

Properties are

- ① $\lambda \propto \frac{1}{m}$, hence lighter the particle, greater is the wavelength.
- ② $\lambda \propto \frac{1}{v}$, smaller the velocity, greater will be the wavelength associated.
- ③ As $v \rightarrow \infty$, $\lambda \rightarrow 0$
- ④ As $v \rightarrow 0$, $\lambda \rightarrow \infty$ which means no wave is associated. For wave to be associated, particle must be in motion.
- ⑤ Matter waves do not depend on the charge of the particle. Particle can be charged or uncharged, but in motion.
- ⑥ Velocity of matter wave is not constant but depends on the velocity of particle generating them.

$$V_p = \frac{c^2}{v}$$

- ⑦ Matter waves are waves of probability.

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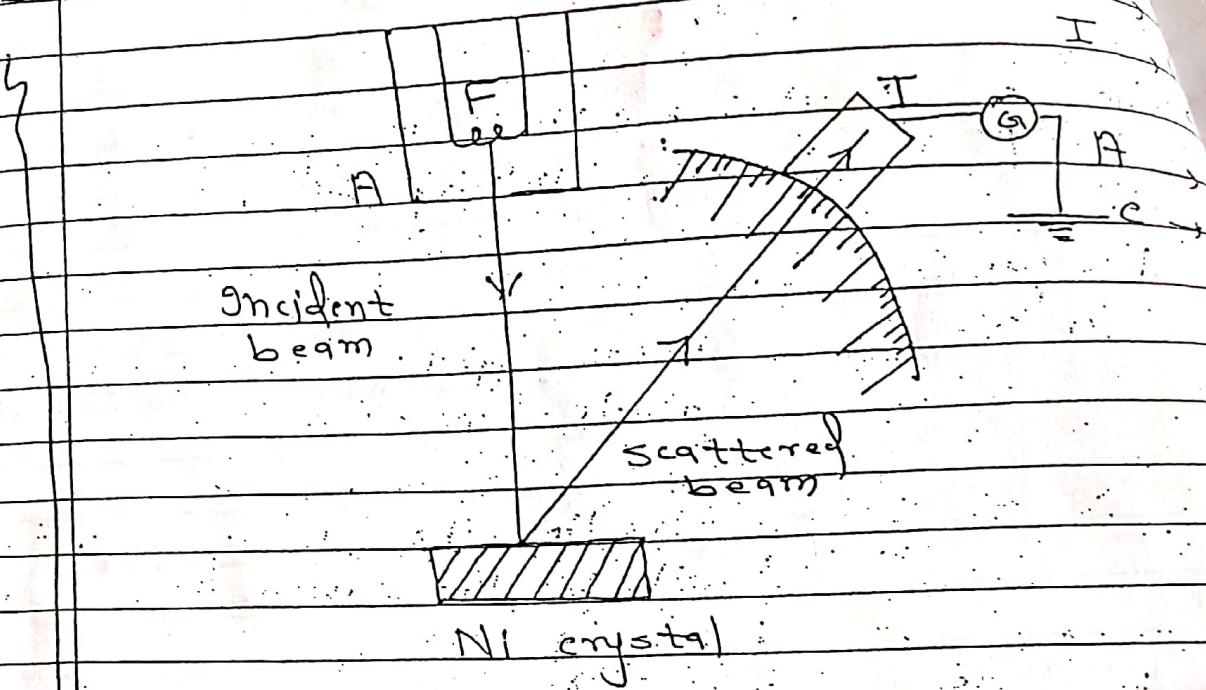
- (1) $\lambda \propto \frac{1}{m}$, hence lighter the particle, greater is the wavelength
- (2) $\lambda \propto \frac{1}{v}$, smaller the velocity, greater will be the wavelength associated
- (3) As $v \rightarrow \infty$, $\lambda \rightarrow 0$
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$$V_p = \frac{c^2}{v}$$

- (7) Matter waves are waves of probability.

Q.7. Describe Davisson and Germer's experiment in support of De-Broglie's hypothesis.

Ans.



Davisson and Germer performed an experiment on electron diffraction to prove wave nature of electrons. Two important factors are:

- ① It gives evidence for De-Broglie's hypothesis of matter waves.
- ② With this experiment it helps to determine the wavelength of electrons.

EXPERIMENT

- ① It consists of filament F surrounded by an anode A with a small opening through which electrons are emitted.
- ② A Ni crystal is used to scatter the electrons which has an inter-atomic distance of 2.15 Å units.
- ③ An ionisation chamber (I) is used to measure intensity of scattered electrons in different

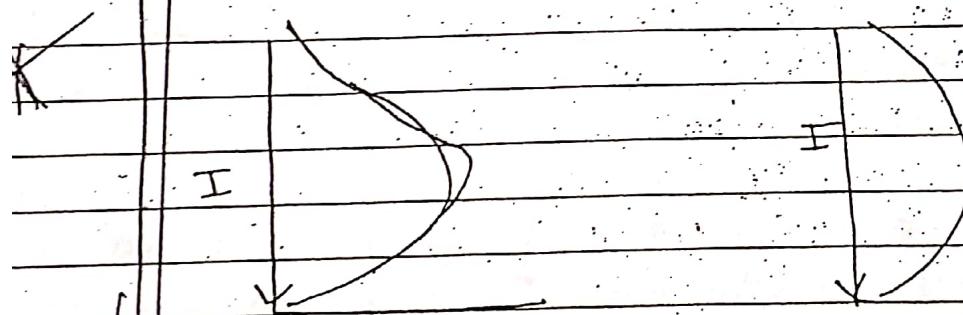
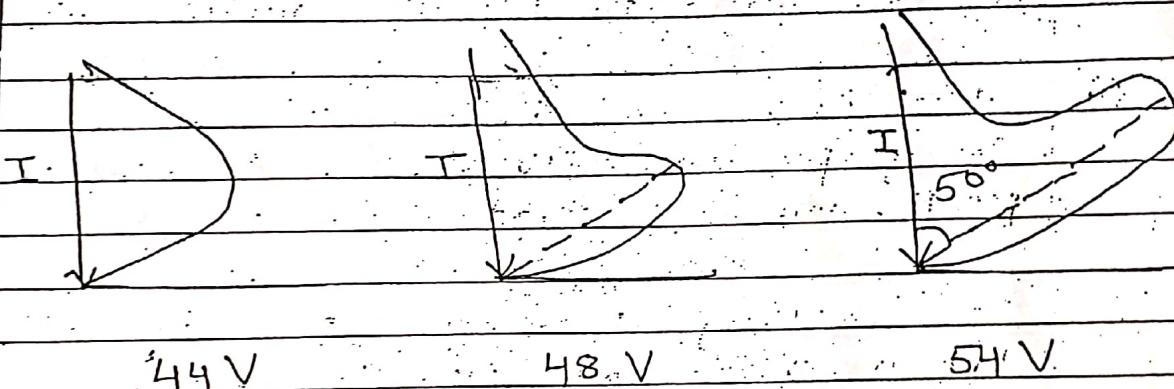
(11)

directions which moves on a circular scale.
(I is connected to sensitive galvanometer)

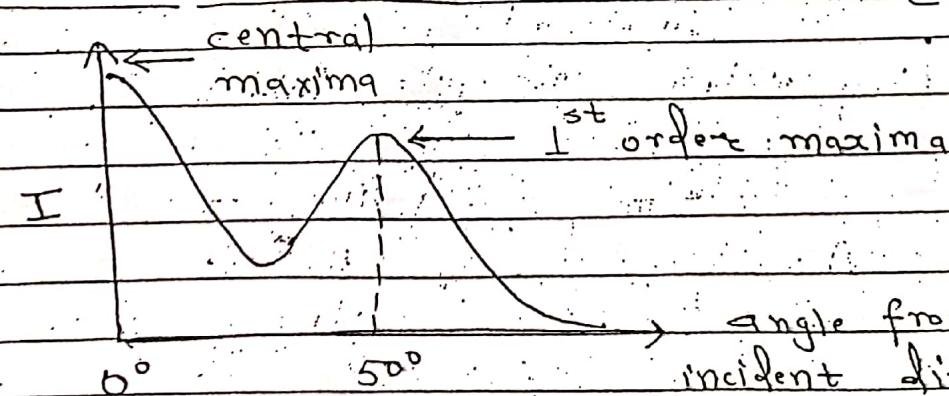
(4) The intensity I of the scattered beam is noted for various positions θ for a particular voltage V.

(5) Polar graphs between Intensity and θ for various voltages are plotted as shown.

OBSERVATIONS



[fig(9)]



[Graph for 54 V anode potential] (fig 5)

OBSERVATIONS

- (1) For 44 V anode potential, the intensity was maximum near the incident direction and gradually decreased to 0 near 90° .
- (2) For 48 V, intensity was maximum near incident dirn which decreased and slightly increased again near 50° .
- (3) The intensity of 1st order maximum found to be pronounced for anode potential of 54 V at an angle of 50° to incident direction.
- (4) For 60 V and 64 V variation were similar to graph for 48 V of 44 V. intensity peak was not that prominent.

Setting accelerating potential at 54 V, the intensity of diffracted electron beam was measured for different positions of the ionisation chamber and a graph was plotted as shown in fig(b).

Pattern is similar to diffraction pattern. Ni crystal acts as diffraction grating. Since e⁻s can be diffracted, they must have De-Broglie's waves associated with it.

SUPPORT TO DE-BROGLIE'S HYPOTHESIS.

Wavelength of e⁻ wave can be found by using Bragg's law.

$$\text{Using } 2d \sin\theta = n\lambda$$

where $d \rightarrow$ interplanar distance

$\theta \rightarrow$ glancing angle

$n \rightarrow$ order of spectrum.

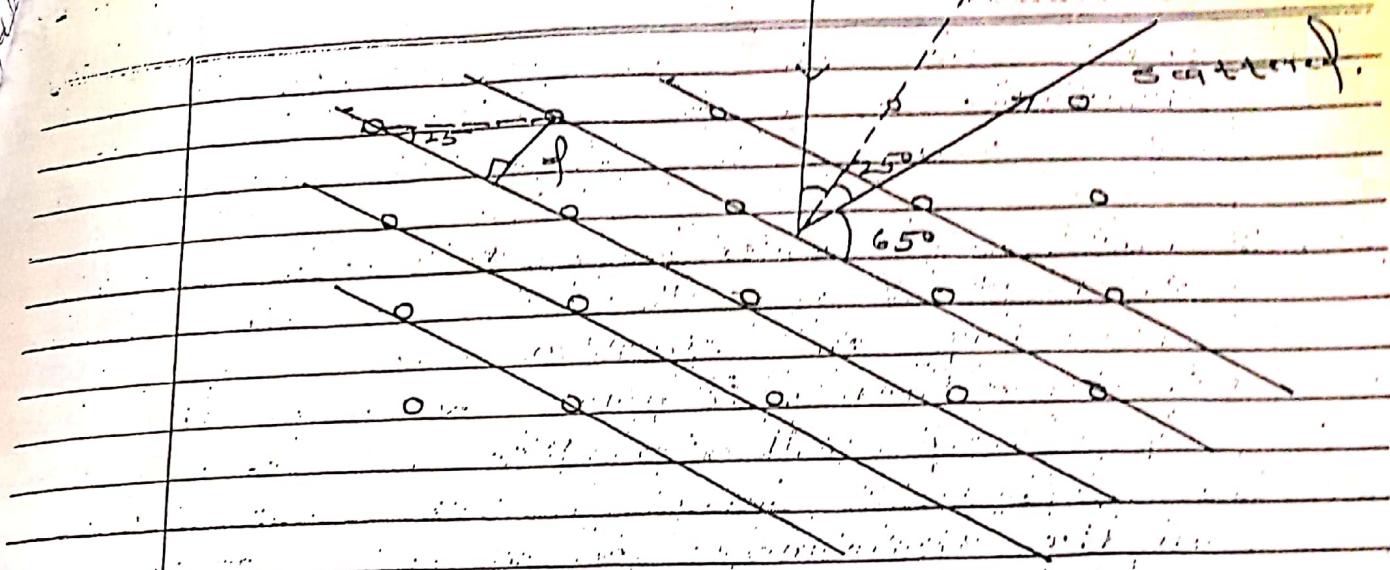


Fig (c)

Amooth

In this case

$$n = 1$$

$$\alpha = 65^\circ \quad (\text{fig c})$$

$$q d = q \sin 65^\circ \pm$$

$$= \frac{215}{0.91} \times 10^{-10} \text{ m} \sin 65^\circ$$

Substituting all these values, in

$$n \lambda = 2d \sin \alpha$$

$$\lambda = 1.65 \text{ \AA}$$

exp

As per De-Broglie's hypothesis

$$\lambda = 12.27 \text{ \AA}$$

hyp

$$= 12.27 \text{ \AA}$$

$$\lambda_{\text{hyp}} = 1.66 \text{ \AA}$$

There is excellent agreement which conf

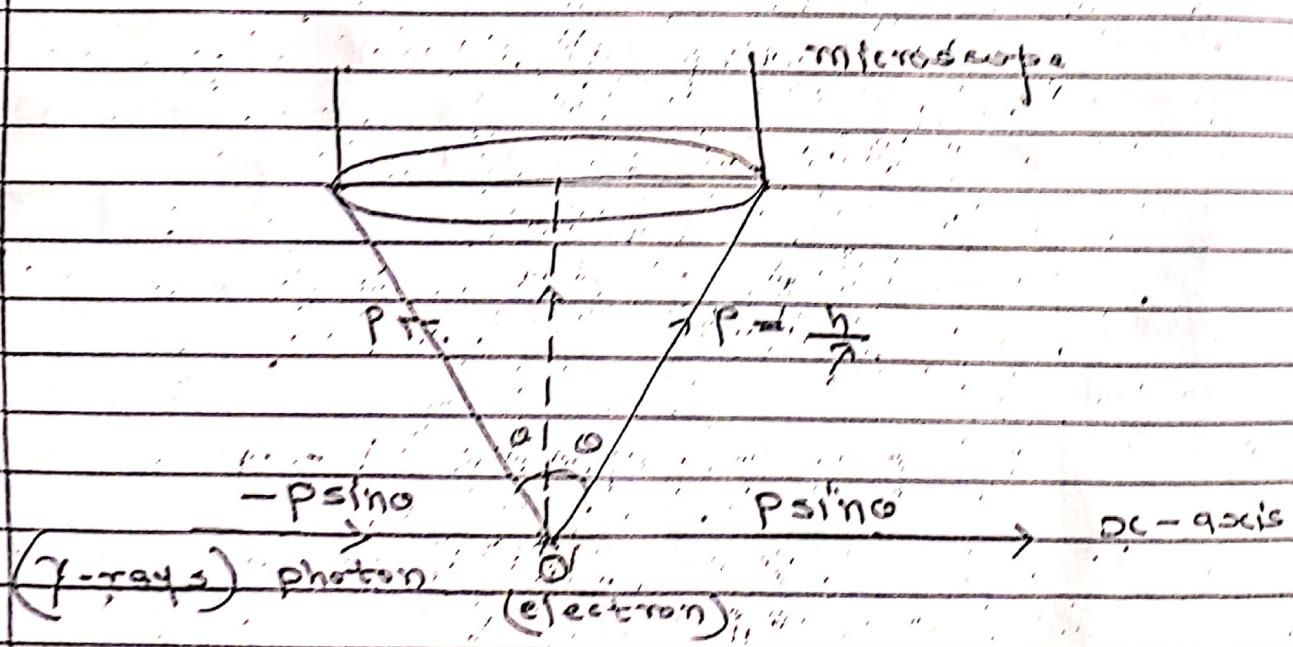
(iv) State Heisenberg's uncertainty principle
Illustrate it by an experiment on an electron by γ -ray scattering.

Ans: Heisenberg's uncertainty principle states that it is impossible to determine accurately and simultaneously the exact position and momentum of a particle of a very small size like an electron. There is always certain uncertainty in the simultaneous measurement of position and momentum of a particle in motion.

$$\text{I. } \Delta x \Delta p \geq h$$

Where $\Delta x \rightarrow$ uncertainty in the position
 $\Delta p \rightarrow$ uncertainty in momentum
 $h \rightarrow$ Planck's constant.

(ii) Illustration of an experiment on an electron by γ -ray scattering.



(scattering of photon by an electron)

- ① Consider an e^- moving along positive x direction. Let it is at point O at time t . At t is illuminated by a γ -ray photon of wavelength λ .
- ② Let α is semivertical angle of the cone of light entering the microscope lens.
- ③ The electron can be observed if atleast one photon scattered enter in the range of microscope.

④ The range

$$\Delta x = \frac{\lambda}{2 \sin \alpha} \quad ①$$

- ⑤ Hence uncertainty in the measurement of position of the electron is Δx , given by eqn ①

- ⑥ initial momentum of photon $= p = \frac{h}{\lambda}$

- ⑦ After scattering it enters the microscope anywhere within the angle 2α , as shown.

- ⑧ The x -component of momentum of scattered photon may be between $+ps \sin \alpha$ and $-ps \sin \alpha$. Hence uncertainty in the measurement of momentum

$$\Delta p = [p \sin \alpha - (-p \sin \alpha)]$$

$$= 2p \sin \alpha$$

$$\Delta p = 2 \frac{h}{\lambda} \sin \alpha \rightarrow ②$$

From ① & ②

$$\Delta x \Delta p = \frac{\lambda}{2 \sin \alpha} \cdot 2 \frac{h \sin \alpha}{\lambda}$$

Q.9 State Heisenberg's uncertainty principle
Illustrate it by an experiment of diffraction at a single slit.

Ans(I) Heisenberg's uncertainty principle states that it is impossible to determine accurately and simultaneously the exact position and momentum of a moving particle of a very small size like an electron.

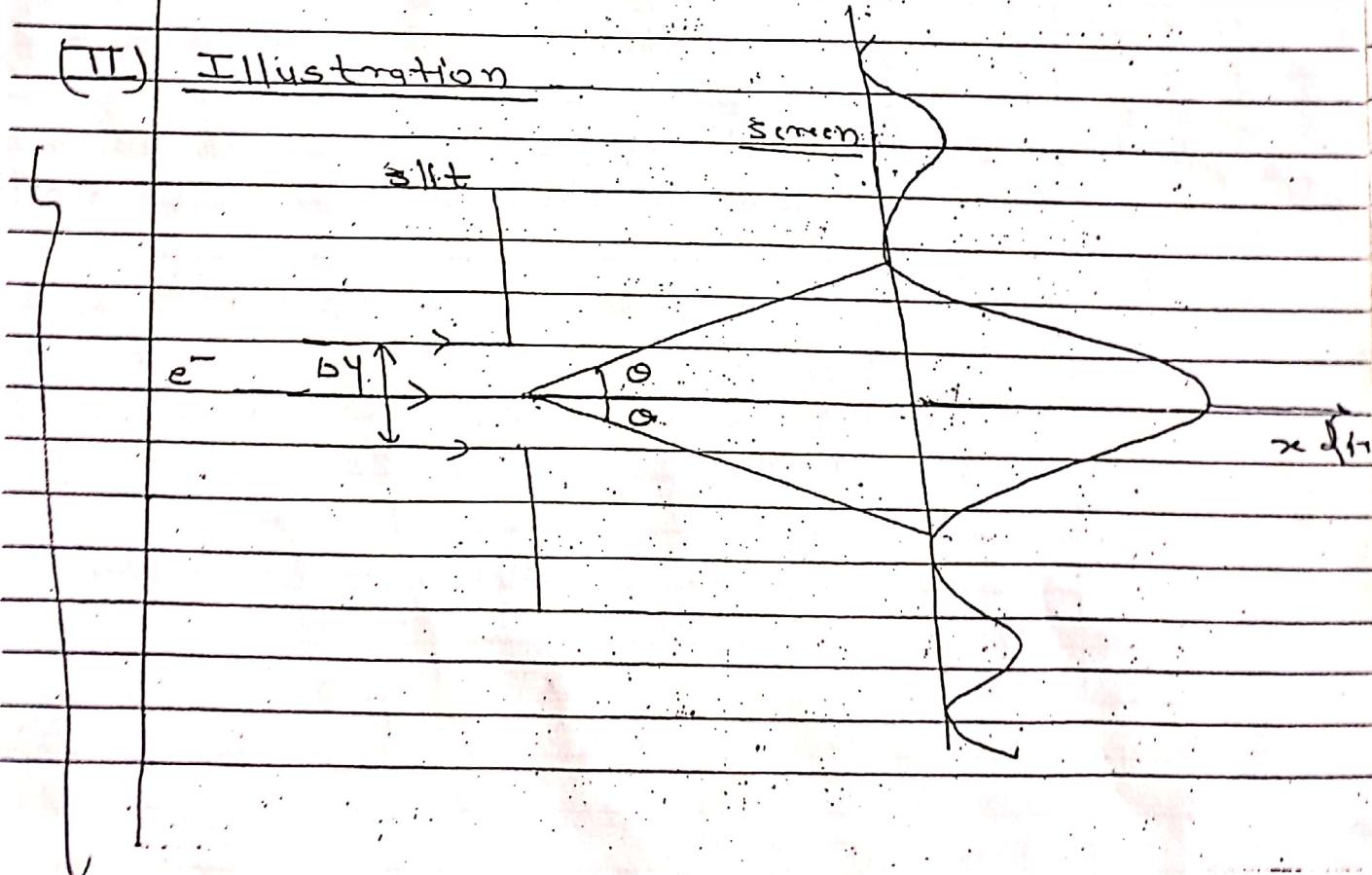
OR

There is always certain uncertainty in the simultaneous measurement of position and momentum of a moving particle on the atomic scale, and

$$\Delta x \cdot \Delta p \geq h$$

Where Δx \rightarrow Uncertainty in the measurement of position
 Δp \rightarrow Uncertainty in momentum
 h \rightarrow Planck's constant.

(II) Illustration



① A beam of electron moving along x -axis and passing through a vertical narrow slit of width Δy . A diffraction pattern is produced on the screen as shown.

② Let the 1st order minima be produced at angle α .

③ Applying minima cond'n for diffraction at a single slit we get

$$a \sin \alpha = n \lambda \quad a \rightarrow \text{slit width.}$$

$$\Delta y \sin \alpha = 1 \times \lambda$$

④ electron can be anywhere in the range Δy . Hence uncertainty in the measurement of position of e^- is Δy , i.e.

$$\Delta y = \frac{\lambda}{\sin \alpha} \quad \textcircled{1}$$

⑤ Let $p = \frac{h}{\lambda}$ is the initial momentum of e^-

⑥ After diffraction at the slit, the electron deviates from the initial path and acquires y -component of momentum that lies between $ps \sin \alpha$ and $-ps \sin \alpha$.

Hence uncertainty Δp_y in the measurement of momentum will be

$$\Delta p_y = [ps \sin \alpha - (-ps \sin \alpha)]$$

$$= 2ps \sin \alpha$$

$$= 2 \cdot h \cdot \frac{\sin \alpha}{\lambda} \quad \textcircled{2}$$

From ① & ②

$$\Delta y \cdot \Delta p_y = \frac{\lambda}{\sin \alpha} \times 2h \sin \alpha$$

Distribution of photon by HVP $\propto \frac{1}{\sin \alpha}$
corresponds to diffraction of wave

there are 2 levels, one higher and one lower level. The two levels which are very close are so close.

Hence it is proved that

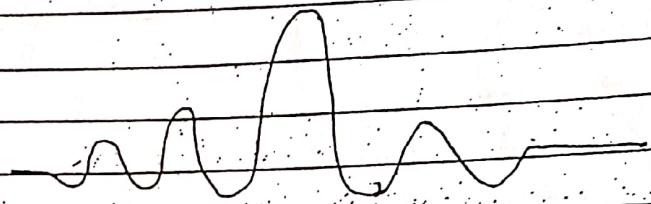
(Q10)

$$\Delta x \Delta p_x > h$$

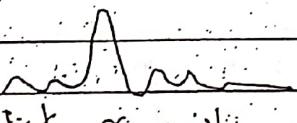
Q.10 What is Heisenberg's uncertainty principle? Give its proof for wave packet.

Ans(I) Same

(II) In wave mechanics a particle is described by a group of waves called a wave packet as shown.



① The particle can be located anywhere within the group at a given time. If the wave group is narrow as shown, particle position can be specified more accurately.



But the wavelength of the wave is not well defined.

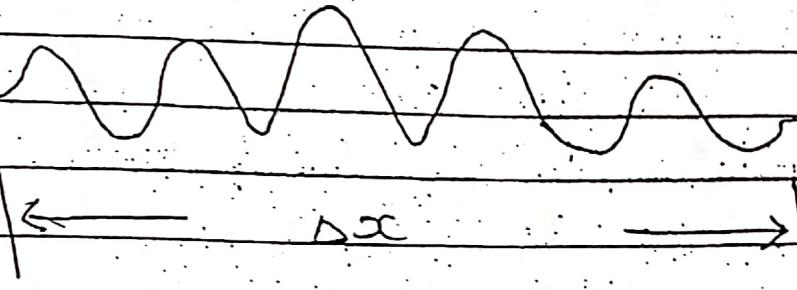
Because momentum is given by

$$p = \frac{h}{\lambda} \quad \text{it is also not}$$

well defined. Hence we can say if position of the particle is measured more accurately, momentum will be less accurate.

③

If a wave group is wider as shown



Where is exactly the particle located will be difficult to find. Hence Δx will be larger.

On the other hand, since λ is well defined, momentum $p = \frac{h}{\lambda}$ can be defined more accurately.

- ④ Hence it is concluded that it is not possible to determine exactly the position and momentum of a moving particle simultaneously.

are 2 ~~higher~~
one higher
level. which is
Q. 1 to explain the physical significance of

(20) Ans(1) The quantity whose variation make up waves is called the wave function ψ , get similar to electric and magnetic field vector case of light waves. ψ

(2) ψ gives info about the probability of finding the particle at a point (x, y, z) and time since probability can't be negative ($-ve$ prob. is meaningless), ψ alone doesn't have any physical significance. Hence

(3) probability $\propto |\psi|^2$

A large value of $|\psi|^2$ means a strong probability of finding the particle and a small value of $|\psi|^2$ means a little probability of existence of particle.

If $|\psi|^2 = 0$ means particle is absent.

(4) ψ may be a complex function having both real and imaginary parts.

$$\psi = A + iB$$

$$\text{Hence } \psi^* = A - iB$$

$$\psi \psi^* = A^2 + B^2 = |\psi|^2$$

(5) Since probability of finding the particle all over the space at all times is unity (100% chances),

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 1$$

(2) probability of finding the particle over limited region in general is

$$\int |\Psi|^2 dv = N^2$$

$$\cdot \int \Psi \Psi^* dv = N^2$$

$$\therefore \int \left(\frac{\Psi}{N}\right) \left(\frac{\Psi^*}{N}\right) dv = 1 = \int \Psi_N \Psi_N^* dv$$

where Ψ_N is called as normalised wave func

(6) Ψ should be normalised function.

(7) Ψ should be single valued func since probability of finding the particle is always single valued.

(8) Ψ must be finite everywhere in space

(9) Ψ and its derivatives are continuous everywhere.

(10) since Ψ is continuous, its derivatives

$\frac{\partial \Psi}{\partial x}$, $\frac{\partial \Psi}{\partial y}$, and $\frac{\partial \Psi}{\partial z}$ are continuous everywhere in space.

Wave function Ψ satisfying the cond's

(6) - (10) is called as well behaved function.

X Q. 2. Derive Schrodinger's time independent wave equation.

Ans(1) To describes behavior of matter wave in mathematical form Schrodinger derived a wave equation.

(2) Eqⁿ gives complete information about energy, momentum & position of the particle.

(3) Eqⁿ to simple harmonic wave moving along x dirn is

$$\frac{\partial^2 y}{\partial t^2} = \frac{v^2}{\partial x^2} \frac{\partial^2 y}{\partial x^2} \quad \text{where } y \rightarrow \text{displacement}$$

if $v \rightarrow$ velocity of wave.

(4) For a wave associated with a particle ~~which~~ can be written as

$$\frac{\partial^2 \psi}{\partial t^2} = U^2 \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right]$$

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

where $\nabla^2 = \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right]$ is

called Laplacian operator.

and $U = \frac{\text{wave velocity}}{\text{velocity of matter waves}}$.

(5) Soln to eqⁿ (1) is

$$\psi(xyz, t) = \Psi_0(xyz) e^{-iwt}$$

$$\text{or} \quad \psi(r, t) = \Psi_0(\vec{r}) e^{-i\omega t} \quad (2)$$

(6) Differentiating eqⁿ (2) w.r.t t

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

$$\therefore \frac{\partial^2 \psi}{\partial t^2} = i^2 \omega^2 (\psi e^{-i\omega t})$$

$$= i^2 \omega^2 \psi$$

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

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

Substituting in eqn. ①

$$\frac{\partial^2 \psi}{\partial t^2} = 4^2 \nabla^2 \psi, \text{ we get.}$$

$$-\omega^2 \psi = 4^2 \nabla^2 \psi.$$

$$\therefore \nabla^2 \psi = -\frac{\omega^2}{4^2} \psi$$

$$\text{or } \nabla^2 \psi + \frac{\omega^2}{4^2} \psi = 0 \quad \text{③}$$

where $\omega = 2\pi\nu$ $\nu \rightarrow$ frequency
 $\text{if } u = \nu \lambda$ $\lambda \rightarrow$ of matter wave

Substituting in ③ we get

$$\nabla^2 \psi + \left(\frac{4\pi^2 \omega^2}{\lambda^2} \right) \psi = 0$$

$$\therefore \nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0. \quad \text{④}$$

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

$$\text{④} \rightarrow \nabla^2 \psi + \left(\frac{4\pi^2 p^2}{h^2} \right) \psi = 0, \quad \text{⑤}$$

$$\text{⑦ Total energy } E = \frac{1}{2} mv^2 + V \quad (V \rightarrow p \cdot E)$$

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

$$= \frac{p^2}{2m} + V$$

$$\therefore p^2 = 2m(E - V)$$

~~X~~ substituting in eqⁿ ⑤, we get

$$\nabla^2 \psi + \left[\frac{4\pi^2}{h^2} \times 2m(E-V) \right] \psi = 0$$

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

This is Schrodinger's time independent eqⁿ.

- ~~X~~ Q.3 Derive Schrodinger's time independent eqⁿ.
- Ans ① To describe behavior of matter wave in mathematical form Schrodinger derived a wave equation.

- ② Eqⁿ gives complete information about energy which momentum and position of the particle as a function of time.

- ③ Schrodinger's (S.T.I.E) is

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

eliminating E we get S.T.D.E.

- ④ The differential eqⁿ for the matter wave with wave velocity u can be written as

$$\frac{\partial^2 \psi}{\partial t^2} = u^2 \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right]$$

or $\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi \quad \text{②}$

- ⑤ Solⁿ to equation ② is

$$\psi(x, t) = \psi_0(x) e^{-iwt} \quad \text{②}$$

(2) Differentiating eqⁿ (3) w.r.t. time t , we get

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

$$\boxed{\frac{\partial \psi}{\partial t} = -i\omega \psi} \quad \boxed{\text{④ } (\psi = \psi_0 e^{-i\omega t})}$$

(7) Now $\omega = 2\pi\nu$

$$= \frac{2\pi E}{\hbar} \quad (E = h\nu)$$

Substituting in eqⁿ (4), we get

$$\frac{\partial \psi}{\partial t} = -i\left(\frac{2\pi E}{\hbar}\right)\psi$$

$$\text{OR } i \frac{\partial \psi}{\partial t} = \frac{2\pi E}{\hbar} \psi$$

$$\text{OR } \boxed{E\psi = i\hbar \frac{\partial \psi}{\partial t}} \quad \textcircled{5}$$

(8) Eqⁿ ① i.e S.T.I-E can be written as

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

$$\text{Div } \frac{\hbar^2}{8\pi^2m} \nabla^2\psi + E\psi - V\psi = 0 \quad \textcircled{6}$$

Substituting ⑤ in ⑥

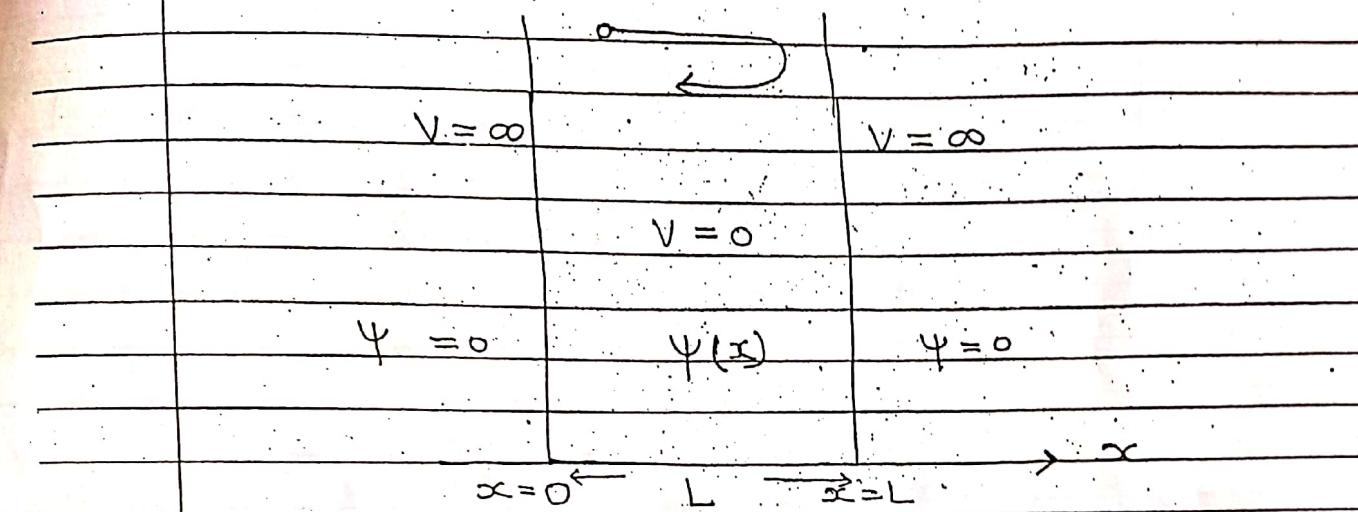
$$\boxed{\frac{\hbar^2}{8\pi^2m} \nabla^2\psi + \frac{i\hbar}{2\pi} \frac{\partial \psi}{\partial t} - V\psi = 0}$$

~~off~~

This is called S.T.D.E.

Q. 4 Derive an expression for the energy levels and wave function of a particle enclosed within infinite deep potential well. (OR Rigid box), show necessary waveforms.

Ans



(1) Consider a particle enclosed in a box of length L and allowed to move only along x -axis.

(2) For a rigid box, the potential energy at the walls of the box is ∞ i.e. $V = \infty$

(3) Inside the box, particle is free to move, hence for simplicity its potential energy is constant.

For simplicity let it is zero. ($V = 0$)

(4) As the particle can't cross walls of infinite potential, its probability of finding outside the box is zero. Hence

$$\psi = 0 \quad \text{for } x \leq 0$$

$$\text{if } \psi = 0 \quad \text{for } x \geq L$$

(5) Particle can be anywhere within the box. Hence we have to find out wave function ψ

within the box i.e from

2b
2

$$0 < x < L$$

(6) Soln (for Energy)

(I) Schrodinger's time independent wave equation in one dimension (i.e along x) is

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0 \quad (1)$$

(7) Substituting $V = 0$ (inside the box)

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E \psi = 0$$

$$\text{i.e. } \frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad (2)$$

$$\text{where } k^2 = \frac{8\pi^2 m}{h^2} E \quad (3)$$

(III) General soln to eqn (2) is

$$\psi(x) = A \sin kx + B \cos kx \quad (4)$$

(where A & B are constants)

constants can be determined by applying boundary conditions (B.C) i.e

$$\psi(0) = 0 \quad \text{at } x = 0$$

$$\text{if } \psi(L) = 0 \quad \text{at } x = L$$

Putting $\psi(x) = 0$ at $x = 0$ in eqn (4)
we get

$$\psi(0) = A \sin k \cdot 0 + B \cos k \cdot 0$$

$$0 = 0 + B$$

$$\therefore B = 0$$

Hence eqn (4) becomes

$$\psi(x) = A \sin kx + 0$$

$$\psi(x) = A \sin kx$$

III Applying second B.C i.e

$$\begin{aligned} \psi(x) &= 0 & x &= L \\ \text{i.e } \psi(L) &= 0 & x &= L \\ \text{eqn (6) becomes} \end{aligned}$$

$$\begin{aligned} \psi(L) &= A \sin kL \\ 0 &= A \sin kL \end{aligned}$$

$$\rightarrow \begin{aligned} \text{either } A &= 0 \\ \text{or } \sin kL &= 0 \end{aligned}$$

$A \neq 0$, because if $A = 0$

$$\psi(x) = A \sin kx = 0$$

\rightarrow particle is absent which contradicts the fact that the particle is within the box.

Therefore $\sin kL = 0$

$$\text{i} \quad : \quad kL = n\pi \quad (n = 1, 2, 3, \dots)$$

$$\text{ii} \quad k = \frac{n\pi}{L} \quad (n \neq 0 \text{ some})$$

(IV) (7) in (3) gives

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

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

$$\boxed{\therefore E = \frac{n^2 h^2}{8m L^2}}$$

8

CONCLUSIONS

① From eqn ③ it can be seen that particle's energy is ~~discrete~~ can have certain fixed energy values like

$$E_1 = \frac{\hbar^2}{8mL^2} \quad \text{for } n=1$$

$$E_2 = \frac{4\hbar^2}{8mL^2} \quad \text{for } n=2$$

and so on. Hence energies are quantized.

In classical mechanics, any arbitrary energy value is allowed.

② Since $\gamma \neq 0$, energy can never be zero. This means ~~system~~ in any system, atoms are always in the vibrating mode.

In classical mechanics, zero energy is allowed for a system. It is called as ground state energy.

③ Energy is inversely proportional to square of the length of the box, i.e. mass of the particle.

WAVE FUNCTION

From eqn ⑥ Wave function

$$\psi(x) = A \sin kx \quad (B=0) \quad ①$$

Applying normalisation cond

$$\int_0^L |\psi(x)|^2 dx = 1 \quad ②$$

$$A^2 \int_0^L \sin^2 kx dx = 1 \quad ③$$

$$A^2 \int_0^L \sin^2(n\pi)x dx = 1 \quad ④$$

$$\text{Using } \cos 2\theta = 1 - 2 \sin^2 \theta$$

$$\sin^2 kx = \frac{1 - \cos 2kx}{2}$$

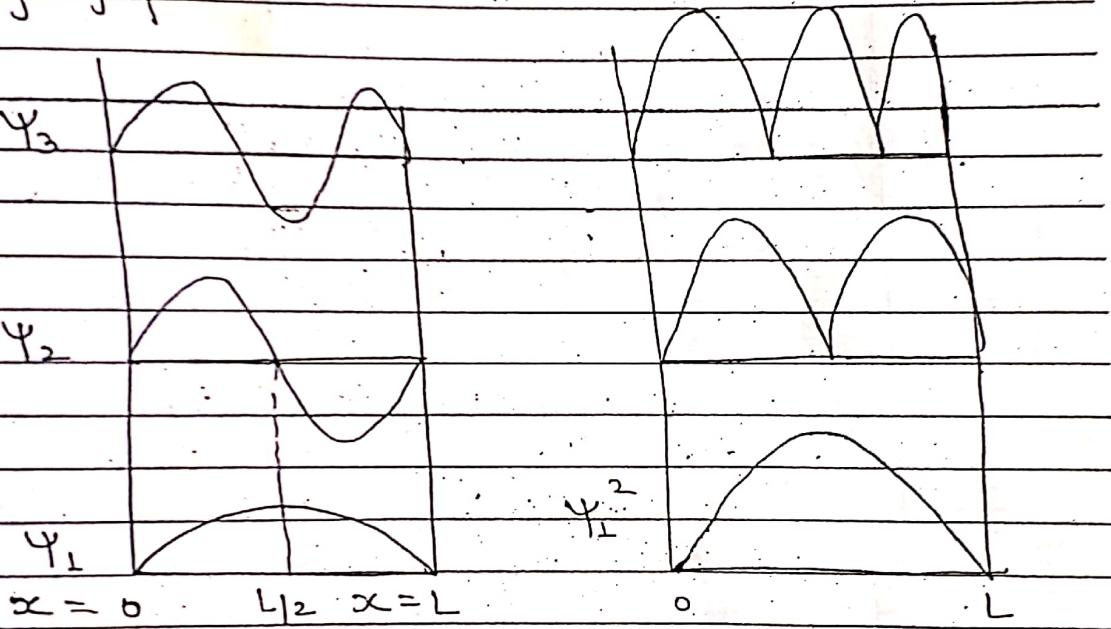
Substituting in eqn (3) and simplifying, we get

$$A = \sqrt{\frac{2}{L}}$$

Hence

$$\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$$

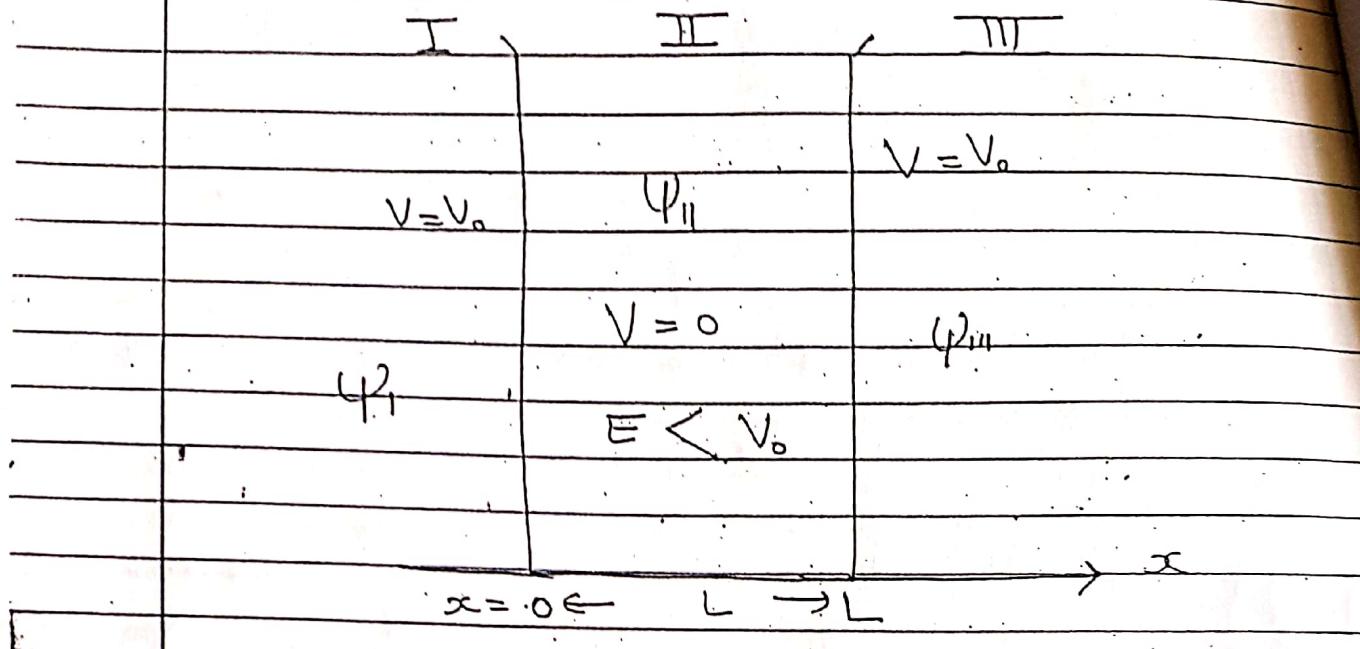
Plotting the graph of wave fun' Ψ , we get following graph



Wave functions.

Probability densities

Q.5 Discuss particle in a non-rigid box
(or finite potential well)



① Consider a particle enclosed in a box of length L and allowed to move along x -axis.

② For a non-rigid box, potential energy at the wall of the box is finite. i.e.

$$V = V_0$$

③ Inside the box particle is free to move. Hence

$$V = 0$$

④ Let the energy of the particle inside the box is E and

$$E < V_0$$

⑤ As per classical mechanics if $E < V_0$, particle can never be found outside the box. But

⑥ As per quantum mechanics though $E < V_0$,

particle can penetrate or tunnel through the box. Hence hence there is some fixed probability of finding the particle outside the box. Hence

$\Psi \neq 0$ in regions I & III also.

(1) Let $V = V_0$ outside the box

& $V=0$ inside the box

(2) Let Ψ_I , Ψ_{II} , & Ψ_{III} are the wave functions corresponding to regions I, II and III.

(3) Soln

(I) For region I, Schrödinger's equation is

$$\frac{d^2\Psi_I}{dx^2} + \frac{8\pi^2m}{h^2} (E - V_0) \Psi_I = 0 \quad (1)$$

For region II

$$\frac{d^2\Psi_{II}}{dx^2} + \frac{8\pi^2m}{h^2} (E - 0) \Psi_{II} = 0 \quad (2)$$

& for region III

$$\frac{d^2\Psi_{III}}{dx^2} + \frac{8\pi^2m}{h^2} (E - V_0) \Psi_{III} = 0 \quad (3)$$

(II) Eqn (1), (2) & (3) can be written as

$$\frac{d^2\Psi_I}{dx^2} - k^2 \Psi_I = 0 \quad (4) \quad k^2 = \frac{8\pi^2m(E-V_0)}{h^2}$$

$$\frac{d^2\Psi_{II}}{dx^2} + k^2 \Psi_{II} = 0 \quad (5) \quad k^2 = \frac{8\pi^2mE}{h^2}$$

$$\frac{d^2\Psi_{III}}{dx^2} - k^2 \Psi_{III} = 0 \quad (6) \quad -k^2 = \frac{8\pi^2m(E-V_0)}{h^2}$$

Soln to eqn (4), (5) & (6) is

$$\Psi_I(x) = A e^{ikx} + B e^{-ikx} \text{ for } x \leq 0$$

$$\Psi_{II} = P e^{ikx} + Q e^{-ikx} \text{ for } 0 < x < L$$

$$+ \Psi_{III} = C e^{kx} + D e^{-ikx} \text{ for } x > L$$

where A, B, P, Q, C, D are constants to be determined.

(IV) Applying Boundary cond'n

$$(i) \text{ as } x \rightarrow \infty, \Psi(x) \rightarrow 0 \quad (\text{less chance for particle to be there})$$

$$(ii) x \rightarrow -\infty, \Psi(x) \rightarrow 0$$

$$(iii) \Psi_I(0) = \Psi_{II}(0)$$

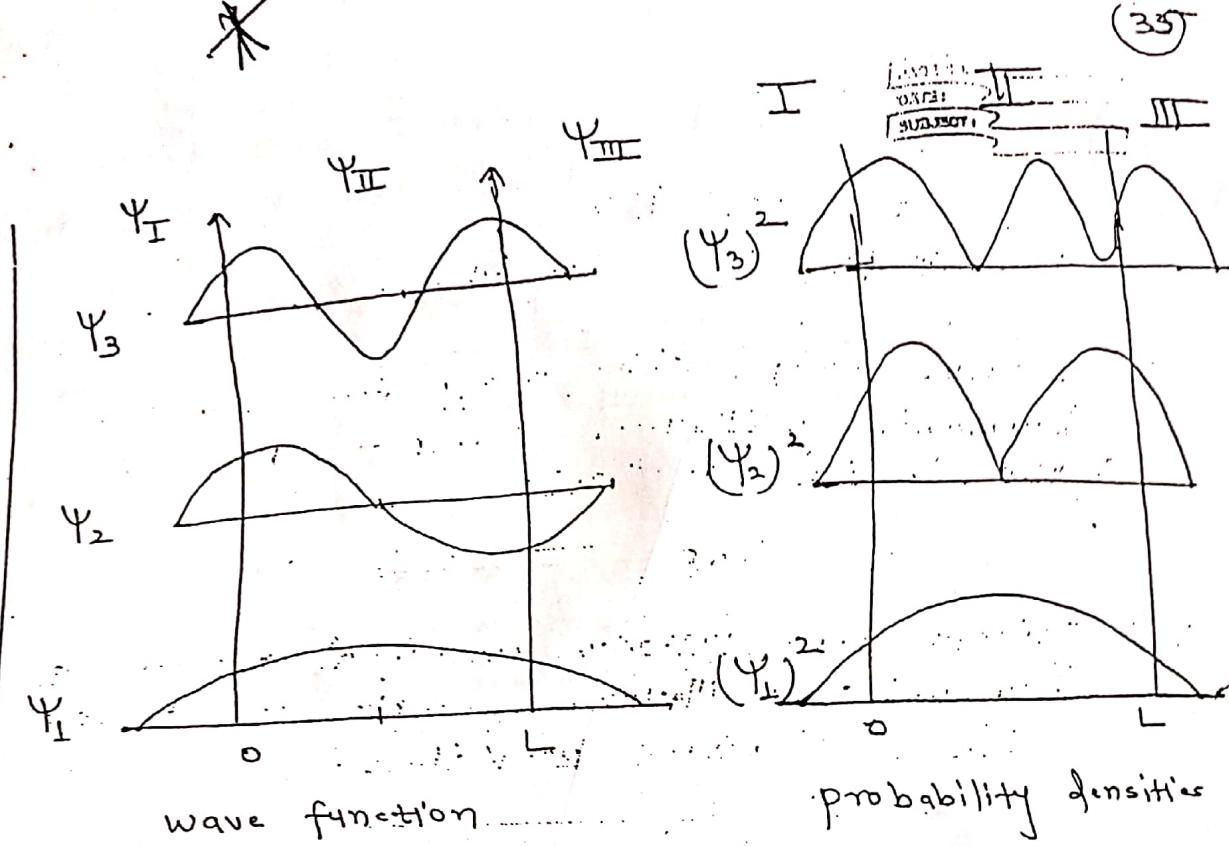
$$(iv) \Psi_{II}(L) = \Psi_{III}(L)$$

$$(v) \left| \frac{\partial \Psi_I}{\partial x} \right|_{x=0} = \left| \frac{\partial \Psi_{II}}{\partial x} \right|_{x=0}$$

$$(vi) \left| \frac{\partial \Psi_{II}}{\partial x} \right|_{x=L} = \left| \frac{\partial \Psi_{III}}{\partial x} \right|_{x=L}$$

Using six boundary conditions, six constants can be determined. Hence wave functions $\Psi_I, \Psi_{II}, \Psi_{III}$ can be known completely.

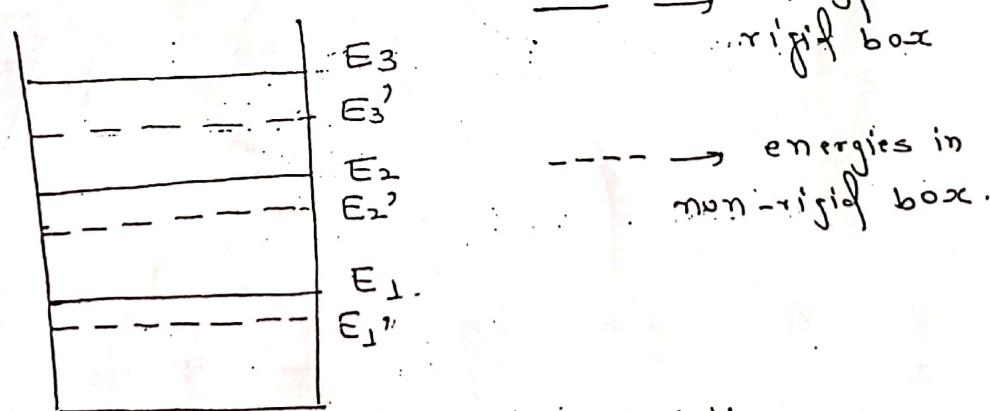
(v) Plotting the graph of wave function Ψ , we get following graph:



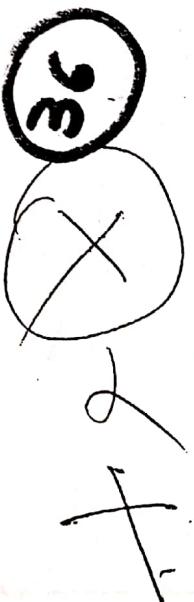
(VI)

CONCLUSIONS

- ① It is seen that wave function Ψ_n are not equal to zero outside the box. This means though the particle energy E is smaller than the value of potential outside the box, it can penetrate through the walls & come out.
- ② Wavelength of the particle are longer ~~than~~ in the non-rigid box than the wavelength when it is in the rigid box.
- ③ A larger wavelength means smaller frequency and hence smaller energy.



- ④ Energies are quantised for $E < V_0$.



Q. 6

5. K.E. of the particle outside the box i.e. (E) is always less than the K.E. inside the

Derive briefly the energy eigen values of a harmonic oscillator. Compare the results with the classical mechanics.

OR

Q. 6. Discuss the quantum mechanical picture of a harmonic oscillator. Compare its predictions with the classical predictions.

OR

Discuss the quantum mechanical model of linear simple harmonic oscillator and show that zero point energy is $\frac{1}{2} \hbar \omega$.

Ans

Simple harmonic oscillator is defined as the periodic motion of a system in which a restoring force acting on it is directly proportional to its displacement and it always acts towards the mean position.

(II)

①

CLASSICAL APPROACH OF S.H.M.

As per def'

$$F = -kx \quad \text{--- (1)} \quad k \rightarrow \text{force constant}$$

We have

$$F = m \ddot{x}$$

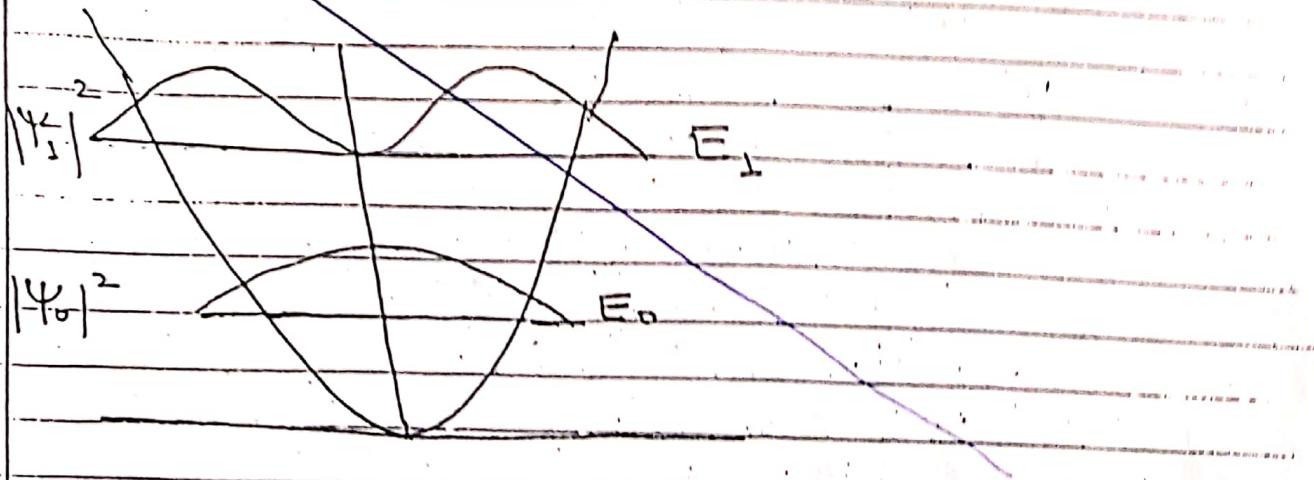
$$m \ddot{x} = -kx \quad \text{--- (2)}$$

From (1) & (2)

$$m \frac{d^2x}{dt^2} = -kx$$

$$\frac{d^2x}{dt^2} + \frac{k}{m} x = 0$$

as shown in the following figure.



① From above graph it is seen that there is certain probability of finding the particle beyond the limits A and $-A$.

This is unique observation in quantum mechanics.

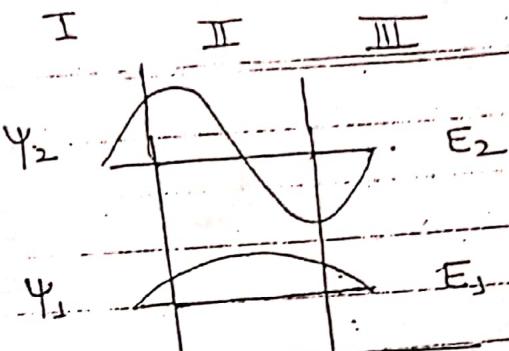
According to classical mechanics probability of finding particle outside the box is zero.

Q.7 Explain Tunneling effect? Illustrate with example. What is a tunnel diode?

Ans(I) According to classical mechanics a particle having energy E less than the potential barrier at the walls can never be found outside the box.

$V = V_0$		$V = V_0$
$\Psi = 0$	Ψ	$\Psi = 0$
	$E < V_0$	

By quantum mechanics says that even though particle can't jump the walls, it will tunnel through and there is fixed probability of finding the particle outside the box as shown.

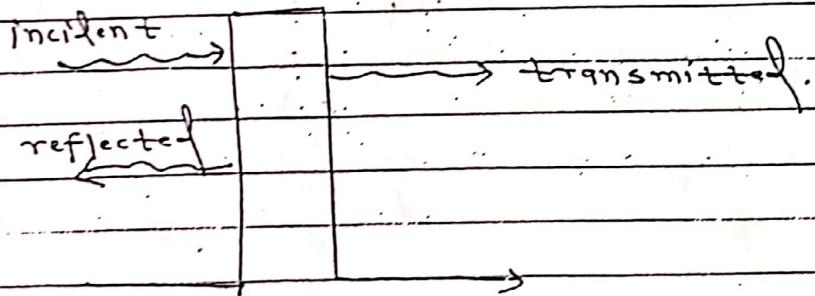


This is called as tunneling effect.
This effect is the result of wave nature of particle.

Particle nature of matter can't explain this phenomenon. It can be seen with the analogy of light in optics.

When light is incident, travelling through a rarer medium, the part of the ray gets reflected and part gets transmitted. This can be explained on the basis of wave theory of light only.

Similarly on the atomic scale when the particle is incident on the potential barrier, part of it gets reflected and part get transmitted through as shown, which proves wave nature of matter.



II Examples.

I- Alpha decay

The best example is α -decay. An α particle whose kinetic energy is a few MeV can escape from its nucleus whose potential wall is almost 25 MeV high. The probability of escape is very small, otherwise it has to strike the wall more than 10^{38} times.