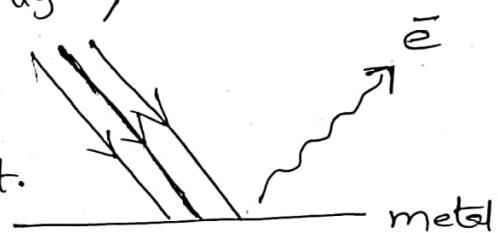


UNIT IV Dual Nature of Matter and Radiation

Photo electric effect: photo electric effect was discovered by Hertz and explained by Einstein. When U.V light (or) monochromatic e.m radiation falls on the surface of metals like Li, Na, K etc, then the metal surface emits electrons. This phenomenon is known as P.E.E. The emitted electrons are called photo electrons and the metal that emits electrons is known as photometal. The current (U.V light) constituted with the flow of these electrons is known as photo current.



Threshold frequency (ν_0): The minimum frequency of photo radiation at which a photo electron is emitted but no K.E is called Threshold frequency.

Threshold wavelength (λ_0): The maximum possible value of wavelength of incident radiation at which photo electrons are emitted with no K.E is called threshold wavelength.

Work function (W): The minimum amount of light energy required to pull (or) remove an electron from the metal surface is called work function (W). It can be measured in electron Volt.

'W' is constant for a given metal. Its value changes from metal to metal. For Na, W is 1.9 eV.

$$\therefore W = h\nu_0 = h \frac{c}{\lambda_0}, \quad h \rightarrow \text{Planck's Constant}$$
$$\nu_0 \rightarrow \text{Threshold frequency}$$
$$c \rightarrow \text{Velocity of light in Vacuum}$$
$$\lambda_0 \rightarrow \text{Threshold wavelength.}$$

$$W = \frac{12400}{\lambda_0 (\text{in } \text{\AA})}$$

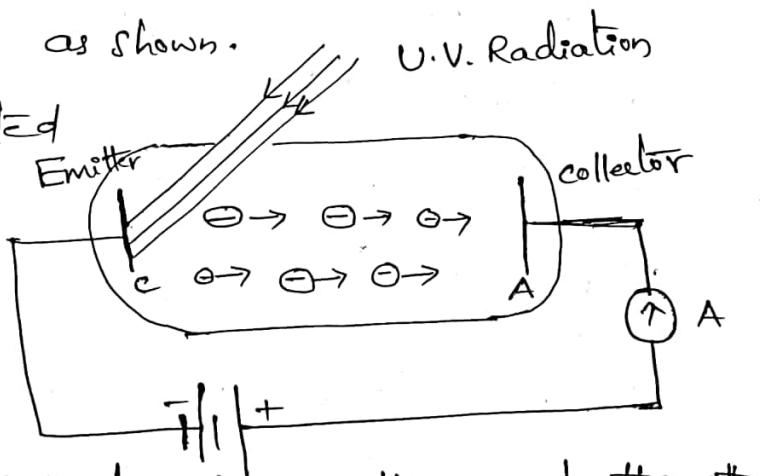
This formula holds good if λ_0 is in \AA and 'W' is e.V.

Hertz and Lenard observations on P.E.E.

The experimental set up is as shown.

It consists of an evacuated glass tube. Two electrodes are placed at the two ends of a glass tube.

out of two electrodes (zinc plates) one will act as Cathode (or) emitter and the other will act as Anode (or) collector.



Monochromatic light of short wavelength is allowed to fall on the Cathode, then electrons will get emitted. So, when light falls on photo sensitive plate electrons get emitted from emitter and get attracted towards the other metal plate (Anode).

Therefore, electric current is setup between Cathode and Anode due to the flow of electrons. This current is called photo current which can be measured by

(2)

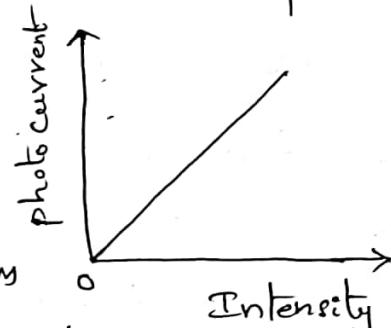
Ammeter. This experiment was helpful in studying the variation of photo current as we change the frequency of incident radiation (or) as we change the intensity of light (or) as we change the P.D between the two plates.

We will see the conclusions of this experiment.

Conclusion 1

Variation of photo current with intensity of light.

To explain the variation of photo current with intensity of radiation, first the frequency of light was kept fixed and the P.D between the plates was also kept fixed. Then it was observed like this when the intensity of light was increased, the photo current was also increases linearly with time. photo current means the no. of photo electrons per unit time. As the intensity of incident light was increased, the no. of photo electrons per second also increased with time. As the photo electrons per second increases, photo current also increases.



Conclusion: 2

Variation of photo current with Potential.

Now let us study variation of current with P.D between

the two plates.. When we talk about the potential there are two types. one is +ve potential and the other one is -ve potential.

'+ve' and '-ve' potentials:

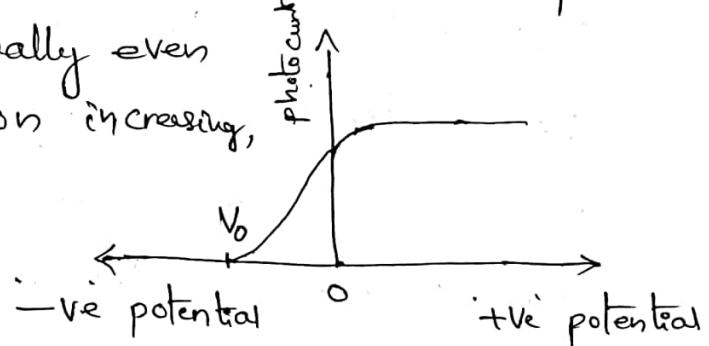
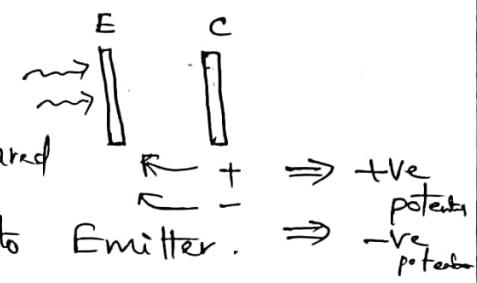
If we keep the collector at higher potential compared to emitter. i.e collector is +ve w.r.t. Emitter. This is +ve potential. Similarly if we keep the Collector at lower potential as compared to emitter potential.

Now look at the first scenario. ie '+ve' potential. If the collector is +ve, then electrons emitted from emitter will get attracted by collector. So electrons will keep flowing towards collector. Hence photo current increases. Gradually even if the +ve potential keeps on increasing, the photo current is same.

i.e. photo current becomes saturated because no more free photo electrons to flow.

If we look at the scenario - 2, ie '-ve' potential. If the collector is at -ve potential w.r.t. emitter. ie the collector was at lower potential. Therefore, the electrons flowing from emitter will be repelled by collector. So, photo current will decrease.

It was found, at a particular value of -ve potential (Retarding potential), the photo current drops to zero.



The $-ve$ potential at which the photo current drops to zero is called stopping potential (V_0). (3)

$$\therefore K_{\max} = eV_0$$

The maximum K.E of photo electron can be written as

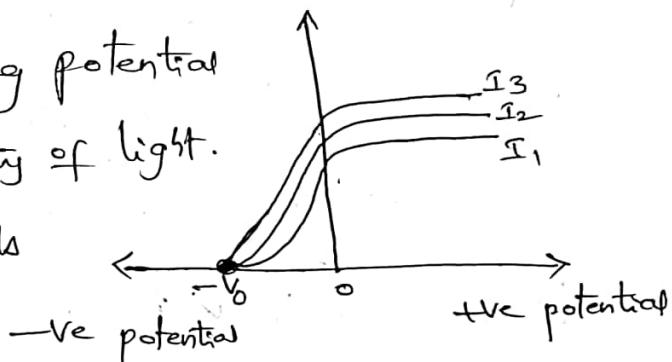
$$K_{\max} = eV_0 \quad (\because F = E q)$$

for a given frequency of incident radiation, stopping potential is independent of intensity.

Let us see, how the intensity of light varies with V_0 .

This shows that the stopping potential does not depends on intensity of light.

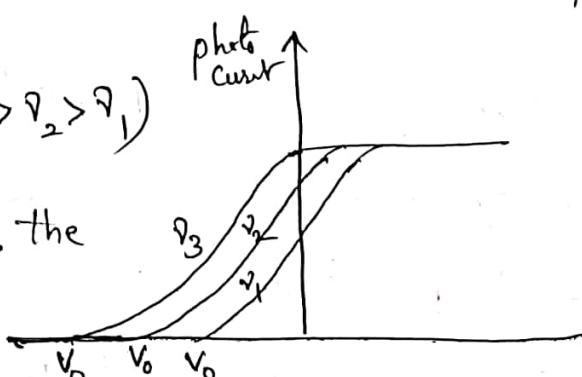
But saturation current depends upon with intensity of light.



Conclusion-3: Variation of photo current with frequency of radiation.

The variation of photo current with frequency of radiation is as shown.

As the frequency of incident radiation changes, the stopping potential changes. $(\nu_3 > \nu_2 > \nu_1)$

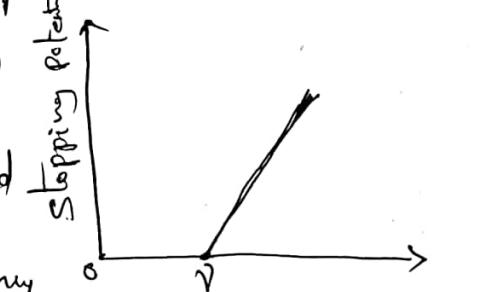


For maximum frequency, V_0 is more, for minimum frequency V_0 is less. The photo current does not change.

$$\therefore V_o \propto \nu$$

∴ photo current is independent of frequency of incident radiation. For a frequency lesser than specific value, no photo electric emission took place.

By drawing a curve between V_o & ν



it was observed that there should be a minimum value of frequency (ν_0) for incident radiation, so that photo current will take place. That minimum frequency is called threshold frequency (ν_0). It is also observed that increasing the frequency will also effect the stopping potential (V_o).

The minimum frequency of incident radiation below which photo electric emission does not occur is called threshold frequency (ν_0).

Photo Electric Equation of Einstein

Einstein proposed particle theory of light.

According to Einstein the radiation consists of small particles called photons. Each particle has energy $E = h\nu$, where $h \rightarrow$ Planck's constant, $\nu \rightarrow$ frequency

(4)

Einstein gave an equation which was able to satisfactorily explain all the observed behaviour of photoelectric effect called Einstein photo electric equation.

Einstein told when radiation falls on the metal plate, that means photons of each energy $E = h\nu$ falls on the electrons of metal surface. So each photon will interact with electrons and absorbed by the electron. The electron gains that amount of energy $h\nu$.

If the amount of energy which the electron gains is greater than the work function of the metal, then the electron will escape out of metal plate.

∴ According to him $h\nu = \omega + K \cdot E_{\max}$

i.e., the incident photon energy is partly used to overcome the work function and remaining energy will be in the form of $K \cdot E_{\max}$.

$$\therefore h\nu = h\nu_0 + \frac{1}{2}mv^2 \quad (\because \omega = h\nu_0)$$

$$\begin{aligned}\therefore \frac{1}{2}mv^2 &= h\nu - h\nu_0 \\ &= h(\nu - \nu_0) \\ &= h\left(\frac{c}{\lambda} - \frac{c}{\lambda_0}\right)\end{aligned}$$

$$\boxed{\therefore \frac{1}{2}mv^2 = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)}$$

This is called Einstein photo electric equation.

Laws of P. E. Emission and explanation based on Einstein photo electric equation:

Ist law: The max. Velocity of emitted photo electron is independent of intensity of incident radiation.

Explanation: Einstein photo electric equation is given by

$$h\nu = \omega + \frac{1}{2}mv^2 \Rightarrow \boxed{\frac{1}{2}mv^2 = h\nu - \omega}$$

∴ It is clear that $\frac{1}{2}mv^2$ and hence the max. velocity of electron is independent of intensity of light.

If the intensity of incident radiation increases, the no. of photons striking per unit area increases.

∴ The no. of collisions increases and hence the no. of photo electrons emitted increases. Due to this photo electric current increases with the increase in intensity of incident radiation. As there is no change in the nature of collision, there is no change in the max. Velocity of emitted photo electron.

IInd law, The max. Velocity (max. K.E) of emitted photo electron increases with the increase in the frequency of incident radiation.

Explanation: W.R.T $h\nu = \omega + \frac{1}{2}mv^2$
For a given metal, ω is constant.

$$\therefore h\nu \propto \frac{1}{2}mv^2 \Rightarrow \nu \propto V^2$$

$$\therefore \boxed{V = \sqrt{\nu}}.$$

∴ As V increases, then V also increases and concluded that $V \propto \sqrt{V}$.

IIIrd law: For every metal surface there exist a threshold frequency above which only photo electric emission takes place.

$$N \cdot K \cdot T \quad h\nu = W + \frac{1}{2}mv^2$$

According to IInd law of photoelectric emission, Velocity of emitted photo electron increases with the increase in frequency of incident radiation. Also, if $\nu \downarrow \infty$, then V also decreases and at a particular frequency of incident radiation the Velocity of emitted photo electron becomes zero. This frequency at which the Velocity of emitted photo electron becomes zero is known as threshold frequency or critical frequency. It depends on the nature of metal used.

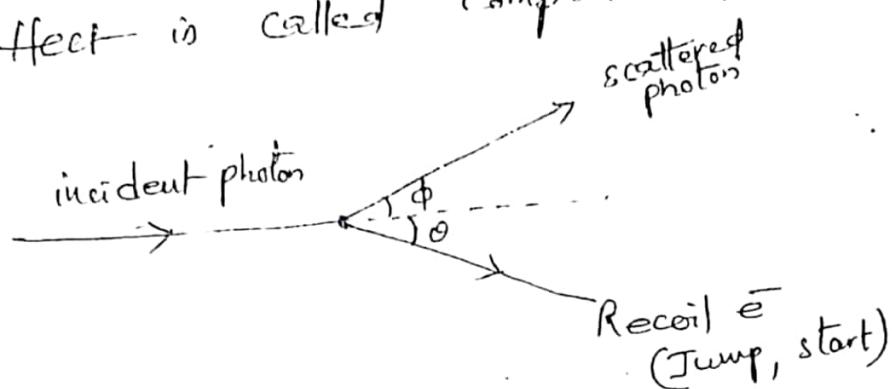
4th law: There is no time lag in the process of photoelectric emission. i.e as and when the photon falls on atom, it emits the photo electron immediately.

Explanation: Einstein photo electric equation is derived based on the assumption that a perfectly elastic Collision takes place between photon & the atom. Any elastic collision takes place in about 10^{-8} sec. ∴ No time lag during this process.

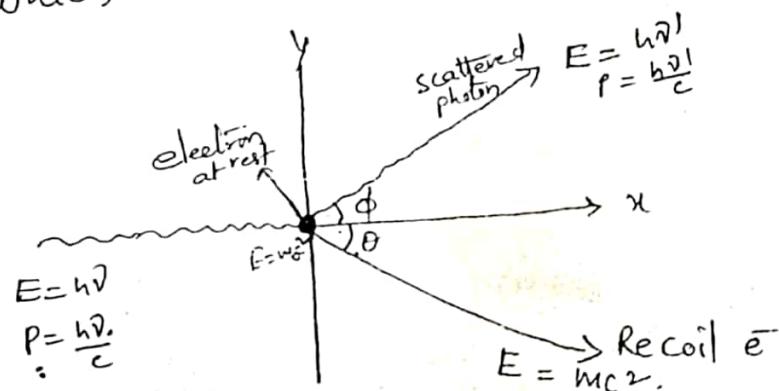
Compton effect :- When a monochromatic beam of x-rays is allowed to fall on certain substances of low atomic weight like Carbon, the x-ray beam is scattered and it consists of two components.

- ① The radiation having same wavelength as that of the incident radiation.
- ② The other radiation with a higher wavelength compared to the incident wavelength.

The phenomenon of change in wavelength of the scatter of x-rays is called Compton shift. This effect is called Compton effect.



During the scattering process, Compton assumed that incident photon collides with a free electron in the scattering material. The photon transfers some of its energy to the electron which recoils with this kinetic energy



Consider a photon of energy $\underline{h\nu}$ collides elastically with a free electron.

Energy before collision

Energy of incident photon = $\hbar\nu$

" of \bar{e} at rest = m_ec^2

T.E before collision = $m_ec^2 + \hbar\nu$

Energy after collision

Energy of scattered photon = $\hbar\nu'$

" of recoil electron = $m_ec'^2$

T.E after collision = $m_ec'^2 + \hbar\nu'$

According to law of conservation of energy,

T.E before collision = T.E after collision

$$\boxed{\hbar\nu + m_ec^2 = \hbar\nu' + m_ec'^2} \quad \text{--- (1)}$$

As the momentum is a Vector Quantity,

x and y components of momentum before and after collisions should be calculated.

Momentum before Collision

X-component

Momentum of photon = $\frac{\hbar\nu}{c}$

" of electron = 0

T.M along X-axis = $\frac{\hbar\nu}{c} + 0$
= $\frac{\hbar\nu}{c}$

Y-component

Momentum of photon = 0

" of \bar{e} = 0

T.M along Y-axis = 0.

Momentum after Collision

X-component

Momentum of scattered photon = $\frac{\hbar\nu'}{c}$

" of recoil \bar{e} = $m_e v \cos\theta$

T.M along X-axis = $\frac{\hbar\nu'}{c} \cos\theta + m_e v \cos\theta$

Y-component

Momentum of scattered photon = $\frac{\hbar\nu'}{c} \sin\theta$

" of recoil, \bar{e} = $-m_e v \sin\theta$

T.M along Y-axis = $\frac{\hbar\nu'}{c} \sin\theta - m_e v \sin\theta$

Applying law of conservation of momentum.

T.M before Collision = T.M after collision

$$\text{along } x\text{-axis, } \frac{h\vec{v}}{c} = \frac{h\vec{v}'}{c} \cos\phi + m\vec{v} \cos\theta \quad \text{--- (2)}$$

$$\text{along } y\text{-axis, } 0 = \frac{h\vec{v}'}{c} \sin\phi - m\vec{v} \sin\theta \quad \text{--- (3)}$$

$$\text{multiplying (2) with } c, \text{ then } h\vec{v} = h\vec{v}' \cos\phi + m\vec{v} c \cos\theta$$

$$\text{multiplying (3) with } c, \text{ then } 0 = h\vec{v}' \sin\phi - m\vec{v} c \sin\theta$$

The above equations can be changed to

$$m\vec{v} c \cos\theta = h\vec{v} - h\vec{v}' \cos\phi$$

$$m\vec{v} c \sin\theta = h\vec{v}' \sin\phi$$

Squaring and adding these two, we get

$$m^2 v^2 c^2 = [h\vec{v} - h\vec{v}' \cos\phi]^2 + [h\vec{v}' \sin\phi]^2$$

$$m^2 v^2 c^2 = h^2 v^2 + h^2 v'^2 \cos^2\phi - 2 h^2 v v' \cos\phi + h^2 v'^2 \sin^2\phi$$

$$\therefore m^2 v^2 c^2 = h^2 v^2 + h^2 v'^2 - 2 h^2 v v' \cos\phi \quad \text{--- (4)}$$

$$\text{consider (1), } h\vec{v} + m\vec{v} = h\vec{v}' + m\vec{v}'$$

$$\Rightarrow m\vec{v}' = (h\vec{v} - h\vec{v}') + m\vec{v}'$$

$$\text{Squaring on both sides, } m^2 \vec{v}'^2 = [(h\vec{v} - h\vec{v}') + m\vec{v}']^2$$

$$m^2 \vec{v}'^2 = (h\vec{v} - h\vec{v})^2 + m^2 \vec{v}^2 + 2(h\vec{v} - h\vec{v}) \cdot m\vec{v}'$$

$$m^2 \vec{v}'^2 = h^2 v^2 + h^2 v'^2 - 2 h^2 v v' + m^2 \vec{v}^2 + 2(h\vec{v} - h\vec{v}) m\vec{v}'$$

--- (5)

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subtract (5) from (8)

$$m^{\nu}c^{\nu} [c^{\nu} - v^{\nu}] = -2h^{\nu}\gamma\gamma^1 + 2h^{\nu}\gamma\gamma^1 \cos\phi + 2(h^{\nu} - h^1) m_0 c^{\nu} \\ + m_0^{\nu} c^{\nu} \quad \text{--- (6)}$$

We know that from theory of relativity,

$$m = \frac{m_0}{\sqrt{1 - \frac{v^{\nu}}{c^2}}} \Rightarrow [m_0^{\nu} c^{\nu} = m^{\nu} (c^{\nu} - v^{\nu})]$$

Substitute this value in (6), we get

$$\cancel{m_0^{\nu} c^{\nu} \cdot c^{\nu}} = -2h^{\nu}\gamma\gamma^1 + 2(h^{\nu} - h^1) m_0 c^{\nu} + m_0^{\nu} c^{\nu} + 2h^{\nu}\gamma\gamma^1 \cos\phi$$

$$\therefore 0 = -2h^{\nu}\gamma\gamma^1 + 2(h^{\nu} - h^1) m_0 c^{\nu} + 2h^{\nu}\gamma\gamma^1 \cos\phi$$

$$0 = -2h^{\nu}\gamma\gamma^1 (1 - \cos\phi) + 2(h^{\nu} - h^1) m_0 c^{\nu}$$

$$+ 2h^{\nu}\gamma\gamma^1 (1 - \cos\phi) = + 2(h^{\nu} - h^1) m_0 c^{\nu}$$

$$\therefore \frac{2(h^{\nu} - h^1)}{m_0 c^{\nu}} = \frac{2h^{\nu}\gamma\gamma^1}{m_0 c^{\nu}} = \frac{1}{\gamma\gamma^1} - \frac{1}{\gamma}$$

$$\therefore \frac{1}{\gamma\gamma^1} - \frac{1}{\gamma} = \frac{2(1 - \cos\phi)}{m_0 c^{\nu}}$$

Multiply with 'c', we get,

$$\frac{c}{\gamma\gamma^1} - \frac{c}{\gamma} = \frac{hc}{m_0 c^{\nu}} (1 - \cos\phi)$$

$$\boxed{1 - \gamma = \frac{hc}{m_0 c} (1 - \cos\phi)}$$

This is Compton shift.

de-Broglie's hypothesis:

In 1924, de-Broglie extended dual nature to material particles like electrons, protons and neutrons. According to his hypothesis when particles are accelerated then those will be spread out like a wave with a certain wavelength. He gave simple mathematical equations to support his hypothesis as follows.

According to Planck's theory, the energy of a photon whose frequency ν can be expressed as $E = h\nu$

According to Einstein mass-energy relation $E = mc^2$, m - mass of a photon, c - velocity of a photon.

from these two $h\nu = mc^2$

$$\text{ie } \frac{h\nu}{c} = mc \Rightarrow \lambda = \frac{h}{mc} = \frac{h}{m\nu} = \frac{h}{P}$$

(PTO)

In the same way according to de-Broglie hypothesis if an electron of charge e , mass m is moving with a velocity v in the presence of the potential V , then the wavelength associated with that electron can be expressed as $\lambda = \frac{h}{mv} = \frac{h}{p}$, which is called de-Broglie's wave equation.

The energy of electron in terms of potential can be expressed as $E = eV$

The K.E. of an electron $K.E = E = \frac{1}{2}mv^2$

$$\therefore eV = \frac{1}{2}mv^2 \Rightarrow mv^2 = \frac{2eV}{m}$$

$$\therefore mv^2 = 2meV \Rightarrow p^2 = 2meV$$

$$\therefore p = \sqrt{2meV}$$

Now de-Broglie wave equation becomes,

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times V}}$$

$\boxed{\therefore \lambda = \frac{12.27}{\sqrt{V}} \text{ Å}}$. This is the wavelength associated with an electron in presence of P.D.

Matter Waves: According to de-Broglie's hypothesis, when the material particles like electrons are accelerated, then those will be spread out like waves called Matter waves.

- Properties:-
- ① The motion of the particles generate matter waves.
 - ② Lighter is the ~~Velocity~~ of the particle greater will be the wavelength associated with it.
 - ③ Smaller is the Velocity of the particle, greater will be the wavelength associated with it.
 - ④ These waves are a new kind of waves. They are not electro magnetic waves.
 - ⑤ The Velocity of matter waves depends on the Velocity of matter particles. i.e. it is not a constant.
 - ⑥ The Velocity of matter waves is greater than the Velocity of light.

wave function: -

In Quantum Mechanics, the motion of any atomic particle is described by a variable quantity which is known as a wavefunction. It is represented by ψ . It is a function of both position and time.

Physical significance:-

- ① It relates the wave and particle nature.
- ② ψ gives the information about the particle behaviour.
- ③ ψ is a complex quantity. so it can be expressed as $\psi = a+ib$. Hence its complex conjugate can be represented by $\psi^* = a-ib$.
- ④ The product of ψ and ψ^* ie $|\psi\psi^*|$ or $|\psi|^2 = a^2+b^2$, is a real quantity and positive. This $|\psi|^2$ represents the probability density, denoted by P . This means that the probability of finding a particle

at a particular position.

⑤ The probability of finding a particle in a closed volume dV is represented by $P = \int |\psi|^2 dV$ (or) $\int (\psi\psi^*) dV$ where $dV = dx dy dz$.

⑥ If $P=1$, then the condition is called normalisation property. i.e $\int \psi\psi^* dx dy dz = 1$ i.e there is 100% chance of finding a particle within the volume.

⑦ The wave function ψ has no physical meaning whereas as the probability density has a definite physical meaning.

*Heisenberg Uncertainty Principle:-

The product of uncertainties in determining the position and momentum of a particle is approximately equal to Planck's constant.

If Δx is the uncertainty in determining the position of a particle and Δp is the uncertainty in determining the momentum. Then

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

The uncertainty principle can also be applicable to conjugate variables. i.e $\Delta E \cdot \Delta t \geq \frac{\hbar}{4\pi}$ and

$\Delta J \cdot \Delta \theta \geq \frac{\hbar}{4\pi}$, where $\Delta E, \Delta t$ are uncertainties in energy and time while ΔJ and $\Delta \theta$ are angular momentum and angle.

In classical mechanics, a moving particle at any instant has a fixed position in space and a definite momentum which can be determined if the initial values are known.

In wave mechanics, the particle is described in terms of a wave packet.

When the wave packet is small (Localised), the position of a particle may be fixed but the wavelength ' λ ' is not fixed and hence the momentum is not fixed. (since $\lambda = \frac{h}{p}$). Because the wave is localised (or) finite

and beyond the points A and B 
no wave is present & it is also keeps on changing and hence λ is not fixed.

(λ keeps on changing)

On the other hand, when the wave packet is large. i.e the wave look like extended wave through out space. Hence the wavelength ' λ ' is fixed and hence momentum can be fixed. ($\therefore \lambda = \frac{h}{p}$) 
 λ is constant)

Extended wave
in space.

Because the wave is not a localised wave (or) it is extended wave in space and hence the position is not fixed (or) uncertainty.

Therefore, it can be concluded that the certainty in momentum involves the uncertainty in position and the certainty in position involves uncertainty in momentum.

Applications:

① Non existance of electron in nucleus.

We know that the size of the nuclei is of the order of $10^{-15} m$.

If an electron is present with in the nuclei, the uncertainty in its position should not exceed 10^{-15} m . Using Heisenberg uncertainty relation,

The uncertainty in momentum of electron is

$$\text{given by } \Delta P \geq \frac{\hbar}{4\pi} \times \frac{1}{\Delta x}$$

$$\therefore \Delta P \geq \frac{6.62 \times 10^{-34}}{4 \times \frac{2}{7} \times 10^{15}}$$

$$\therefore \Delta P \geq 0.5266 \times 10^{-19} \text{ kgm/sec.}$$

This means that the momentum of the electron in the nucleus must be at least of the order of $0.5266 \times 10^{-19} \text{ kgm/sec.}$

using relativistic formula, $E^2 = p^2 c^2 + m_0^2 c^4$

The energy of electron is given by $E^2 = p^2 c^2 + m_0^2 c^4$

$$\therefore E = (0.5266 \times 10^{-19} \times 3 \times 10^8)^2 + [9.11 \times 10^{-31} \times (3 \times 10^8)^2]^2$$

$$\therefore E = 100 \text{ MeV}$$

This means that if the electron exists inside the nucleus, it should have the energy of the order of 100 MeV.

But the electrons emitted during Beta decay of radioactive nuclei have energies less than 5 MeV. Hence it is evident that electrons do not exist in the nucleus.

② finite width of spectral lines:-

From Heisenberg uncertainty principle of energy and time relation, we have $\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$

Since the life time of electron in an excited state is finite ($\approx 10^{-8}$ sec), the energy level of an atom is $\Delta E \geq \frac{h}{4\pi \cdot \Delta t}$,

Schrodinger's time independent wave equation:

Having got convinced with the de-Broglie's concept of matter waves, Schrodinger developed a wave equation for moving particles like electrons. Schrodinger equation is a fundamental equation in Quantum Mechanics, which describes the behaviour of matter waves.

Let a particle of mass m in moving with a velocity v , then it is associated with a wave. Let ψ be the wave function of the particle.

The equation for a simple harmonic wave travelling in x -direction is $y = A \sin(\omega t - kx)$

Similarly, the wave function ψ associated with the moving particle be written as,

$$\psi(x, t) = \psi_0 \sin(\omega t - kx), \text{ where } \psi_0 \rightarrow \text{Amplitude}$$

$$\omega = \frac{2\pi}{T} = 2\pi\nu$$

Diff. this equation w.r.t x , $K = \frac{2\pi}{\lambda}$, propagation vector.

$$\frac{d\psi}{dx} = (-K) \psi_0 \cos(\omega t - kx)$$

$$\frac{d^2\psi}{dx^2} = (-K)(-K) \psi_0 [-\sin(\omega t - kx)]$$

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$$\therefore \frac{d^2\psi}{dx^2} = -k^2 \psi_0 \sin(\omega t - kx)$$

$$= -k^2 \psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2 \psi \quad \text{and hence} \quad \boxed{\frac{d^2\psi}{dx^2} + k^2 \psi = 0}$$

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

$$\Rightarrow \frac{d^2\psi}{dx^2} + \left(\frac{2\pi}{d}\right)^2 \psi = 0 \quad (\because k = 2\pi/d)$$

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2}{d^2} \psi = 0 \quad \text{--- ①}$$

But from de-Broglie's hypothesis $\lambda = \frac{h}{mv}$

$$\text{then } d^2 = \frac{h^2}{m^2 v^2} \quad \text{--- ②}$$

$$\text{put ② in ①, we get } \frac{d^2\psi}{dx^2} + \frac{4\pi^2}{\left(\frac{h^2}{m^2 v^2}\right)} \psi = 0$$

$$\therefore \frac{d^2\psi}{dx^2} + \frac{4\pi^2}{h^2} (m^2 v^2) \psi = 0 \quad \text{--- ③}$$

The total energy of the particle $E = K.E + P.E$

for moving particle $K.E = \frac{1}{2} mv^2$ and

let $V(r)$ be the potential energy of electron.

$$\text{thus } E = K.E + P.E \Rightarrow E = \frac{1}{2} mv^2 + V(r)$$

$$\Rightarrow \frac{1}{2} mv^2 = E - V(r)$$

$$mv^2 = 2 [E - V(r)]$$

$$\Rightarrow m^2 v^2 = 2m [E - V(r)] \quad \text{--- ④}$$

put ④ in ③, we get $\frac{d^2\psi}{dx^2} + \frac{4\pi^2}{h^2} 2m [E - V(r)] \psi = 0$

$$\text{ie } \frac{d^2\psi}{dx^2} + \frac{4\pi^2}{h^2} 2m [E - V(r)] \psi = 0$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} [E - V(r)] \psi = 0 \quad \dots \textcircled{5}$$

In Quantum mechanics, most frequently $\hbar/2\pi$ occurs as \hbar . ie $\hbar = \frac{h}{2\pi}$, $\Rightarrow h = \hbar \times 2\pi$

$$\text{Hence } h^2 = \hbar^2 \times 4\pi^2 \quad \dots \textcircled{6}$$

put ⑥ in ⑤, we get $\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2 \times 4\pi^2} [E - V(r)] \psi = 0$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(r)] \psi = 0}$$

This is the one dimensional Schrodinger's time independent wave equation.

This equation can be extended in 3-Dimensional

$$\text{ie } \left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} \right) + \frac{2m}{\hbar^2} [E - V(r)] \psi = 0$$

$$\text{ie } \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \psi + \frac{2m}{\hbar^2} [E - V(r)] \psi = 0$$

$$\Rightarrow \boxed{\nabla^2 \psi + \frac{2m}{\hbar^2} [E - V(r)] \psi = 0}, \text{ where } \nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

In this equation as the time factor does not appear and hence it is called time independent.

Schrodinger's time dependent wave equation

Consider a particle of mass m moving along x -axis. Then the wave function associated with the moving particle be taken as $\psi(x)$.

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

$$\therefore \psi(x) = A e^{i(kx - \omega t)} \quad \text{--- (1)}$$

Let the energy of the particle be $E = K + E_F$

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

To replace the terms k and ω in equation (1), we can use $p = \hbar k$ and $E = \hbar \omega$.

put $k = \frac{p}{\hbar}$ and $\omega = E/\hbar$ in (1),

$$\text{we get, } \psi(x) = A e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)}$$

$$\begin{aligned} \therefore p &= \hbar k = \frac{\hbar}{2\pi} \times \frac{2\pi}{l} \\ p &= \frac{\hbar}{l} \Rightarrow l = \hbar/p \\ \text{and} \\ E &= \hbar \omega = \frac{\hbar}{2\pi} \times 2\pi f \\ \therefore E &= \hbar f \end{aligned}$$

$$\therefore \psi(x) = A e^{i\hbar(px - Et)} \quad \text{--- (3)}$$

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

$$\frac{d\psi}{dx^2} = -\frac{p^2}{\hbar^2} A e^{i\hbar(px - Et)}$$

$$\therefore \frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2} \psi \Rightarrow \boxed{p^2 \psi = -\hbar^2 \frac{d^2\psi}{dx^2}} \quad \text{--- (4)}$$

Again Consider $\frac{d\psi}{dt} = \left(-\frac{iE}{\hbar}\right) A e^{i/t} (px - Et)$

$$\therefore \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi \quad [\because \psi = A e^{i/t} (px - Et)]$$

$$\therefore E\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

$$\therefore E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad \text{--- (5)}$$

Consider the equation ②, $E = \frac{p^2}{2m} + V$

Take ψ on both sides, $\therefore E\psi = \frac{p^2\psi}{2m} + V(\psi)$

put ④ & ⑤ in this equation,

$$\therefore i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi$$

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = i\hbar \frac{d\psi}{dt}}.$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right] \psi = i\hbar \frac{d\psi}{dt}$$

Here $\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right] \psi = H$, H is called Hamiltonian operator

$$\boxed{H\psi = E\psi} \quad (\because E = i\hbar \frac{d}{dt})$$

\therefore Time dependent Schrodinger's wave equation

can be written as $\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = i\hbar \frac{d\psi}{dt}$

(a)

$$H\psi = E\psi$$

In 3-Dimension, it becomes,

$$\boxed{\frac{-\hbar^2}{2m} \nabla^2\psi + V\psi = i\hbar \frac{d\psi}{dt}}$$

* particle in a potential Box:-

suppose an electron of mass 'm'

moves back and forth in

a one dimensional crystal of

length 'L' parallel to x-direction. At the two ends of the crystal is at $x=0$ and at $x=L$

two potential walls of infinite height exist,

so that the particle may not penetrate the

walls. Assume that the P.E of the crystal is

constant. Let us assume the P.E of the

electron inside the crystal is zero.

As the particle is inside the potential box, the

probability of the particle inside the crystal

is equal to one. i.e. $|\psi(x)|^2$ or $|\psi|^2 = 1$ and

out side the potential box, the probability

$P = |\psi|^2 = 0$, Hence $\psi(x) = 0$ for $0 \geq x \geq L$.

This study will show Quantum nos., discrete

Values of energy, the wave function associated with particle

Consider one dimensional Schrödinger time independent wave equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0$$

for a free particle, $V(x) = 0$.

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

$$\text{Let } \frac{2m}{\hbar^2} E = k^2, \quad \text{--- (1)}$$

$\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0$ This is a second order differential equation in terms of ' ψ '.

It has a solution of $\psi(x) = A \sin kx + B \cos kx$

To find A and B, apply boundary condition

$$\textcircled{1} \quad \psi(0) = 0 \quad \text{at } x=0 \quad \textcircled{2} \quad \psi(L) = 0 \quad \text{at } x=L$$

Applying boundary condition $\textcircled{1}$, we get

$$0 = B \Rightarrow \boxed{B=0}$$

Applying boundary condition $\textcircled{2}$, we get

$$A \sin kL = 0 \Rightarrow kL = n\pi$$

$$\therefore k = \frac{n\pi}{L} \Rightarrow k^2 = \frac{n^2\pi^2}{L^2} \quad \text{--- (2)}$$

from $\textcircled{1}$ & $\textcircled{2}$

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

$$\therefore E_n = \frac{n^2 \pi^2 h^2}{2mL^2} = \frac{n^2 \pi^2 \times h^2}{4\pi^2 \times 2mL^2} = \frac{n^2 h^2}{8mL^2}$$

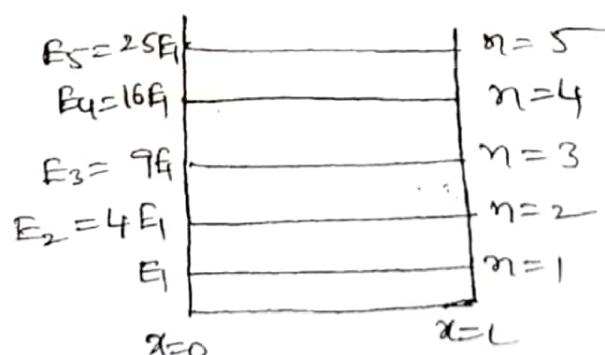
$$\boxed{E_n = \frac{n^2 h^2}{8mL^2}} \rightarrow \textcircled{3}$$

Equation \textcircled{3} indicates that a particle in the box can take discrete values of energy for $n=1, 2, 3, \dots$ ie energy is quantised.

These discrete values of energy are called Eigen values of energy or allowed energy states.

The no. n is called Quantum no.

From equation \textcircled{3}, the energy is inversely proportional to mass of the particle and square of the length of the potential box.



Wave function ψ :

wave function $\psi = A \sin kx$

$$\psi(x) = A \sin \left(\frac{n\pi}{L} \right) x$$

To find 'A', apply normalisation property,

$$\text{N} \int_0^L |\psi|^N dx = 1$$

$$\therefore \int_0^L A^n \sin^n\left(\frac{n\pi}{L}x\right) dx = 1$$

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

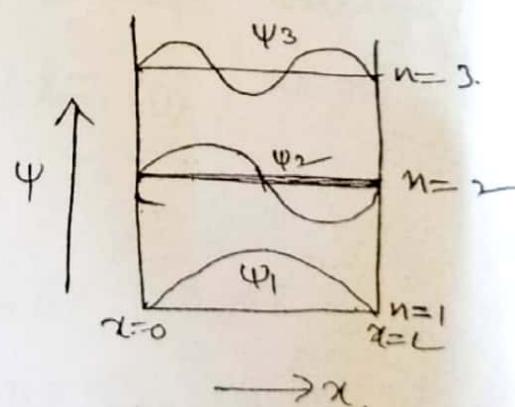
$$\therefore A^n \left[\frac{1}{2} [x]^L + 0 \right] = 1 \Rightarrow A^n = \frac{2}{L} \\ \Rightarrow A = \sqrt{\frac{2}{L}}$$

\therefore wave function $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$.

for $n=1$, ψ_1 has two nodes at $x=0$ and at $x=L$

for $n=2$, ψ_2 has 3 nodes at $x=0, \frac{L}{2}, L$

for $n=3$, ψ_3 has 4 nodes at $x=0, \frac{L}{3}, \frac{2L}{3}, L$



Probability density :-

We know that $P = \frac{2}{L} \sin^2\left(\frac{n\pi}{L}x\right)$

This is maximum when $\left(\frac{n\pi}{L}\right)x$ is $\frac{n\pi}{2}$, for $n=1, 3, 5$

$$\therefore \frac{n\pi}{L} x = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots$$

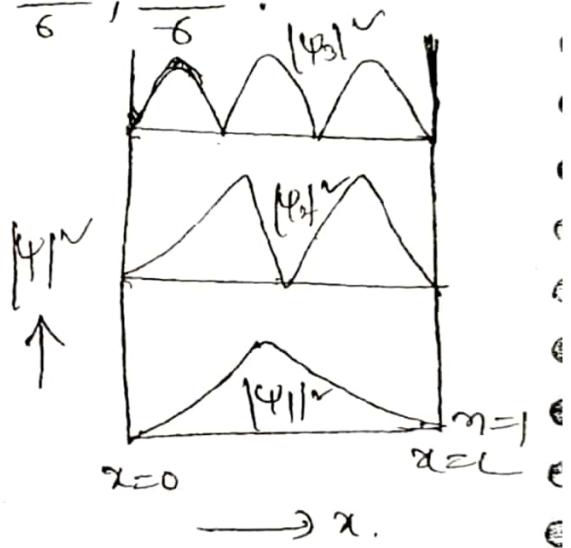
$$x = \frac{L}{2n}, \frac{3L}{2n}, \frac{5L}{2n}, \dots$$

for $n=1$, the most probable position of the particle is at $x=L/2$

for $n=2$, the most probable position of the particle is at $x=\frac{L}{4}, \frac{3L}{4}$

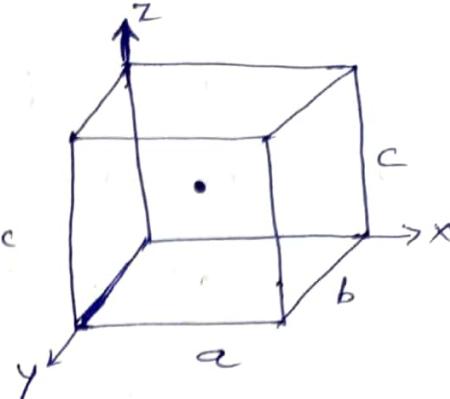
for $n=3$, the most probable position of the particle is at $x=\frac{L}{6}, \frac{3L}{6}, \frac{5L}{6}$.

These are as shown.



Particle in 3-Dimensional Potential box

Let us consider a particle of mass 'm' moving in a 3-dimensional rectangular box having sides 'a, b, c' along x, y and z-axes as shown in figure.



The P.E. of the particle inside the box will be zero. The P.E. of the particle outside the box will be ∞ .

The Schrodinger time independent wave equation for a particle moving inside the box is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} E \psi = 0 \quad \text{--- (1)}$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + \frac{8\pi^2 m}{h^2} E \psi = 0$$

$$\Rightarrow \boxed{\nabla^2 \psi + \frac{8\pi^2 m}{h^2} E \psi = 0}, \text{ where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

This is Second order diff. equation, where the wave function ψ is a function of co-ordinates (x, y, z)
 $\Rightarrow \psi(x, y, z)$ is a product of 3-functions each depending on just one coordinate

$$\therefore \psi(x, y, z) = X_x Y_y Z_z \quad \text{--- (2)}$$

Take double derivative w.r.t 'x' ones.

$$\frac{\partial^2 \psi}{\partial x^2} = yz \frac{d^2 x}{dx^2} \quad \text{--- (a)}$$

and take double derivative w.r.t. y and z again, then we get

$$\frac{\partial^2 \psi}{\partial y^2} = xz \frac{d^2 y}{dy^2} \quad \text{--- (b)} \quad \frac{\partial^2 \psi}{\partial z^2} = xy \frac{d^2 z}{dz^2} \quad \text{--- (c)}$$

put (a), (b) & (c) in equation (1),

$$yz \frac{d^2 x}{dx^2} + xz \frac{d^2 y}{dy^2} + xy \frac{d^2 z}{dz^2} + \frac{8\pi^2 m}{h^2} E \psi = 0$$

$$yz \frac{d^2 x}{dx^2} + xz \frac{d^2 y}{dy^2} + xy \frac{d^2 z}{dz^2} + \frac{8\pi^2 m}{h^2} E XYZ = 0$$

Dividing through out by XYZ , we get

$$\frac{1}{x} \frac{d^2 x}{dx^2} + \frac{1}{y} \frac{d^2 y}{dy^2} + \frac{1}{z} \frac{d^2 z}{dz^2} + \frac{8\pi^2 m}{h^2} E = 0$$

$$\frac{1}{x} \frac{d^2 x}{dx^2} + \frac{1}{y} \frac{d^2 y}{dy^2} + \frac{1}{z} \frac{d^2 z}{dz^2} = -\frac{8\pi^2 m E}{h^2} \quad (\text{cont.})$$

$$\text{i.e. } \frac{1}{x} \frac{d^2 x}{dx^2} = -\frac{8\pi^2 m E_x}{h^2} \quad \text{--- (a)}$$

$$\frac{1}{y} \frac{d^2 y}{dy^2} = -\frac{8\pi^2 m E_y}{h^2} \quad \text{--- (b)}$$

$$\frac{1}{z} \frac{d^2 z}{dz^2} = -\frac{8\pi^2 m E_z}{h^2} \quad \text{--- (c)}$$

Re-arrange (a), (b) and (c)

$$\frac{d^2 x}{dx^2} + \frac{8\pi^2 m}{h^2} E_x \cdot x = 0 \quad \text{and} \quad \frac{d^2 z}{dz^2} + \frac{8\pi^2 m}{h^2} E_z \cdot z = 0$$

$$\frac{d^2 y}{dy^2} + \frac{8\pi^2 m}{h^2} E_y \cdot y = 0$$

Total energy of a particle in all 3-directions

$$E = E_x + E_y + E_z \quad \dots \text{--- (3)}$$

We already know that equations for 1-D box.

$$x = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a}\right)x, \quad y = \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi}{b}\right)y \quad \text{and}$$
$$z = \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi}{c}\right)z$$

$$\text{and } E_x = \frac{n_x^2 h^2}{8ma^2}, \quad E_y = \frac{n_y^2 h^2}{8mb^2}, \quad E_z = \frac{n_z^2 h^2}{8mc^2}$$

The wave function in 3-D box becomes,

$$\psi = XYZ$$

$$\therefore \psi = \sqrt{\frac{2}{a}} \cdot \sin\left(\frac{n_x \pi}{a}\right)x \cdot \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi}{b}\right)y \cdot \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi}{c}\right)z$$
$$\therefore \boxed{\psi = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_x \pi x}{a}\right) \cdot \sin\left(\frac{n_y \pi y}{b}\right) \cdot \sin\left(\frac{n_z \pi z}{c}\right)}$$

This is the expression for wave function.

The expression for energy $E = E_x + E_y + E_z$.

$$\therefore E = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$
$$\therefore \boxed{E = \frac{h^2}{8m} \left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right]}$$

This is the expression of energy of a particle in 3-D potential box.

postulates of Quantum Mechanics

The relationship between quantum mechanics and operators has helped to present the concepts in the form of some postulates.

They are

① The state of a system in Q.M is described by a wave function $\Psi(x,y,z,t)$ where $x, y, z \rightarrow$ are 3-coordinates, $t \rightarrow$ time

For a wave function ' ψ ' to describe any physical system, the following boundary conditions must be satisfied.

(a) $\psi(x)$ as well as $\frac{d\psi}{dx}$ must be finite

(b) $\psi(x)$ as well as $\frac{d\psi}{dx}$ must be continuous.

(c) $\psi(x)$ as well as $\frac{d\psi}{dx}$ must be single valued

(d) $\psi(x)$ must satisfies Born's condition.

i.e., The probability of finding a particle in a given volume element $dx dy dz$ is given

by $|\psi|^2 dx dy dz$ or $\psi \psi^* dx dy dz$

If the particle is somewhere in the space then the probability be equal to 1.

$$\text{i.e. } \int \psi \psi^* dx dy dz = 1$$

This is called Normalisation property.

- ② Every observable physical property of a system can be characterized by a linear operator. For example, The position (A) is characterized by an operator (\hat{A}). When this operator operates on a wave function ψ , then the result is $\hat{A}\psi = a\psi$, where a is observable quantity known as eigen value of operator.

The following table shows some quantum mechanics operators corresponding to different classical observable quantities.

Classical Quantity	Quantum Mechanical Operator
Cartesian components of position x, y, z	$\hat{x}, \hat{y}, \hat{z}$
position Vector \mathbf{r}	$\hat{\mathbf{r}}$
momentum P	$-i\hbar \nabla$
Cartesian components of linear momentum P_x, P_y, P_z	$-i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z}$
Total energy E	$i\hbar \frac{\partial}{\partial t}$

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③ When an operator \hat{A} is operated on a wave function ' ψ ', an average result obtained is given by $\langle \hat{A} \rangle = \frac{\int \psi^* A \psi dx dy dz}{\int \psi \psi^* dx dy dz}$

If the wave function ' ψ ' is normalized to unity, then the denominator is equal to 1.

$$\text{Then } \langle A \rangle = \int \psi^* A \psi dx dy dz$$

$$\text{For example, } \langle P_x \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} dx dy dz$$

$$\langle P_y \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial y} dx dy dz$$

$$\langle P_z \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial z} dx dy dz$$

$$\langle E \rangle = i\hbar \int \psi \psi^* \frac{\partial \psi}{\partial t} dx dy dz$$