Quantum mechanics

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de- Broglie Hypothesis :-

→ It discusses dual nature of light.

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

h - plank's constant
p - momentum.
λ - wavelength.

Consider $E = h\nu$

but $E = mc^2$ (Einstein energy - mass equation)

$\therefore$ also

$$p = mc.$$

$$\therefore p = \frac{mc^2}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}.$$

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

Properties of Matter wave :-

1. Matter waves are produced by the motion of the particles and are independent of the charge. Hence, they are neither Electromagnetic nor acoustic waves but are new kind of waves.
2. They do not require medium for propagation. Therefore can travel through vacuum.
3. Smaller the velocity of particle, longer is the wavelength of the matter wave associated with it.
4. The lighter the particle, the longer is the wavelength of the matter wave associated with it.
5. The velocity of matter waves depends on the velocity of the material particle and is not constant quantity.
6. They exhibit diffraction phenomenon as any other waves.

② Phase velocity & Group velocity

Phase velocity :

consider a wave.

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

$$u_{phase} = \frac{\omega}{k}$$

If a point is imagined to be marked on a travelling wave, then it becomes a representative point for a particular phase of the wave and the velocity with which it is transported owing to the motion of the wave. is called phase velocity.

Group velocity :-

two or more waves slightly diff velocity. superimposed. The resultant pattern causes variation in amplitude and is called as wave packet ~~or~~ wave group.

for electromagnetic wave,

phase velocity $u = \nu\lambda$. and $E = h\nu$.

$$\therefore u = \frac{E}{h} \cdot \lambda$$

$$= \frac{mc^2}{h} \cdot \frac{h}{m \cdot v}$$

$$\boxed{u = \frac{c^2}{v}}$$

⇒ phase velocity of de Broglie wave associated with the particle moving with velocity greater than c.

⇒ This difficulty can be overcome by assuming that each moving particle is associated with a group of waves or wave packet rather than a single wave.

so if $y_1 = a \sin(\omega_1 t - k_1 x)$

$y_2 = a \sin(\omega_2 t - k_2 x)$

then $y = y_1 + y_2$

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

$\Delta\omega = \omega_1 - \omega_2$

$\Delta K = k_1 - k_2$

$\omega = \frac{\omega_1 + \omega_2}{2}$

$K = \frac{k_1 + k_2}{2}$

$\boxed{\text{then } \frac{\Delta\omega}{\Delta K} = G}$ → G - Group velocity.

(3) Wave f^n and physical interpretation

→ Let ψ associated with system of e^- then $|\psi|^2 d\tau$ is considered as a measure of density of e^-.

→ $|\psi|^2 d\tau$ provides probability of finding the e^- in certain volume $d\tau$.

$|\psi|^2$ – probability function.

→ $\int |\psi|^2 d\tau = 1$ particle must be somewhere in the volume τ.

→ ψ has no meaning but $|\psi|^2$ has.

→ ψ characterises the state of the system.

→ $\psi = A + iB$ (ψ is usually complex no.)

A → real, B → real

→ Condition of Normalizat^n:

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

★ Condition for well behaved wave f^n s:-

(i) ψ must be finite! Even if $x \to \pm\infty$, ψ must be be finite and defined.

(ii) ψ - must be single valued :- Only one value of is allowed at a point.

(iii) ψ - must be continuous:- ψ and $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}$ & $\frac{\partial \psi}{\partial z}$ should be continuous across any boundary.

Uncertainty principle

⟹ "Quantum mechanics doesn't ~~a~~ simultaneously permit the determination of position and momentum of a particle accurately.

Mathematically:

$$\Delta x . \Delta p_x \geq \hbar$$

or $$\Delta x . \Delta p_x \geq \frac{h}{2\pi}$$

Δx – uncertainty in position

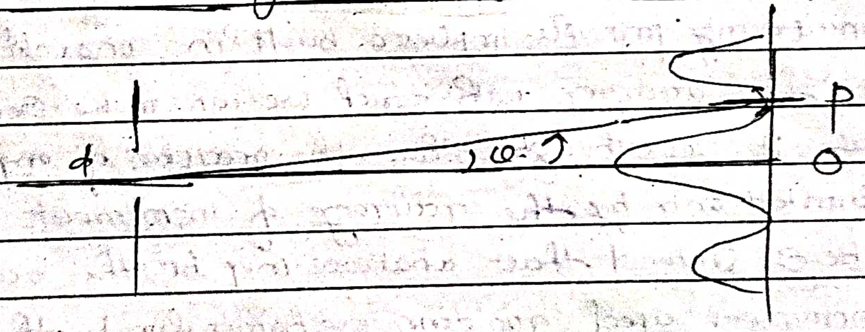
Δp_x – " in momentum

Other forms:

$$\Delta E . \Delta t \geq \hbar$$

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

⟹ Uncertainty in Electron Diffraction Expt.



Consider, P represent first order minimum.

condition for 1st order minima is

$$\sin\theta = \frac{\lambda}{d}$$

Consider photon with well defined momentum passes through slit. After it passes through slit the positn is known within an uncertainty which is equal to its slit width.

$$\therefore \Delta y = d.$$

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After passing through slit, photon has its value uncertain or it makes an angle θ with horizontal
$\therefore$ uncertainty in y-component of momentum is at least as large as $p\sin\theta$

$$\therefore \Delta p_y \geq p \cdot \frac{\lambda}{d}$$

$$\because p = \frac{h}{\lambda} \quad \text{(de-Broglie)}$$

$$\therefore \Delta p_y \geq \frac{h}{\lambda} \cdot \frac{\lambda}{d}$$

$$\geq \frac{h}{d}$$

$$\geq \frac{h}{\Delta y}$$

$$\boxed{\therefore \Delta y \cdot \Delta p_y \geq h}$$

In Good agreement with
$\Delta y \, \Delta p_y \geq \hbar$.

The uncertainty principle implies a built-in, unavoidable limit to the accuracy with which we can make measurement. Classically, it was thought that the precision of any measurement was limited only by the accuracy of instruments but Heisenberg showed that whatever may be the accuracy of the instrument used, quantum mechanics limit the precision when two properties are measured at the same time.
The quantities are called conjugate quantities in Quantum mechanics which has Energy x time dimensions.
$\therefore$ pair (i) position - Momentum, (ii) Energy-time (iv) also
(iii) Angular momentum & angular displacement. time-freq

One - Dimensional Time Dependent Schrodinger eq^n

Schrödinger develops a similar theory like Newton's law in classical mechanics.

A particle moving with velocity v and mass m is $\lambda = \frac{h}{p}$

The wave eq^n for de-Broglie wave can be written as.

$$\psi = A \cdot e^{-i\omega t}$$

A - Amplitude.
ω - angular $freq^n$.

what is schrodinger wave eq^n:-
Schrodinger reasoned that debroglie wave associated with e^- would resemble the classical wave of light and developed wave eq^n that describe the behaviour of matter waves. The eq^n describe the wave property of e^- and also predicts particle like behaviour.

for a 1-D case, the classical wave eq^n has the following form.

$$\frac{d^2\psi}{dx^2} = \frac{1}{v^2}\frac{d^2\psi}{dt^2} \quad \text{—— (1)}$$

y - displacement, v - velocity of wave.

$$\therefore y(x,t) = A \cdot e^{-i(kx - \omega t)} \quad \text{... sol}^n \text{ of the wave}$$

where,

$$\omega = 2\pi\nu$$

From eq^n (1), we can write the wave eq^n as

$$\frac{d^2\psi}{dx^2} = \frac{1}{v^2}\frac{d^2\psi}{dt^2}$$

$\omega = vk$. v = phase velocity

sol^n of the above eq^n.

$$\psi(x,t) = A \cdot e^{-i[Et - px]/\hbar}$$

Now. diff. w.r.to t.

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

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

$$\therefore \frac{\partial\psi}{\partial t} = \frac{-i}{\hbar} E \psi \quad \text{—— (2)}$$

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Similarly diff. w.r.to x.

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\right)$$

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

$$\frac{\partial^2\psi}{\partial x^2} = A \cdot e^{-i(Et - px)/\hbar} \cdot \frac{ip}{\hbar} \cdot \left(\frac{ip}{\hbar}\right)$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{-p^2}{\hbar^2}\psi \quad \text{--- } (3)$$

In classical mechanics, $E = \frac{p^2}{2m}$

Let there be a field where particle is present. Depending on its position in the field, the particle will possess P.E. V.

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

$$\text{or} \quad \frac{p^2}{2m} = E - V$$

$$\therefore \frac{p^2}{2m}\psi = E\psi - V\psi \quad \text{--- } (4)$$

from eq^n (2) from eq^n (3)

$$E\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t} \qquad p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}$$

from eq^n (4).

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

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

This is <u>one-D</u> time dependent eq^n.

Time independent - Schrodinger wave eq^n

Consider potential energy is stationary or independent of time

i.e. $V(x)$ only (position dependent only)

$\therefore$ $\psi(x,t)$ can be written as,

$$\psi(x,t) = \psi(x) \cdot \phi(t)$$

$\therefore$ eq^n

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$ can be written as.

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

Divide both side by $\phi(t) \cdot \psi(x)$

$$\underbrace{-\frac{\hbar^2}{2m} \cdot \frac{1}{\psi} \cdot \frac{\partial^2\psi(x)}{\partial x^2} + V(x)}_{\text{LHS function of } x \text{ only}} = \underbrace{i\hbar \cdot \frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}}_{f^n \text{ of } t \text{ only}}$$

eq^n is in variable separable form.

LHS & RHS must be equal to a constant.

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

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

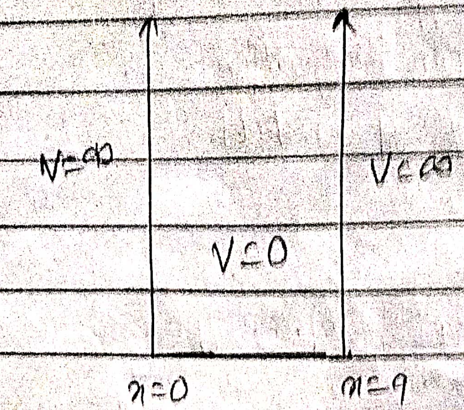
or

$$i\hbar \cdot \frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = E$$

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

Application of Schrodinger wave eq^n

* particle enclosed in a infinitely deep potential well (particle in a rigid box) :-



let m = mass of particle.

particle moving in x- direction from x=0 to a.

potential energy is infinite outside the box.

∴ from schrodinger eq^n.

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

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

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

∴ multiply both side by $\frac{2m}{\left(\frac{h}{2\pi}\right)^2}$

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

→ let $K^2 = \frac{8\pi^2 mE}{h^2}$

$$\therefore \frac{d^2\psi}{dx^2} + K^2\psi = 0$$

The sol^n are

$$\psi = A\cos Kx + B\sin Kx$$

when, $x = 0$, $\psi = 0$.

$\therefore 0 = A$

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

$\therefore 0 = A \cdot \cos ka + B \sin ka$

$\because A = 0$.

$\Rightarrow B \sin ka = 0$

$B \neq 0$.

$\therefore \sin ka = 0$.

$\underline{ka = n\pi}$

$\therefore ka = \cancel{\sqrt{\frac{2mE}{\hbar}}} \cdot a = \cancel{n\pi}$

$\sqrt{\frac{8\pi^2 mE}{h^2}} \cdot a = n\pi$

$\frac{8\cancel{\pi^2} mE}{h^2} \cdot a^2 = n^2 \cancel{\pi^2}$

$\therefore E = \cancel{n^2 \pi^2} \frac{n^2 h^2}{8ma^2}$ $[n = 1, 2, 3 \ldots]$

$$\boxed{E_n = \frac{n^2 h^2}{8ma^2}}$$

$$\boxed{E_n \propto n^2}$$

—o—

$$\boxed{\psi_n = B \sin\left(\frac{n\pi}{a}\right) \cdot x}$$

Calcu function

$\because \psi_n = B \sin \frac{n\pi x}{a}$

$\therefore \int_{-\infty}^{\infty} |\psi_n|^2 dx = \int_0^a |\psi_n|^2 dx$

$= B^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) . dx.$

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

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

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

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

$= \frac{B^2}{2} \left[(x)_0^a - \frac{a}{2n\pi} \left(\sin \frac{2n\pi x}{a} \right)_0^a \right]$

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

$1 \quad = \frac{B^2}{2} [a]$

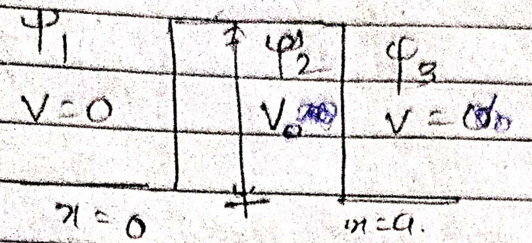
$\therefore \int_{-\infty}^{\infty} |\psi|^2 dx = 1$

$$\boxed{B = \sqrt{2/a}}$$

$$\therefore \boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}}$$

This is the wave f^n for particle in a box with infinite potential

* Particle in a finite potential well / Barrier and Tunneling effect



→ Classically, if a particle strike to a hard wall its not possible to find it on other side of wall. But, Quantum mechanics, has complete opposite sol^n to offer.

let $V = V_0$ – (Height of the potential barrier)
a – thickness of the barrier.

• Case :- if particle coming from LHS & $E < V$ particle will be reflected.
To found inside the wall, $E \geq V$.

But Quantum mechanically if $E < V$, ~~∃ a~~ there are chances of particle to be found in the barrier on RHS. ~~Such~~ This process is called Tunnelling

1-D schrödinger eq^n:

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

⇒ for LHS, let $\psi = \psi_1$ and $V = 0$.

$$\frac{d^2\psi_1}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi_1 = 0. \quad \text{—— (1)}$$

for RHS $\psi = \psi_3$, & $V = 0$.

$$\frac{d^2\psi_3}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi_3 = 0 \quad \text{—— (2)}$$

for $E < V$ and $V = V_0$, $\psi = \psi_2$

$$\psi_2 : \frac{d^2\psi_2}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V_0)\,\psi_2 = 0 \quad (3)$$

Eqⁿ (1) & (2) implies that

$$\psi_1 = A\cdot e^{ikx} + B\cdot e^{-ikx}$$
$$\psi_3 = C\cdot e^{ikx} + D\cdot e^{-ikx}.$$

But for eqⁿ (3)

$$\frac{d^2\psi_2}{dx^2} - \frac{8\pi^2 m}{h^2}(V - E)\,\psi_2 = 0$$

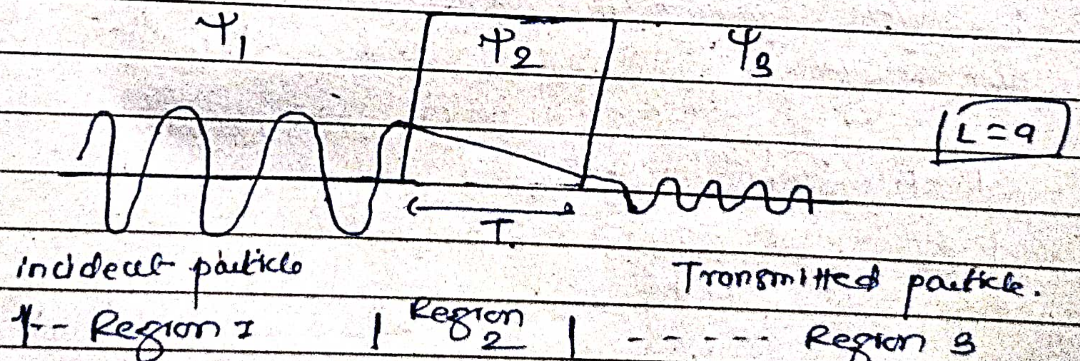
& eqⁿ.

$$\psi_2 = L e^{kx} + M e^{-kx}$$

$\downarrow$

represents exponentially decaying wave

Transmission co-efficient :-



$$T = G\cdot e^{-2kL} = \left[\frac{16E}{V_0}\left(1 - \frac{E}{V}\right)\right] e^{-2L\sqrt{8\pi^2 m(V_0 - E)}}$$

$$\boxed{T = G\cdot e^{-2kL}}$$

so, G - constant,

T decreases rapidly with increasing barrier width L

L mean a here.

* Tunnelling effect Examples

(i) α- Decay:

Energy of α- particle ≈ 4 to 9 MeV.
when such decay takes place the forces in the nucleus set up a potential barrier of ≈ 30 MeV.
∴ The process is happening through Tunnelling so α- particle with energy 4-9 MeV can cross the potential barrier of 30 MeV.

(ii) Tunnel diode

Tunnel diode is semi-conductor diode. The current in this device is largely due to tunneling of electrons through a potential barrier. The rate of tunnelling or current can be controlled over a wide range ~~of~~ by varying the height of the barrier, which is done by varying the applied voltage.

(iii) Scanning Tunnelling electron Microscope:-

→ Instrument invented by Gerd Bining ~~and~~ in 1979.
Helmrich Roharer
and awarded Nobel prize in physics.

→ STM uses electron Tunnelling to produce images of the surfaces down to the scale of individual atoms.

→ If two conducting samples are brought in close approximity, with a small but finite distance between them, el- from one sample flow into the other if the distance is of the order of the spread of the electronic wave fn. into space. This is said that the electrons "tunnel" through the barrier into the adjacent sample.

→ for electrons, the barrier width which may be overcome by via tunnelling process is of the order of nm; i.e. of the order of several atomic spacing

→ The probability of an e^- to get through the tunneling barrier decreases with exponentially with the barrier width. i.e tunneling current is extremely sensitive to measure of the distance betn two conducting samples.