Quantom Mechanics

Intro → Classical

→ Trajectory :- State descriptor od Newtonian physics

→ Evolution od the state :- Use Newton's second law

→ Principle od causality :- Two identical systems with the same initial conditions, subject to the same ~~movement~~ measurement will yield the same result.

Intro → Quantum

→ Act as both particles and waves → called wave-particle duality.

→ It is a conglomeration od several possible outcomes od measurement od physical properties → use language od Probability theory.

→ An observer cannot observe a microsopic system without altering some od it's properties. Neither one can predict how the state od system will change

→ Quantization od energy is yet another property od "microscopic" Particles

de-Broglie

Relation from relativity

$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ & $E = mc^2$ $\left[\begin{array}{l} m_0 \to \text{~~Rest~~ mass (Rest)} \\ m \to \text{(Motion) mass} \end{array} \right]$

$E^2 = m^2c^4\left[1-\frac{v^2}{c^2}\right] + p^2c^2 = m_0^2c^4 + p^2c^2$

$E = h\nu$, $E = pc$ [For Application od photon $m_0 = 0$]

$p = \frac{h\nu}{c} = \frac{h}{\lambda} = \frac{E}{c}$

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

Hypothesis

He proposed that Frequency and wavelength can be associated with an electron's energy & momentum.

$$E = pc = h\nu = \frac{hc}{\lambda}$$

Consider a particle with kinetic energy 'K'

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

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

then wavelength,

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}$$

In terms of 'V' (potential difference)

$$\frac{1}{2}mv^2 = qV \rightarrow p^2 = 2mqV \Rightarrow p = \sqrt{2mqV}$$

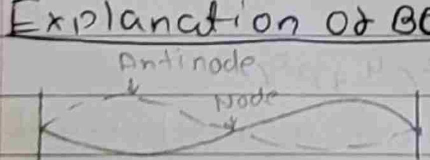
$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mqK}}$$

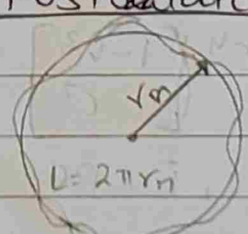
$q = e$ [for electron]

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

$$\lambda = \frac{12.28}{\sqrt{V}} \times 10^{-10}\ m$$

Explanation of BOHR's second Postualate of Quantization





For electron moving in the n^{th} orbit,

$$2\pi r_n = n\lambda$$

$n = 1, 2, 3 \ldots$

i.e, Circumference od orbit should be integral multiple od de-broglie wavelength od electron moving in n^{th} orbit.

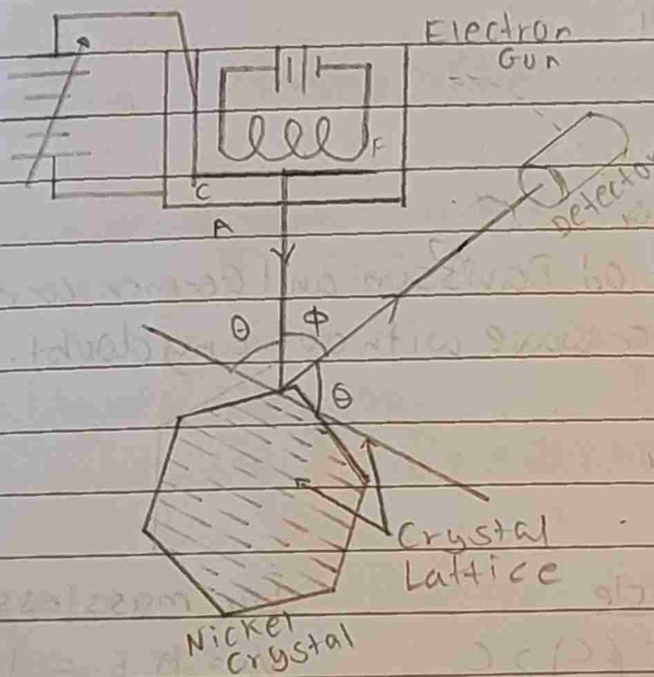
we know,

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

$$\frac{2\pi r_n}{n} = \frac{h}{mv_n}$$

$$\boxed{mv_n r_n = \frac{nh}{2\pi}}$$

Davisson-Germer experiment



→ A beam od eletrons emitted by the electron gun is made to fall on nickel crystal cut along cubical axis at a particalar angle

→ The scattered beam od electrons is received by the detector which can be rotated at any angle.

→ The energy od incident beam od electrons can be varied by changing the applied voltage to the electron gun.

→ Intensity od scattered bean od electron is found to be max. when angle od scattering (φ) is 50° and accelerating potential is 54V

$\theta + 50 + \theta = 180$

$\boxed{\theta = 65^\circ}$

$d = 0.91 Å$ → For Ni crystal

$n = 1$ → First principal Maximum.

Bragg's Equation,

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

$\lambda = 2 \times 0.91 \times \sin 65^\circ$

$\boxed{\lambda = 1.65 Å}$ - ①

Now,

Using de broglie,

$\lambda = \frac{h}{\sqrt{2meV}} = \frac{12.28 \times 10^{-10}}{\sqrt{54}}$ Am $= \boxed{1.66 Å}$ - ②

Since ① ~~≈~~ ≈ ②,

~~This result thus~~

Thus the result od Davisson and Germer condirms the de-broglie concept od matter wave without any doubt.

Phase velocity

$V_P = \lambda \nu$

For massive particle

$V_P = \frac{h}{mv} \times \frac{mc^2}{h} = c\left(\frac{c}{v}\right) > c$

For massless particle.

$V_P = \frac{h}{p}\frac{E}{h} = \frac{1}{p}\frac{pc}{1} = c$

Phase velocity does not describe particle motion.

Properties od matter Waves

→ Associated with moving particles.

→ Wavelength inversely propotional to mass and velocity.

→ Independent od nature od charge.

→ Niether electromagnetic nor mechanical waves.

→ Associated with Probability of finding particle
→ Phase velocity is not significant for the matter waves.
→ ~~A velocity is not significant for the matter waves.~~
→ A velocity called group velocity is significant ~~of~~ for the matter waves
→ Quantity associated is called wavefunction
$\Psi(x, y, z, t) = A + iB$
→ $|\Psi|^2$ is real and called probability of finding the particle.

Normal wave	Matter wave
→ Are disturbance in space	→ Disturbance is $\Psi(x,y,z,t)$
→ Carry energy from one place to another	→ Probability amplitude Ψ
→ Often will obey the classical wave equation	→ Probaility density $P(x,y,z,t) = \|\Psi\|^2$

Not a difference

Group velocity

$\Psi_1 = A\cos(\omega t - kx)$

$\Psi_2 = A\cos[(\omega+\Delta\omega)t - (k+\Delta k)x]$

$\Psi = \Psi_1 + \Psi_2$

$\Psi = 2A\cos\frac{1}{2}[(2\omega+\Delta\omega)t - (2k+\Delta k)x]\cos\frac{1}{2}\{(\Delta\omega)t - (\Delta k)x\}$

with $\Delta\omega \ll \omega \ll k$

$$\boxed{\Psi = 2A\cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right]\cos[\omega t - kx]}$$

Phase velocity = wave velocity of carrier : $\boxed{V_p = \frac{\omega}{k}}$

group velocity = wave velocity of envelope : $\boxed{V_g = \frac{\Delta\omega}{\Delta k}}$

For more than two wave contributions : $\boxed{V_g = \frac{d\omega}{dk}}$

$$\omega = 2\pi\nu = 2\pi \frac{E}{h} = \frac{2\pi}{h}\left[\frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}}\right]$$

$$K = \frac{2\pi}{\lambda} = \frac{2\pi}{h}(mv) = \frac{2\pi}{h}\left[\frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}\right]$$

$$V_g = \frac{d\omega}{dK} = \frac{d\omega/dv}{d\omega/dx} \quad -(1)$$

$$\frac{d\omega}{dv} = \frac{2\pi\, m_0 c^2 v}{h(1-v^2/c^2)^{3/2}} \quad -(2)$$

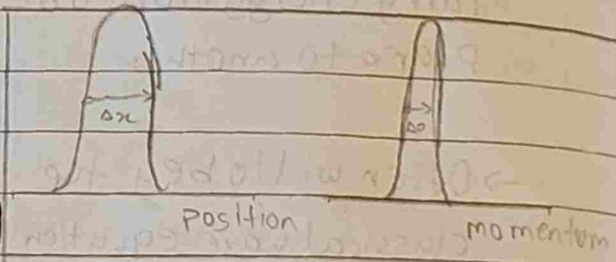
$$\frac{dK}{dv} = \frac{2\pi\, m_0 c^2}{h(1-v^2/c^2)^{3/2}} \quad -(3)$$

$\boxed{V_g = v}$ [From (1), (2) & (3)]

Heisenberg's Uncertainty Principle

It is not possible to precisely specify a particle's position & momentum at the same time

$\Delta x \Delta p_x \geq \hbar/2$	Other forms: [2D]
$\Delta y \Delta p_y \geq \hbar/2$	1. Energy-time: $\Delta E \Delta t \geq \frac{h}{2\pi}$
$\Delta z \Delta p_z \geq \hbar/2$	2. Ang. Post-Ang momentu.:
	$\Delta\theta \Delta L \geq \frac{h}{2\pi}$ [In 3D $h/4\pi$]



Implication

→ It is impossible to know both the position & momentum exactly ie, $\boxed{\Delta x = 0}$ & $\boxed{\Delta p = 0}$

→ These uncertanities are inherent in the physical world and have nothing to do with the skill of observer

$\boxed{\hbar = 1.054 \times 10^{-34} \text{ [J.s]}}$

→ Because 'h' is so small, these uncertainties are not observable in mormal everyday situations.

→ Example of Baseball

- A pitcher throws a 0.1 kg baseball at 40 m/s
- So momentum is $0.1 \times 40 = 4$ kg m/s
- Accuracy of 1%: $\Delta P = 0.01 P = 4 \times 10^{-2}$ kg m/s

- The uncertainty in Position is then
$\Delta x \geq \frac{h}{4\pi \Delta P} = 1.3 \times 10^{-33}$ m

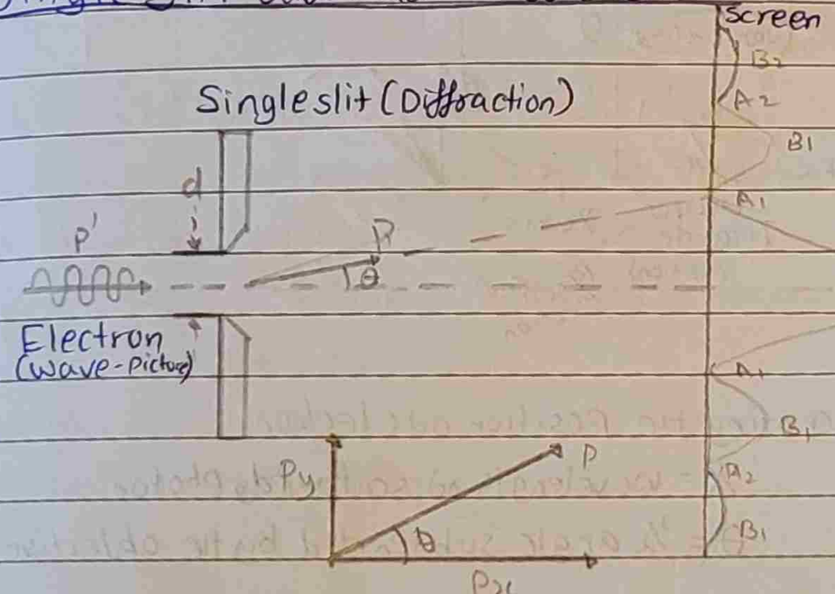
- No wonder one does not observe the effect of the uncertainty principle in everyday Life!

→ Example of Electron

- The electron which has mass 9.11×10^{-31} Kg travelling at 40m/s
- So momentum = 3.6×10^{-29} Kgm/s
and ~~its~~ $\Delta P = 3.6 \times 10^{-31}$ Kg m/s
- The uncertainty in postion is then
$\Delta x \geq \frac{h}{4\pi \Delta P} = 1.4 \times 10^{-4}$ m

Proof

Single slit diffraction of electron



B_0 : central maximum
B_1 : Secondary maxima
A_n : minima

⇒ Before entering the slit, the electron has a definite momentum 'p' and after passing through the slit the electrons get diffracted

For First minima,

$\Delta x \sin\theta = \lambda \quad [\because d\sin\theta = n\lambda]$ — ①

$\Delta x = \dfrac{\lambda}{\sin\theta}$ — ②

Since electron can be anywhere in the diffraction pattern from $-\theta$ to θ

$\therefore$ Uncertainty od electron,

$\Delta p = p\sin\theta - p\sin(-\theta) = 2p\sin\theta$

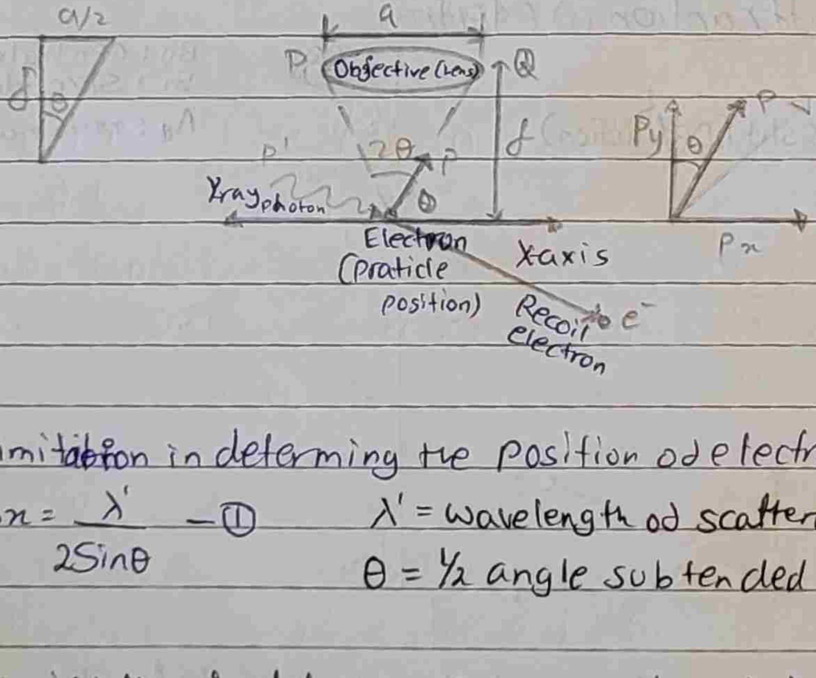
$\Delta p = \dfrac{2h}{\lambda}\sin\theta$ — ③

From ② & ③

$\Delta x \Delta p = \dfrac{\lambda}{\sin\theta} \times \dfrac{2h}{\lambda}\sin\theta = 2h$

$\boxed{\Delta x \Delta p \not> h}$

Gamma-ray microscope



a) Limitation in determing the position od electron.

$\Delta x = \dfrac{\lambda'}{2\sin\theta}$ — ①

λ' = wavelength od ~~scattered~~ scattered photon

θ = ½ angle subtended by the objective at the object

b) Limitation in determing the momentum od electron.

$p = \dfrac{h}{\lambda} \rightarrow$ Incident photon

$p' = \dfrac{h}{\lambda'} \rightarrow$ scattered photon

For OQ,

$p' = \frac{h}{\lambda'} \sin\theta$ → Along x-axis [scattered photon]

$p'' = \frac{h}{\lambda} - \frac{h}{\lambda'} \sin\theta$ → Along x-axis [imparted to the electron]

For OP,

$p_1' = -\frac{h}{\lambda'} \sin\theta$ → Along x-axis [scattedphoton]

$p_1'' = \frac{h}{\lambda} - \left(-\frac{h}{\lambda'} \sin\theta\right) = \frac{h}{\lambda} + \frac{h}{\lambda'} \sin\theta$ → Along x axis [Impartedtothe electron]

$\therefore \Delta P_x = \frac{h}{\lambda} + \frac{h}{\lambda'} \sin\theta - \frac{h}{\lambda} + \frac{h}{\lambda'} \sin\theta$

$\Delta P_x = \frac{2h}{\lambda'} \sin\theta$ — (2)

From (1) & (2)

$\Delta x \Delta P_x = \frac{\lambda'}{2\sin\theta} \times \frac{2h}{\lambda'} \cancel{\sin\theta} \sin\theta = h$

$\boxed{\Delta x \Delta P_x \geq h}$

Application

Non existence od electron in the nucleus

→ Size od nucleus = 10^{-14} m

→ If electron is present in the nucleus uncertainty in the position od electron $\Delta x = 10^{-14}$ m

$\Delta x \Delta p \geq \hbar$

$\Delta p \geq \frac{1.055 \times 10^{-34}}{10^{-14}}$

$\boxed{\Delta p = 1.05 \times 10^{-20} \text{ kg m/s}}$

→ The mim. momentum od the electron must be at least equal to uncertainty ~~od~~ in momentum.

$P = \Delta P = 1.05 \times 10^{-20}$ kg m/s

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

$E = pc$

$$E \approx \frac{1.05\times10^{-20}\times3\times10^{8}}{1.6\times10^{-19}} \text{ MeV} = 20 \text{ MeV}$$

Kinetic energy

Classical

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

Quantum operator

$$p^2 - \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

In 3D,

$$T = \frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] = \boxed{\frac{-\hbar^2}{2m}\Delta}$$

Schrödinger equation

→ Time-dependent

$$\frac{\partial \psi}{\partial t} = Ae^{i(kx-\omega t)}\times(-i\omega) = -i\omega\psi = -i\,2\pi\frac{h}{E}\psi = \boxed{-\frac{iE}{\hbar}\psi}$$

$$\boxed{\therefore i\hbar\frac{\partial\psi}{\partial t} = E\psi} \quad -① \leftarrow \text{(Energy operator)}$$

Similarly,

$$\frac{\partial\psi}{\partial x} = Ae^{i(kx-\omega t)}\times(ik) = ik\psi = \frac{ip}{\hbar}\psi$$

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

Multiply both side by $\hbar^2/2m$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\psi = \boxed{K\psi} \quad -②$$

$V(x)\,\psi(x,t) = V\psi$ [$V(x)$ → potential energy operator]

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t)} \rightarrow [STDE]$$

→ Time - Independent

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

Dividing by $\phi(x) f(t)$

$$i\hbar \frac{1}{f}\frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m\phi}\frac{\partial^2 \phi}{\partial x^2} + V(x) = S$$

we get,

$$\boxed{S = \hbar\omega = E}$$

~~$i\hbar$~~

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

Multiple by $\phi(x)$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \phi}{\partial x^2} + V(x)\,\phi(x) = E\,\phi(x)} \rightarrow (STIE)$$

$$\boxed{H = -\frac{\hbar^2}{2m}\Delta + V} \rightarrow (\text{Remember})$$

→ Applied to free praticle

- Considera particle of mass 'm' moving along +ve x axis.
- Particle is said to be free if it is not under the influence of
- any force or field
- ∴ $V = 0$ [Potential energy]

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

$$\boxed{V = 0}$$

①

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0$$

$$\boxed{\hbar = \frac{h}{2\pi}}$$

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

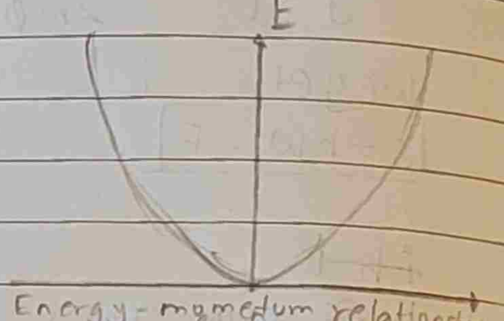
Let $K^2 = \frac{8\pi^2 mE}{h^2}$

$$\frac{\partial^2 \psi}{\partial x^2} + K^2 \psi = 0$$

$$\psi = A e^{iKx} + B e^{-iKx}$$

Since there is no boundary conditions A, B and K can have any values

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



Energy-momentum relationship for a free particle

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

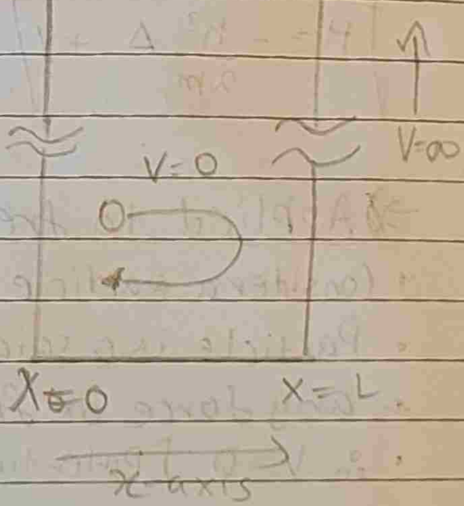
→ Since 'K' has no restriction, 'E' has no restriction.

→ Free particle can have any value of Energy.

Motion of electron

→ 1D potential well

- Consider a particle (like electron) of mass 'm', moving along positive x-axis between two walls of $V=\infty$ Infinite height, one located at $x=0$ and another at $x=L$
- Let $V=0$ in the region between the two walls and infinity in the region beyon the wall



$V=0$ for $0 \le x \le L$

$V=\infty$ for $x<0$ & $x>L$

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

$V=0$ for $0 \le x \le L$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0$$

The solution od the equation

$\psi = Ae^{ikx} + Be^{-ikx}$ Refer 1

at $x=0$, $\psi=0$ — (I)

at $x=L$, $\psi=0$ — (II)

∴ The correct equation:-

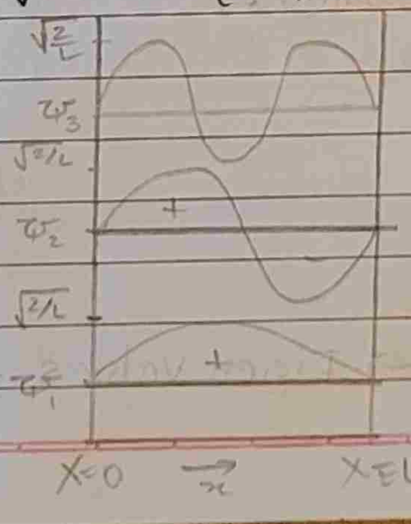
$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ where $m = 1, 2, 3 ---$

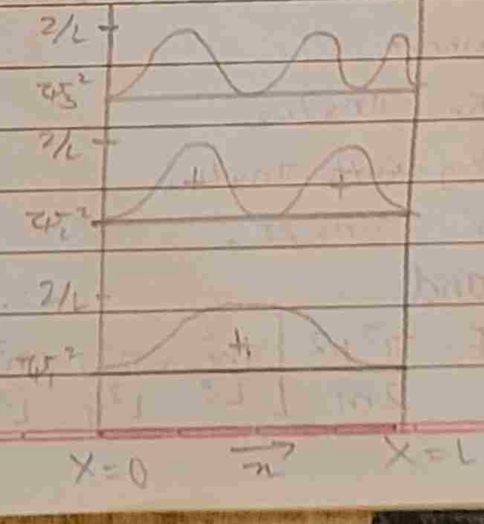
The possible values od ψ are called eigen functions.

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

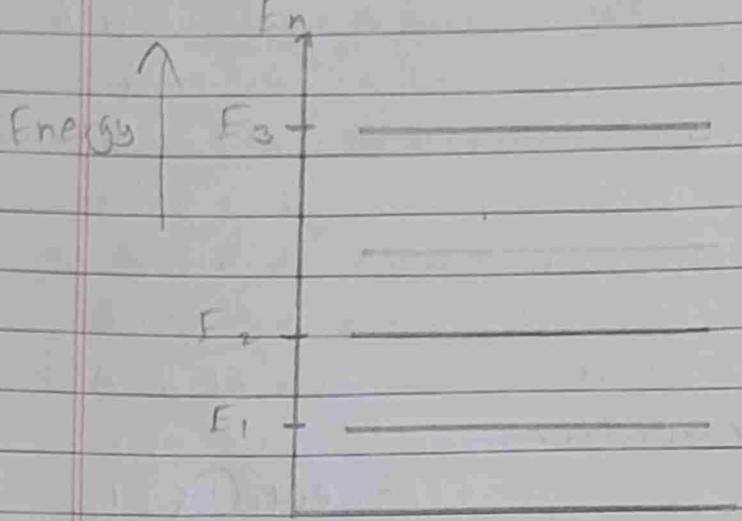
The possible values od energy are called eigen values

$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n x}{L}\right)$ where $n = 1, 2, 3 ---$

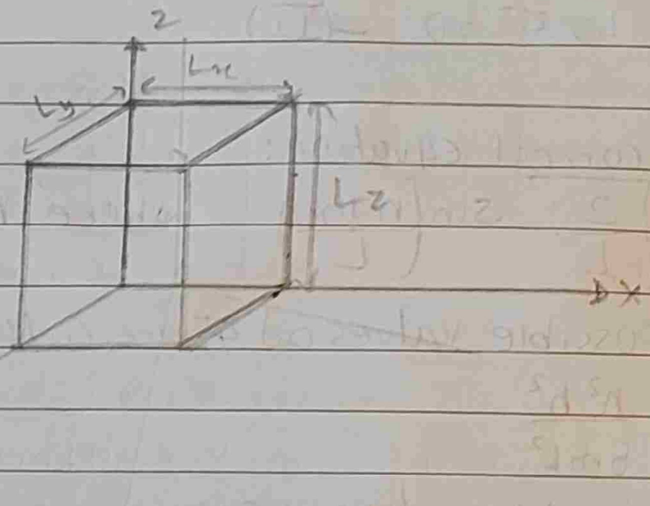




$$E_n = \frac{n^2 h^2}{8mL^2} \quad \text{where } n = 1, 2, 3 \text{ ---}$$



→ <u>3D potential well</u>



→ It's easy to show that:

$\psi(x, y, z) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$

where,

$k_x = \pi n_x / L_x$

$k_y = \pi n_y / L_y$

$k_z = \pi n_z / L_z$

and

$$E = \frac{\pi^2 h^2}{2m} \left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right] \rightarrow \text{Eigen values}$$

When the box is a cube

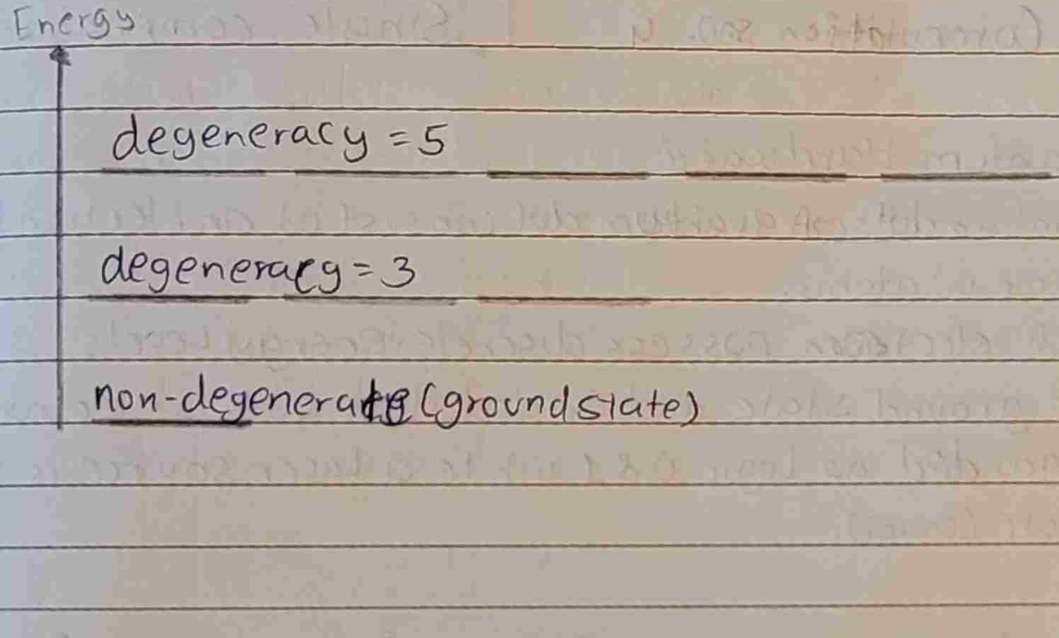
$$E = \frac{\pi^2 h^2}{2mL^2}\left[n_x^2 + n_y^2 + n_z^2\right) \leftarrow \text{Eigen values} \quad L_x = L_y = L_z = L$$

$$\left.\begin{aligned}
\psi_{(x)} &= \sqrt{\frac{2}{L}}\,\sin\left(\frac{n_x \pi x}{L}\right) & n_x &= 1, 2, 3 \ldots \\
\psi_{(y)} &= \sqrt{\frac{2}{L}}\,\sin\left(\frac{n_y \pi y}{L}\right) & n_y &= 1, 2, 3 \ldots \\
\psi_{(z)} &= \sqrt{\frac{2}{L}}\,\sin\left(\frac{n_z \pi z}{L}\right) & n_z &= 1, 2, 3 \ldots
\end{aligned}\right\} \text{Eigen functions}$$

Degeneracy

→ The energy Level is said ~~tobe~~ be degenerate if it corresponds to two or more different measurable states of a quantum system.

→ Conversely, two or more different states of quantum mech. system are said to be degenerate if they give the same value of energy upon measurement.



Quantum computing

→ A quantum computor' is that machine, which utilizes quantum mechanical effect such as super position or quantum entanglement to improve Computational power.

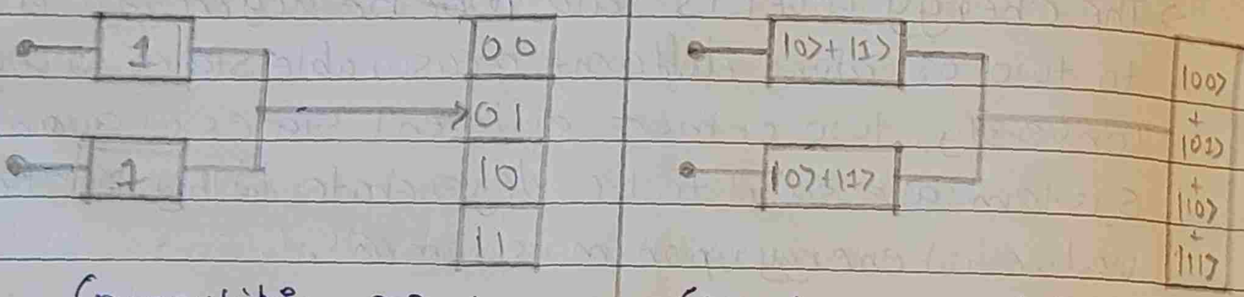
→ ~~Acta~~ classical computer encodes information as a string od binary digits or bits

→ Quantum computers supercharge processing power because they use quantum bits (qubits)

→ Qubits can ~~exis~~ t with two possible states (0 & 1) is represented as:

$|\psi\rangle = a|0\rangle + b|1\rangle$

A classical register | A quantum register



Computation no. 4 | Single computation step

Quantum Hardware

1) Quantum dots:→ A quantum dot consist od an electron trapped in a cage od atoms.

→ Such electron possess discrete energy Levels

→ The ground state and exicted state od this electron are regarded as Logic 0 & 1 while a Laser source is used as a gate (control).

2) Ion traps:→ It uses some ions such as Ca.

→ This Ca atom/ion in it's groundstate & meta stable state is interpreted as logic 0 & 1 respectively.

3) NMR :→ in this qubits are represented by nuclear spin states using nuclei of certain elements

→ A magnetic field is used as gate.

Important differences

Electromagnetic waves	Matter waves
1) EM waves are associated with photon, which has $m_0 = 0$	1) Are associated with all moving material particle having $m_0 \neq 0$
2) A single de-broglie wave can be associated with the particle	2) A single de-broglie wave cannot be associated with the material particle
3) The quantities that vary periodically with space & time are eletric & magnetic fields	3) The quantity that vary periodically with space & time are called wave function.
4) Electric and magnetic fields are real physical quantities and can be measured experimentally	4) The wave function is an abstract mathematical quantity & has no direct physical interpretation.
5) square of field amplitude gives intensity of ~~EM waves~~ Electromagnetic wave.	5) Square of wave function give probability of locating the partical in given ~~interval~~ interval.

Computor

Classical	Quantum
1) Uses semi conductor-based CMOS Logic gate	1) May use atomic, electronic, nuclear or photonic properties.
2) ON/OFF state of CMOS transistor determines logic ~~to~~ 0 or 1	2) Logic 0 or 1 represented by spin up or spin down, ground or exicited state etc
3) Bit can be 0 or 1 at a time	3) Qubit can be 0 and 1 at a time
4) Processor executes bit by bit operator	4) Processor ~~executes~~ operates on all bits simultaneously