

Quantum Mechanics

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Regular old phy.

Newtonian physics → when things get fast → special relativity

When things get small

when things get small & fast

Quantum physics

Quantum field theory

o Wein's Law:

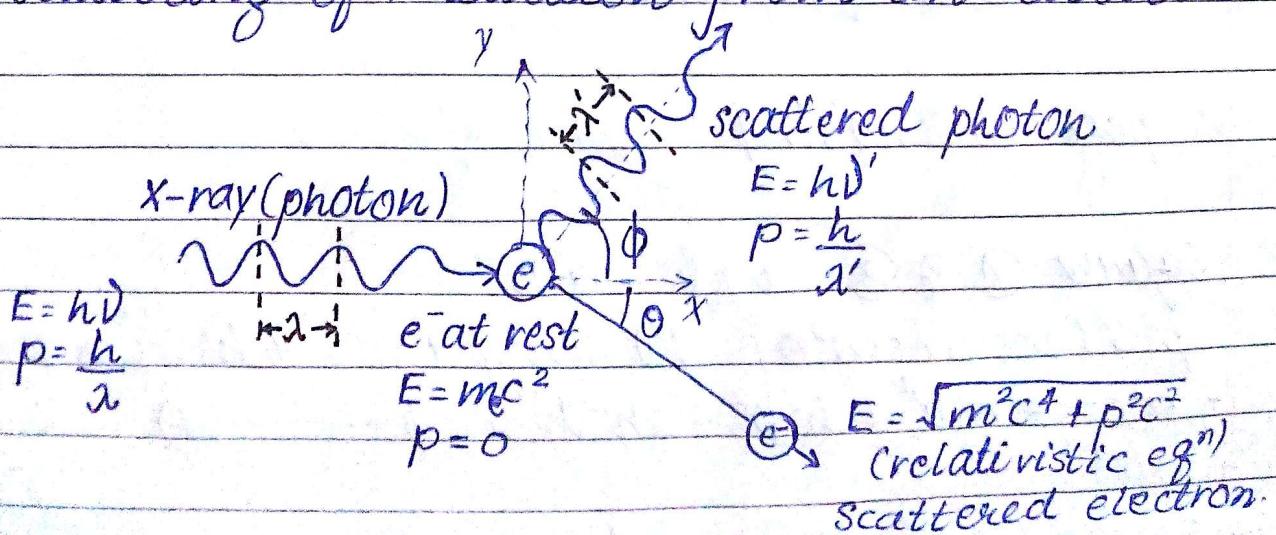
$$\lambda_{\max} \cdot T = b = \text{Wein's constant} \Rightarrow \lambda_{\max} \propto \frac{1}{T}$$
$$= 2898 \mu\text{m Kelvin}$$

Classically, avg. energy of atom = kT
(for Rayleigh-Jeans)

* Compton Effect:

Objective: (1) To show particle nature of light.

(2) Scattering of radiation from an electron.



$E = \sqrt{m^2 c^4 + p'^2 c^2}$
(relativistic eqn)
Scattered electron.

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Loss in energy by x-ray photon = gain in e^- energy
since, its Elastic collision.

$$\therefore (hv - hv') = KE \quad \text{--- (1)}$$

→ Energy and momentum (being vector is conserved in directⁿ of motion as well as \perp dirⁿ) are conserved.

° Case-1 : For dirⁿ of motion:

Initial momentum = final mom.

$$\frac{hv}{c} + 0 = \frac{hv'}{c} \cos\phi + p \cos\theta$$

$$\therefore p = hv - hv' \cos\phi \quad \text{--- (2)}$$

$$x = \frac{hv'}{c} \cos\phi$$

$$y = \frac{hv'}{c} \sin\phi$$

$$x = p \cos\theta$$

$$y = p \sin\theta$$

° Case-2: In \perp directⁿ:

Initial $p =$ Final p

$$0 = \frac{hv' \sin\phi}{c} \mp p \sin\theta -$$

$$\therefore p \sin\theta = hv' \sin\phi$$

Square (2) & (3) and add,

$$\begin{aligned} p^2 c^2 (\cos^2\theta + \sin^2\theta) &= h^2 v'^2 \sin^2\phi + h^2 v^2 + h^2 v'^2 \cos^2\phi - 2h^2 v v' \cos \\ &= p^2 c^2 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' \cos\phi \quad \text{--- (4)} \end{aligned}$$

→ Energy is conserved (Relativistic):

$$E \text{ before collis}^n = E \text{ after collis}^n$$

$$E_{\text{photon}} + E_{e^-} = (E_{\text{photon}} + E_{e^-})_{\text{scattered}}$$

$$= h\nu + mc^2 = h\nu' + \sqrt{m^2c^4 + p^2c^2}$$

from ①,

$$\begin{aligned} KE + mc^2 &= \sqrt{m^2c^4 + p^2c^2} \Rightarrow KE^2 + m^2c^4 + 2mc^2(KE) = m^2c^4 + p^2c^2 \\ \therefore p^2c^2 &= KE^2 + 2mc^2(KE). \\ p^2c^2 &= h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu' + 2h\nu mc^2 - 2h\nu' mc^2 \quad \text{--- (5)} \end{aligned}$$

Substitute p^2c^2 from ④ to ⑤, we get

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

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

$$= mc^2(\nu - \nu') = h\nu\nu'(1 - \cos\phi) \quad ; \quad \nu = \frac{c}{\lambda}$$

$$\therefore mc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) = \frac{h}{\lambda\lambda'}(1 - \cos\phi) \Rightarrow mc(\lambda' - \lambda) = h(1 - \cos\phi)$$

$$\therefore \boxed{\lambda' - \lambda = \frac{h}{mc}(1 - \cos\phi)} \Rightarrow \text{Compton Equation.}$$

λ' = wavelength of scattered photon depends on ϕ

$\because \lambda$ and λ' are diff, Compton effect shows that light behaves as a particle (i.e. particle nature) and not as wave. If it behaved as wave, there would've been no scattering.

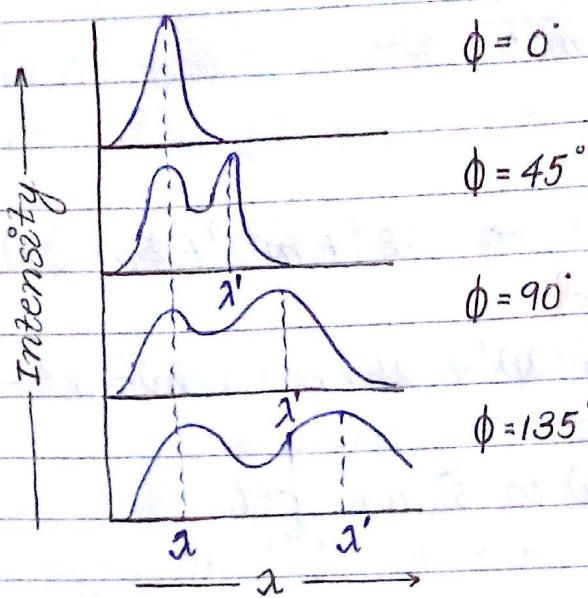
$$\boxed{\lambda_C = \frac{h}{mc}} \Rightarrow \text{Compton constant or Compton wavelength}$$

$$= 2.426 \times 10^{-12} \text{ m}$$

$$= 2426 \text{ pm}$$

$$\lambda = \frac{h}{\gamma mv} = \text{Relativistic De-Broglie wavelength}$$

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



- Q A free e^- cannot absorb a photon. Show this mathematically.
 (Hint: It violates energy-momentum conservation)

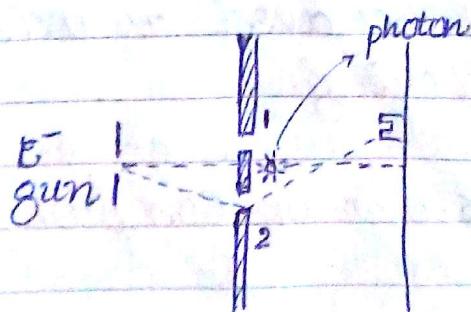
o 2-slit exp. with:

(i) Bullets:

$$P_{12}(\text{bullet}) = P_1 + P_2 \quad (\text{NO interference pattern obtained})$$

(ii) e^- -gun:

$$\begin{aligned}
 P_{12} &= P_1 + P_2 + (\text{extra term}) \text{ due to interference} \\
 &= |\phi_1 + \phi_2|^2 \\
 &= (\phi_1 + \phi_2) * (\phi_1^* + \phi_2^*) \quad ; P_1 = |\phi_1|^2 = \phi_1^* + \phi_1 \\
 &= |\phi_1|^2 + |\phi_2|^2 + \phi_2 \phi_1^* + \phi_1 \phi_2^* \\
 &= P_1 + P_2 + ()
 \end{aligned}$$



$$P'_{12} = P'_1 + P'_2$$

When photon & e^- interact a flash is seen and at screen trick is heard. Flash is seen near a particular slit.

In bullet case interf. occurs but max., minima can't be differentiated due to large size of bullet.

- Case-I (Intensity very high - say 10,000 e⁻ & 10,000 photons)

max. e⁻ scatter and reach screen, click is heard.

No. interference pattern not due to high intensity.

Col-I: e⁻ passing through slit-1

Col-II: e⁻ passing through slit-2

Col-I	Col-II
click &	click &
flash	flash
(1)	(1)
:	:
N'	N

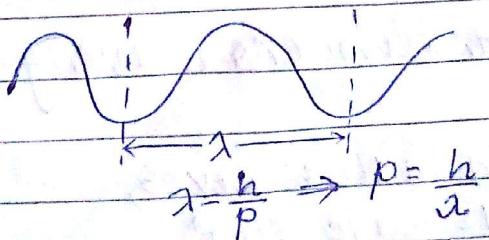
- Case-II (Intensity very low - say 10,000 e⁻ & 1,000 photons)

Interference observed

Col-I	Col-II	Rem. e ⁻
click &	click &	click but
flash	flash	NO flash

- Heisenberg's uncertainty principle:

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi c}$$



$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m}v}$$

$$E_0 = 8.85 \times 10^{-12} \text{ F/m}$$

permittivity of free space
Pa⁻¹⁰ m = 0.53 Å

Q Find λ :

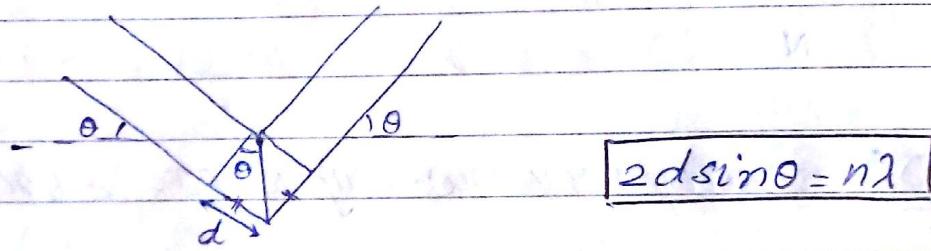
$$(a) m = 46 \text{ gm}, v = 30 \text{ m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{46 \times 10^{-3} \times 30} = \frac{6.63 \times 10^{-32}}{138} = \dots \text{ } 10^{-34} \text{ order}$$

$$(b) m = 9.1 \times 10^{-31} \text{ kg}, v = 2 \times 10^8 \text{ m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 2 \times 10^8} = \dots \text{ } 10^{-12} \text{ order}$$

o Bragg's law:



$n = \text{order}$

if say $n=2$, then in 2d portion 2 max occurs

say $n=1$, then in 2d portion 1 max occurs

due to const. Integ.

→ sound wave = pressure varies

→ water waves = height/amplitude

→ light wave = intensity of electric and magnetic field

} varies periodically.

o Schrodinger's wave funⁿ:

In matter waves,

ψ = wave funⁿ

$|\psi|^2$ = probability amplitude \Rightarrow Dirac notation

$\psi(x, y, z, t)$ = wave funⁿ

The probability of experimentally finding the body described by wave function ψ at point x, y, z at time t is proportional to the value of $|\psi|^2$ there at t

- o Bracket notation

$$\langle \quad \rangle \text{ or } | \rangle \text{ ket}$$

$$\langle \quad |$$

Bra

$$| \rangle = \text{ket}$$

what is known part in ket ($| \rangle$)

$|x=3m\rangle$ would be the state of particle known to be at positⁿ $x=3cm$

$|p\rangle$ particle has momentum p

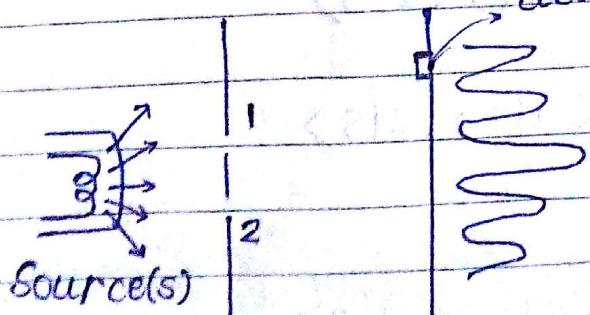
$|x=3, x=5\rangle$ particle is at $x=3$ & $x=5$ — x not possible

$|\psi\rangle$ system in state ψ & is therefore called the state vector

$$\langle \quad | = \text{Bra}$$

represents the final state or lang. in which you wish to express content of set.

Probability amplitude = $\langle \text{Final state} | \text{Ini. state} \rangle$



$$\rightarrow y = A \sin(kx - \omega t) = \text{wave eqn}$$

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

Ex: A particle with definite energy is moving from known position r_1 to r_2 . Find probability amplitude?

Soln: Definite energy \Rightarrow it has momentum (say \vec{p})

$$\langle r_2 | r_1 \rangle = \frac{e^{i\vec{p} \cdot \vec{r}_{12}/\hbar}}{r_{12}} ; \hbar = \frac{h}{2\pi}$$

$$\text{where, } \vec{r}_{12} = \vec{r}_2 - \vec{r}_1$$

$\langle r_2 | r_1 \rangle$ = prob. to find particle at r_2 .

$p^2 c^2 = E^2 - m^2 c^4$ is also valid here \because def. energy.

• How fast de-Broglie wave travels?

$$v_p = \lambda \nu \quad \dots \quad (1)$$

$$\left(v_p = \frac{c^2}{\nu} \right) \quad \dots \quad (2)$$

for matter waves
if $v \neq c$

$\therefore v_p > c$ but v_p can't be $> c$.

phase velocity

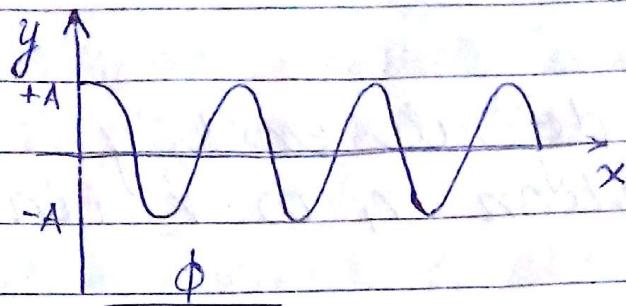
$$\lambda = \frac{h}{p} = \frac{h}{\gamma m v} \quad \dots \quad (3) \quad E = h\nu = \gamma m v c^2 \quad \dots \quad (4)$$

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

from (1), (3), (4),

$$\therefore v_p = \frac{\gamma m c^2}{h} \times \frac{h}{\gamma m v} = \frac{c^2}{v} = \dots \quad (2)$$

o Phase velocity:



(Assump: wave in $-x$ -dir)

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

$$\psi = A \cos(\omega t - kx)$$

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

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

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

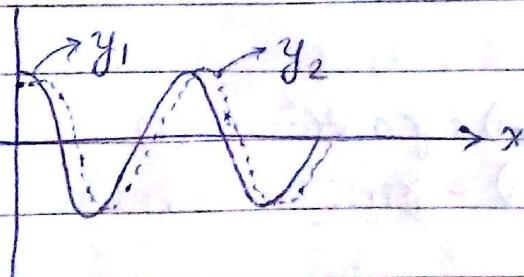
diff. w.r.t t

$$\boxed{\frac{dx}{dt} = \frac{\omega}{k} = v_p} = \lambda$$

o Group velocity:

$$y_1 = A \cos(\omega t - kx)$$

$$y_2 = A \cos((\omega + \Delta\omega)t - (k + \Delta k)x)$$



$$y = y_1 + y_2 = A(\cos\alpha x + \cos\beta x) = 2A \cos\left(\frac{(2\omega + \Delta\omega)t}{2}\right) \cos\left(\frac{\Delta k x}{2}\right)$$

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

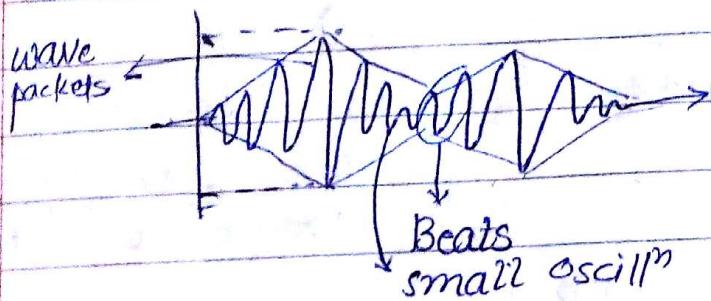
$$2\omega + \Delta\omega \approx 2\omega \quad \text{&} \quad 2k + \Delta k = 2k$$

→ large scale oscillation

$$\therefore y = 2A \cos(\omega t - kx) \cos\left(\frac{\Delta\omega t}{2} - \frac{\Delta k x}{2}\right) = \psi$$

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

superimposed waves



Inside waves = large f
outside waves = small f

$$\frac{\Delta\omega t}{2} - \frac{\Delta k x}{2} = \text{const.} \Rightarrow \frac{dx}{dt} = \frac{\Delta\omega}{\Delta k} = v_g \quad \text{group velocity}$$

- Reln b/w v_p & v_g :

$$v_g = \frac{d\omega}{dk} = \frac{d(v_p k)}{dk}$$

$$v_g = v_p + k \frac{dv_p}{dk}$$

→ in terms of λ ,

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

→ in dispersive medium.

medium in which wavelength λ
wave-dependent v_p is

for const. v_p ,

$$\frac{dv_p}{d\lambda} = 0$$

$\Rightarrow v_g = v_p$ → in non-dispersive medium.

what is group velocity for matter waves?

$$v_g = \frac{d\omega}{dk} \quad \omega = 2\pi\nu$$
$$k = \frac{2\pi}{\lambda}$$

$$\hbar\nu = \gamma mc^2 \quad ; \quad \gamma = \sqrt{1 - \frac{v^2}{c^2}}$$

$$J = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}} \times h}$$

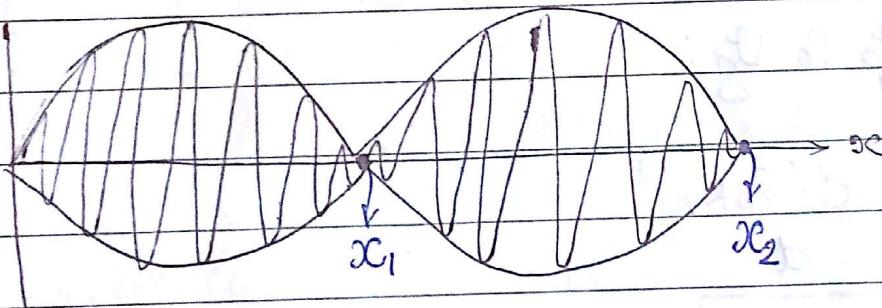
$$g = \frac{\hbar}{\gamma mv}$$

$$J = \frac{mc^3}{h\sqrt{c^2 - v^2}}$$

$$\frac{d\omega}{d\nu} = \frac{2\pi mc^3}{h} \left(\frac{d}{d\nu} \left(\frac{1}{\sqrt{c^2 - v^2}} \right) \right)$$

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/d\nu}{dk/d\nu} = \frac{(2\pi\gamma m)}{n}$$

$v_g = v$ = particle veloc.



Eqⁿ:

$$y = y = 2A \underbrace{\cos\left(\frac{\Delta k x_1}{2} - \frac{\Delta \omega t}{2}\right)}_{\text{Amplitude modulation}} \cos(k x_1 - \omega t) \quad (1)$$

Amplitude modulation

for $t = t_0$ ($t=0$), $A(0) = 0$

$$\text{Amplitude for } x_1: 2A \cos\left(\frac{\Delta k x_1}{2} - \frac{\Delta \omega t_0}{2}\right) = 0$$

$$\text{Amplitude for } x_2: 2A \cos\left(\frac{\Delta k x_2}{2} - \frac{\Delta \omega t_0}{2}\right) = 0$$

phase diff b/w x_1 & x_2 ,

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

Now multiply \hbar both sides,

$$\hbar \Delta k \Delta x = \hbar 2\pi$$

$$[p = \hbar k] \rightarrow \text{we know it}$$

$$\Delta p \Delta x = \hbar ; \hbar = \frac{\hbar}{2\pi}$$

$\langle \rangle$ = expectⁿ

$$\Delta x = [\langle x^2 \rangle - \langle x \rangle^2]^{1/2} \quad \left. \begin{array}{l} \text{uncertainties in position} \\ \text{momentum} \end{array} \right\}$$
$$\Delta p = [\langle p_x^2 \rangle - \langle p_x \rangle^2]^{1/2}$$

= Wave function:

Wave fⁿ has no significance

→ Well behaved wave funⁿ

① ψ must be cont. and single valued.

② $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must be continuous and single valued.

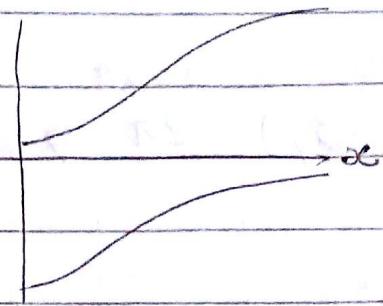
③ ψ must be normalizable which means ψ must go to zero as $x \rightarrow \pm\infty, y \rightarrow \pm\infty, z \rightarrow \pm\infty$ in order that the $\int |\psi|^2 dV$ overall space be a finite constant.

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi(x, y, z)|^2 dV = 1 ; dV = dx dy dz$$

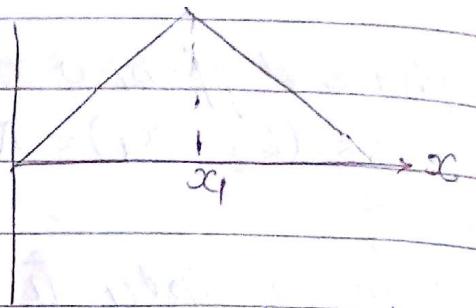
④ One can multiply $\psi(r, t)$ by a constant "N" so that $N\psi$ satisfies the normalizable condition.

$$|N|^2 \int_{-\infty}^{\infty} |\psi(r, t)|^2 dV = 1$$

Q (i)



(ii)

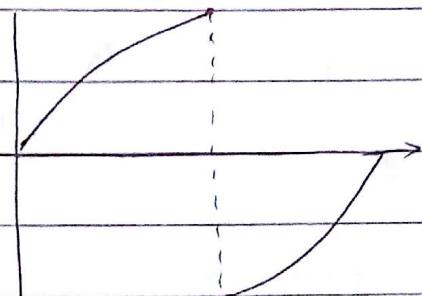


Not wave fun
(well behaved)

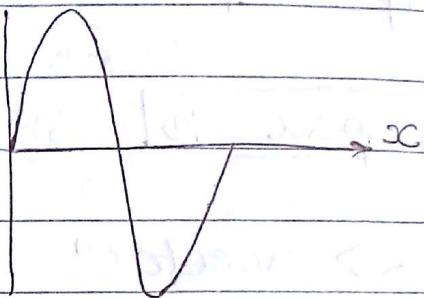
∴ NOT single valued

✓ well behaved due to
conditⁿ (2)

(iii)



(iv)



✓ well behaved
∴ not continuous

✓ well behaved wave
function

$$\begin{aligned} \text{(ii)} \quad \Psi = A \sec x & \quad \left. \begin{array}{l} \text{x well-behaved} \\ \text{wave f}^n \end{array} \right\} \\ \Psi = A \tan x & \\ \Psi = A e^{ax^2} & \\ \Psi = A e^{-ax^2} & \quad \left. \begin{array}{l} \text{well-behaved} \\ \text{wave f}^n \end{array} \right\} \end{aligned}$$

Q Normalize the wave fⁿ: $\Psi = A e^{-ax^2}$ (or find A)?

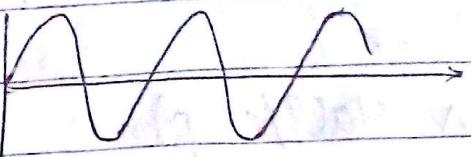
Solⁿ: Given that:

$$\int_{-\infty}^{\infty} e^{-2ax^2} dx = \sqrt{\frac{\pi}{2a}}$$

$$\therefore |A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 1 \Rightarrow |A|^2 \left(\sqrt{\frac{\pi}{2a}} \right)^2 = 1 \Rightarrow |A| = \left(\frac{2a}{\pi} \right)^{1/4} = A$$

$$\therefore \text{Normalized wave f}^n: \left(\frac{2a}{\pi} \right)^{1/4} e^{-ax^2}$$

Time dependent Schrödinger Equation (TDSE):



$$\psi = A e^{-i(-Kx + \omega t)}$$

$E = \hbar\omega$ and $p = \hbar k$.

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

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

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

$$\frac{\partial \psi}{\partial t} = \frac{-iE}{\hbar} \psi \quad \text{--- (2)}$$

Total energy $\rightarrow E = KE + PE$

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

Multiply ψ ,

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

from 2 and (3),

$$-\frac{i\hbar}{\hbar} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi \quad (\text{Now, } -i = \dot{x})$$

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

In 3D:

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

$$\hat{E} \Psi(r, t) = \hat{H} \Psi(r, t) \quad (\text{ } \hat{A} = \text{Hall/cap})$$

where, $\hat{E} = i\hbar \frac{\partial}{\partial t}$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + U \text{ (in 3D)} \quad \text{or} \quad \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U \text{ (in x-dir)}$$

$$[\hat{E} \Psi = \hat{H} \Psi] ; \quad \hat{E} = i\hbar \frac{\partial}{\partial t}$$

Time-independent Schrödinger Eqⁿ (T.I.S.E):

$$\Psi(x, t) = A e^{-i(Et - kx)}$$

$$\Psi(x, t) = A e^{-\frac{i}{\hbar}(Et - px)} \quad \text{(i)}$$

By using separation of variable technique, we can write eqⁿ (i) as:

$$\Psi(r, t) = \Psi(x) \phi(t)$$

$$\Psi(r, t) = \Psi(x) e^{-iEt/\hbar} \quad \text{(ii)}$$

If we substitute eqⁿ - (ii) in TDSE:

$$\frac{i\hbar}{\partial t} (\Psi(x) e^{-iEt/\hbar}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} (\Psi(x) e^{-iEt/\hbar}) + U(x) \Psi(x) e^{-iEt/\hbar}$$

$$= i\hbar \left(-\frac{iE}{\hbar} \right) \Psi(x) e^{-iEt/\hbar} = -\frac{\hbar^2}{2m} e^{-iEt/\hbar} \frac{\partial^2}{\partial x^2} (\Psi(x)) + U(x) \Psi(x) e^{-iEt/\hbar}$$

$$E \Psi(x) e^{-iEt/\hbar} = " + "$$

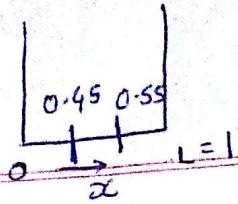
divide above eqⁿ by, $e^{-iEt/\hbar}$

we get:

$$\therefore E \Psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U(x) \Psi(x) \quad \left. \right\} \text{T.I.S.E.}$$

$$\therefore E \Psi(x) = \hat{H} \Psi(x)$$

↓ Total energy of particle.



$\langle \hat{I} \rangle = \text{Dirac not}$

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For position of a particle:

Expectation value = $\langle x \rangle$

$$\therefore \langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx \quad \text{In 1D (or } x\text{-dim)}$$

$\int |\psi|^2 dx \rightarrow$ from 3rd condⁿ of well-behaved wave fⁿ, denominator = 1.

$$\therefore \langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi dx$$

$\psi(x) = \begin{cases} ax & 0 \leq x \leq 1 \\ 0 & \text{otherwise.} \end{cases}$ is a well-defined wave;

(i) Find out the probability that the particle can be found between $x = 0.45$ to $x = 0.55$.

(ii) Find out expectation value:

$$\therefore \langle x \rangle =$$

$$(i) \int_{0.45}^{0.55} |\psi|^2 dx = \int_{0.45}^{0.55} a^2 x^2 dx = \left(\frac{a^2 x^3}{3} \right) \Big|_{0.45}^{0.55} = 0.025 a^2$$

$$(ii) \langle x \rangle = \int (x) \times (a^2 x^2 dx) = \int_{0.45}^{0.55} a^2 x^3 dx = \left. \frac{a^2}{4} (x^4) \right|_{0.45}^{0.55} = 0.0126 a^2$$

$$\int_0^1 a^2 x^3 dx = \frac{a^2}{4} \quad (\text{here } \psi^* = ax)$$

How to determine p?

Operator (\hat{o}): \rightarrow denoting operator

$$\hat{o}\psi = a\psi \quad \rightarrow \text{Eigen funⁿ}$$

$$\downarrow \text{operator} \quad \rightarrow \text{Eigen value}$$

Function	Operator
① position	\hat{x}
② momentum	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ (along x-axis) $\hat{p}_y = -i\hbar \frac{\partial}{\partial y} = \frac{\hbar}{i} \frac{\partial}{\partial y}$ $\hat{p}_z = -i\hbar \frac{\partial}{\partial z} = \frac{\hbar}{i} \frac{\partial}{\partial z}$
③ Total Energy (Time dep.)	$\hat{E} = i\hbar \frac{\partial}{\partial t}$
④ Total Energy (Time indep.)	$\hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{U}(x)$ (Hamiltonian operator)
⑤ Total Potential Energy	\hat{U}
⑥ Angular Momentum	$\hat{L}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$ $\hat{L}_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$ $\hat{L}_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$

Product of Operators:

Let \hat{A} and \hat{B} are two operators, and let us operate on a eigen/wave function ψ , then the expression $\rightarrow \hat{A}\hat{B}\psi$.

We can denote $\hat{A}\hat{B}$ by \hat{C} . \hat{C} is product of operator \hat{A} & \hat{B}

Commutation:

If $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ then this is called commutator of \hat{A} & \hat{B} . If $[\hat{A}, \hat{B}] \neq 0$, then one says that \hat{A}, \hat{B} do not commute & if $[\hat{A}, \hat{B}] = 0$, then \hat{A}, \hat{B} commute with each other.

Q Find value of: $[\hat{x}, \hat{y}, \hat{z}, \hat{p}_x]$
 $[\hat{x}\hat{y}\hat{z}, \hat{p}_y]$
 $[\hat{x}\hat{y}\hat{z}, \hat{p}_z]$

An operator equation of the form $[\hat{A}, \hat{B}] = \text{something}$ is called commutation relation.

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

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

$$\hat{p}_x \psi = -i\hbar \frac{\partial}{\partial x} e^{i(kx - \omega t)}$$

$$= -i\hbar \cdot ik \cdot e^{i(kx - \omega t)}$$

$$= -i^2 \hbar k \psi$$

$$\hat{p}_x \psi = (\hbar k) \psi$$

\downarrow eigen value

Ex: For $\hat{E} = +i\hbar \frac{\partial}{\partial t}$

$$\hat{E} \psi = i \frac{\hbar \partial}{\partial t} e^{i(kx - \omega t)}$$

$$= -i\hbar \omega e^{i(kx - \omega t) \times 2}$$

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

$$\hat{E} \psi = (\hbar \omega) \psi$$

\downarrow eigen value

Q Determine the value of $[\hat{x}, \hat{p}]$

Q Determine the value of $[\hat{y}, \hat{p}_x]$

Ans, is zero.

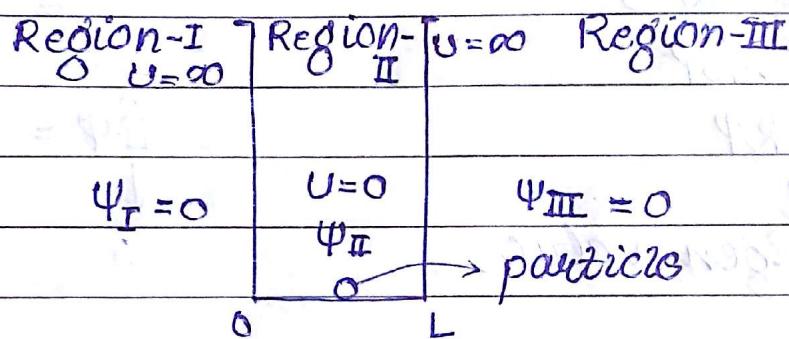
Q Determine the value of $[\hat{x}^2, \hat{p}_x^2]$ — Ans = 0

$$[\hat{x}^2, \hat{p}_x^2]$$

$$\hat{p}_x^2 = (-i\hbar)^2 \times \frac{\partial^2 \psi}{\partial x^2} = -\hbar^2$$

* Particle in a rigid box (1-D):

- ① A particle of mass 'm' trapped in a box with
- ② A particle travelling along x -axis between $x=0$ or $x=L$
- ③ A particle does not loose energy when it collides with such walls, so that its energy stays constant.
- ④ No external force is applied.



Ψ_i = wave fun" for respective regions, for finding particle in that region.

Writing, Time-independent SE for ①

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_I}{\partial x^2} + U \Psi_I(x) = E \Psi_I \quad \text{--- ①}$$

since $U = \infty$, $\Psi_I = 0$

for region ②

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_{II}}{\partial x^2} = E \Psi_{II} \quad \text{--- ②}$$

$$\frac{\partial^2 \Psi_{II}}{\partial x^2} = -\frac{2mE}{\hbar^2} \Psi_{II} \quad \text{--- ③}$$

for region ③,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_{III}}{\partial x^2} + U \Psi_{III}(x) = E \Psi_{III} \quad \text{--- ④}$$

$\therefore U = \infty \therefore \Psi_{III} = 0$

; Only 1 soln exists for region-II,

$$\frac{\partial^2 \Psi_{II}}{\partial x^2} = -k^2 \Psi_{II}(x) \quad \text{--- (5)} \quad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

A general soln for eqn (5),

$$\Psi_{II}(x) = A \cos kx + B \sin kx \quad \text{--- (6)} \quad \text{where,}$$

$A, B = \text{constants}$

Now, applying boundary condn, i.e. wave fun must be zero at end pts. = 0 and L.

∴

$$\text{For } x=0, \Psi_{II}(x=0) = A = 0$$

$$\text{For } x=L, \Psi_{II}(x=L) = 0 -$$

$$\therefore A \cos Lk + B \sin Lk = 0 \quad \therefore \tan Lk = \frac{-A}{B} = 0$$

$$\therefore B \sin Lk = \Psi_{II}(L)$$

$$\text{for, } kx = n\pi, \Psi_{II} = 0 \quad \therefore x = \frac{n\pi}{k} \quad \therefore \text{for } x = L \\ k = \frac{n\pi}{L}$$

$$\Psi_{II}(x) = B \sin \frac{n\pi}{L} x$$

According to normalization condition, $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$

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

wave fn:

$$\therefore \Psi(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi}{L} x \right), & 0 < x < L \text{ (or inside the box)} \\ 0, & \text{otherwise (or outside the box)} \end{cases}$$

For energy,

$$kL = n\pi$$

$$k^2 L^2 = n^2 \pi^2$$

$$\frac{2mE}{\hbar^2} L^2 = n^2 \pi^2$$

$$\therefore E = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \rightarrow \text{Energy is quantized.}$$