05-06-2023

5. QUANTUM MECHANICS

* Quantum Mechanics:-

→ It is a branch of science which describes the 'dynamics of atomic' & 'sub atomic particles'

→ It is used to describe the dynamics of 'microscopic level objects'.

→ Quantum Mechanics have astonishing range of phenomena from 'polymers to semiconductors' from 'superfluids to superconductors' from 'photonics to Lasers' & 'from developing drugs to design of DNA'.

→ There were two independent formulations of quantum mechanics.

1. 'Matrix Mechanics'
2. 'wave Mechanics'

(1) Matrix Mechanics (or) First Formulation :-

→ It was developed by 'Heisenberg' (1925) to describe atomic structure starting from the observed spectral lines.

(2) Wave Mechanics (or) Second formulation :-

→ It was developed by 'Schrodinger' (1926).

→ It is a generalization of 'de Broglie postulate'.

→ It is more intuitive than 'matrix mechanics'.

→ It describes the dynamics of microscopic matter by means of a 'wave equation' [schrodinger equation]

→ In 1927, 'Max Born' proposed his probabilistic interpretation of wave mechanics.

→ Later 'Dirac' formulated quantum mechanics which deals with abstract objects such as 'kets' [state vectors], 'bras' & 'operators'.

* Classical mechanics and its Failures :-

→ It is used to describe the dynamics of 'Macroscopic objects.'

Failures :-

→ classical mechanics failed to explain

1. 'Black body radiation'.
2. 'Photo electric effect'.
3. 'Atomic stability & atomic spectroscopy.'
4. 'Semiconductors & magnetization.'

* Important Events [1900 - 1925] :-

1900 :- Black body Radiation [Max planck].

1905 :- Photo electric Effect [Albert Einstein].

1911 :- Discovery of Atomic Nucleus [E. Rutherford]

1913 :- The Model of Hydrogen Atom [Neils Bohr].

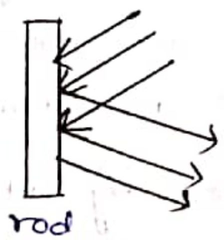
1923 :- The compton effect [A. compton]

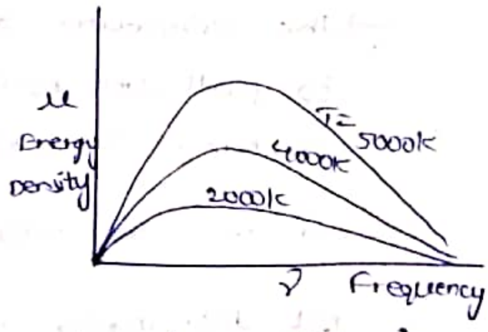
1923 :- The Matter waves [Louis de Broglie].

1925 :- The Quantum pictures [E. Schrodinger & W. Heisenberg].

* Black body Radiation :-

→ A perfect absorber and a perfect emmiter is called 'Black Body.'





→ Planck concluded that the released energy is not continuous.

→ In Nature, there is no perfect Black Body.

* Photo Electric Effect :-

→ Photo electric effect discovered by 'Hertz' and explained by 'Einstein'.

→ The phenomenon of emission of electrons from surface of metal when radiations of suitable frequency fall on it, is called "Photoelectric effect"

→ The emitted electrons are called 'Photoelectrons' & current, so produced is called 'photoelectric current'

→ Alkali metals like Lithium, sodium, etc. show 'photoelectric effect' with 'visible light'.

→ Metals like 'zinc, 'cadmium' etc are sensitive only to 'ultraviolet Light'.

Threshold Frequency :-

→ The Minimum frequency of photo radiation at which a photo electron is emitted is called 'Threshold Frequency'.

* Work Function :-

→ The Minimum amount of light energy required to pull (or) remove an electron from the metal surface is called 'Work function'. [ϕ_0 (or) W_0]

→ It can be measured in 'Electronvolt' [eV]

→ It decreases with the increase on temperature.

$$\boxed{W_0 = h\nu_0 = h\frac{c}{\lambda_0}}$$

$h \rightarrow$ 'Planck's constant'

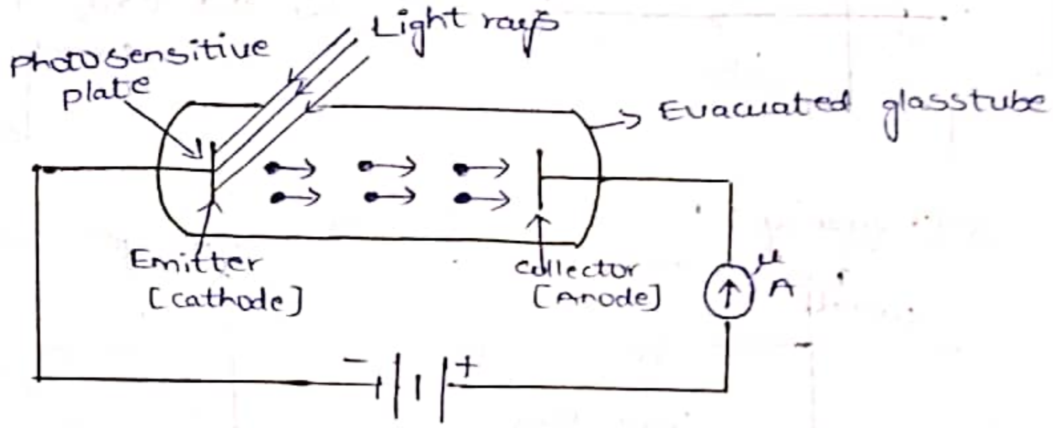
$\nu_0 \rightarrow$ Threshold frequency.

$\lambda_0 \rightarrow$ Threshold wavelength.

$1\,eV = 1.602 \times 10^{-19}\,J$.

* Hertz, Hallwach's and Lenard's observations:-
(or)
Experimental study of PhotoElectric Effect :-

→ The experimental setup is, as follows:



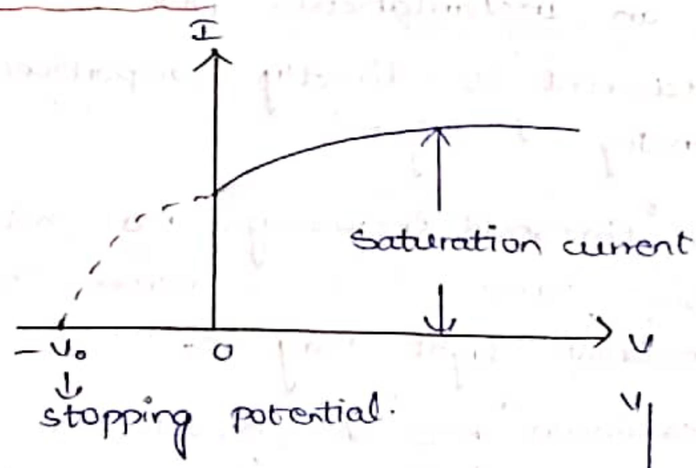
→ Two electrodes are placed at two ends of glass tube. [one is cathode(emitter) & anode(collector)]

→ When Monochromatic Light rays fall on 'cathode', electrons get emitted & attracted towards 'Anode'.

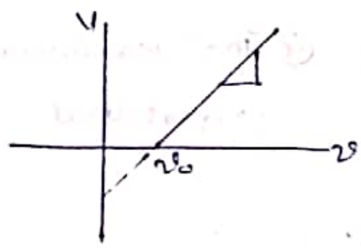
→ Thus photocurrent is setup b/w them.

→ From this experiment we can study
① 'Potential difference'
② 'Intensity of Light'
③ 'Frequency of Light'
④ 'Type of Metal plate'

① Potential Difference :-

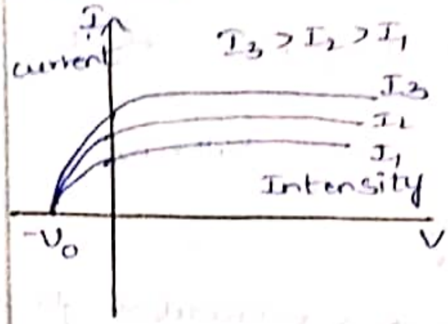


$h\nu = h\nu_0 + eV_0$.



$$\Rightarrow \boxed{V_0 = \frac{h\nu}{e} - \frac{h\nu_0}{e}}$$

(2) Intensity :-

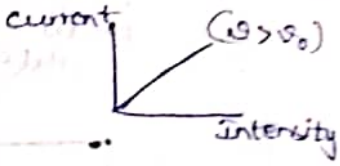


(1) If I(Intensity)↑ but $V < \nu_0$ ⇒ No current

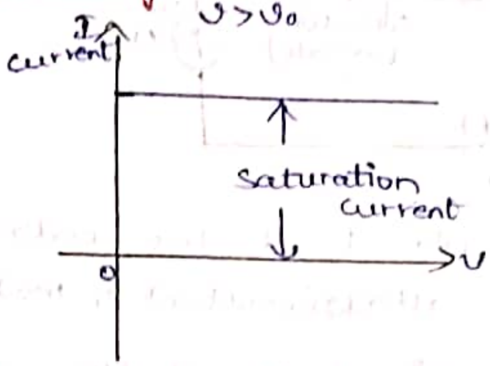
(2) If I↑ and $\nu > \nu_0$ ⇒ current(increases)

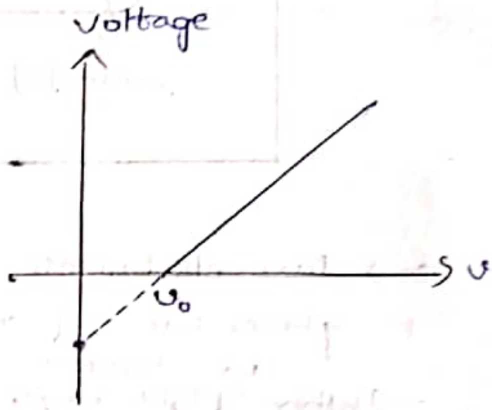
(3) If I↓ and $\nu < \nu_0$ ⇒ No current

(4) If I↓ and $\nu > \nu_0$ ⇒ current (less)

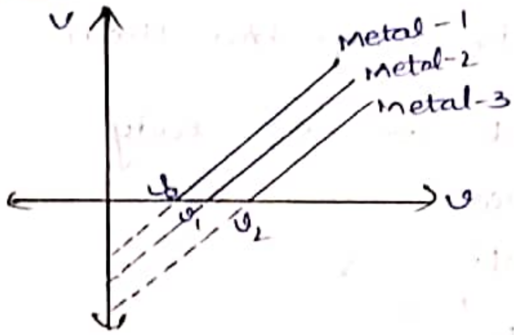


(3) Frequency :-





(4) Metal :-



* Laws of PhotoElectric Emission :-

(1) It is an 'Instantaneous process'

(2) 'Photocurrent' is directly proportional to 'Intensity of Light'

(3) Below 'threshold frequency', no photoelectric emission take place whatever the Intensity of Incident light may be.

(4) The Maximum 'K.E' of photoelectron is directly proportional to 'frequency' of incident light.

* Einstein's Photoelectric equation :-

→ According to Einstein the radiation consists of small particles called 'Photons'.

→ Each particle has energy, '$E = h\nu$'

where, 'h' → 'Planck's constant'

'ν' → 'Frequency'

→ According to him, when the photon of energy ($h\nu$) fall on a metal surface, the energy of the photon is absorbed by the free 'e^-' in the metal.

→ This absorb energy is utilized in 2 ways.

(i) "A part of energy is used by the 'e^-' to overcome the surface barrier."

(ii) "The remaining part of energy is used in giving a velocity to the emitted photo-electron."

→ According to conservation of energy.

$$E = W + K.E$$

$$\Rightarrow [h\nu] = K.E + W$$

$$\Rightarrow K.E = h\nu - h\nu_0 \quad [\because W = h\nu_0]$$

$$\Rightarrow K.E = h(\nu - \nu_0).$$

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$$\Rightarrow eV_0 = h(\nu - \nu_0) \quad [\because K.E = eV_0]$$

$$\Rightarrow V_0 = \frac{h(\nu - \nu_0)}{e}$$

$$\Rightarrow V_0 = \frac{h}{e}\left(\frac{c}{\lambda} - \frac{c}{\lambda_0}\right)$$

$$\Rightarrow \boxed{V_0 = \frac{hc}{e}\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)}$$

(or)

$$\Rightarrow K.E = h(\nu - \nu_0)$$

$$\Rightarrow \frac{1}{2}mu^2 = h(\nu - \nu_0) \quad [\because K.E = \frac{1}{2}mv^2]$$

$$\Rightarrow \frac{1}{2}mu^2 = h\left(\frac{c}{\lambda} - \frac{c}{\lambda_0}\right)$$

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

→ This is called "Einsten photo electric equation."

* Compton Effect :-

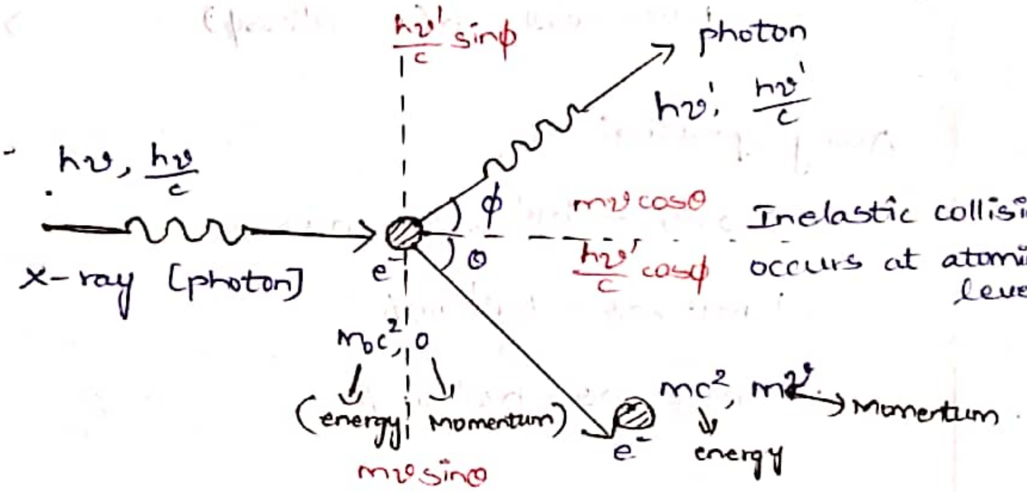
→ 'Einstein' said that when a particle moves around with the speed of light then its mass will changes.

$$\boxed{m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}}$$

'm_0 = mass at rest.'

→ He proved it theoretically.

→ Compton considered an x-ray and it scatters as follows.



Inelastic collision occurs at atomic level.

→ The enery of photon before collision and after collision is different. [Momentum also changes after collision].

→ The 'x-ray' collided with electron then the 'photon' may travels with angle 'ϕ' and 'recoil electron' with 'θ'.

→ Since it is elastic collision, kinetic energy & momentum are conserved.

K.E :-

$$KE_i = KE_f \quad [\because \text{Elastic collision}].$$

$$m_0c^2 + h\nu = mc^2 + h\nu' \quad [\because\ ]$$

$$\Rightarrow h(\nu' - \nu) = (m_0 - m)c^2$$

(or)

$$\Rightarrow h(\nu' - \nu) + mc^2 = m_0c^2$$

Now, $mc^2 = m_0c^2 + h(\nu - \nu')$.

squaring on both sides

$$\Rightarrow m^2c^4 = m_0^2c^4 + h^2(\nu-\nu')^2 + 2m_0c^2(h(\nu-\nu')) \longrightarrow (1)$$

Momentum: $P_i = P_f$ [$\because$ Elastic collision].

Along x-axis:

$$P_i = P_f$$

$$\Rightarrow \frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + m\nu\cos\theta$$

$$\Rightarrow \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\phi = m\nu\cos\theta$$

$$\Rightarrow m\nu c\cos\theta = h(\nu - \nu'\cos\phi) \longrightarrow (2)$$

Along y-axis:

$$\Rightarrow 0 + 0 = \frac{h\nu'}{c}\sin\phi - m\nu\sin\theta$$

$$\Rightarrow m\nu\sin\theta = \frac{h\nu'}{c}\sin\phi$$

$$\Rightarrow m\nu c\sin\theta = h\nu'\sin\phi \longrightarrow (3)$$

Now $eq^n (2)^2 + eq^n (3)^2$

$$\Rightarrow (m\nu c)^2(1) = h^2(\nu - \nu'\cos\phi)^2 + h^2\nu'^2\sin^2\phi$$

$$\Rightarrow (m\nu c)^2 = h^2(\nu - \nu'\cos\phi)^2 + (h\nu')^2\sin^2\phi \longrightarrow (4)$$

We know, $m = \dfrac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$

squaring on both sides

$$\Rightarrow m^2 = \frac{m_0^2}{1-\frac{v^2}{c^2}}$$

$$\Rightarrow m^2 = \frac{m_0^2}{\frac{c^2-v^2}{c^2}} = \frac{m_0^2c^2}{c^2-v^2}$$

$$\Rightarrow m^2(c^2-v^2) = m_0^2c^2 \longrightarrow (5)$$

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Now, (1) − (4)

$$\Rightarrow m^2c^4 - m^2c^2v^2 = m_0^2c^4 + h^2(\nu-\nu')^2 - h^2(\nu - \nu'\cos\phi)^2 - (h\nu')^2\sin^2\phi + 2h(\nu-\nu')m_0c^2$$

$$\Rightarrow m^2c^4 - m^2c^2v^2 = m_0^2c^4 + h^2(\nu^2+\nu'^2-2\nu\nu') - h^2 \times (\nu^2+\nu'^2\cos^2\phi - 2\nu\nu'\cos\phi) - (h\nu')^2\sin^2\phi + 2h(\nu-\nu')m_0c^2$$

$$= m_0^2c^4 + \cancel{h^2\nu^2} + h^2\nu'^2 - 2\nu\nu'h^2 - \cancel{h^2\nu^2} - h^2\nu'^2\cos^2\phi + 2\nu\nu'h^2\cos\phi - (h\nu')^2\sin^2\phi + 2h(\nu-\nu')m_0c^2$$

$$= m_0^2c^4 + \cancel{h^2\nu'^2} - 2\nu\nu'h^2 - \cancel{h^2\nu'^2}(\cos^2\phi+\sin^2\phi) + 2\nu\nu'h^2\cos\phi + 2h(\nu-\nu')m_0c^2$$

$$= m_0^2c^4 - 2h^2\nu\nu' + 2h^2\nu\nu'\cos\phi + 2h(\nu-\nu')m_0c^2.$$

$$\Rightarrow m^2c^2(c^2-v^2) = -2h^2\nu\nu'(1-\cos\phi) + m_0^2c^4 + 2hm_0c^2(\nu-\nu') \longrightarrow (6)$$

From equation (5) & (6)

$$\Rightarrow m_0^2c^4 = -2h^2\nu\nu'(1-\cos\phi) + m_0^2c^4 + 2hm_0c^2(\nu-\nu')$$

$$\Rightarrow m_0^2c^4 - m_0^2c^4 = -2h^2\nu\nu'(1-\cos\phi) + 2hm_0c^2(\nu-\nu')$$

$$\Rightarrow 0 = -2h^2(\nu\nu')(1-\cos\phi) + 2h\,m_0c^2(\nu-\nu').$$

$$\Rightarrow 2h^2\nu\nu'(1-\cos\phi) = m_0c^2(\nu-\nu')\,2h$$

$$\Rightarrow h\nu\nu'(1-\cos\phi) = m_0c^2(\nu-\nu')$$

$$\Rightarrow h(1-\cos\phi) = m_0c^2\left(\frac{\nu-\nu'}{\nu\nu'}\right)$$

$$\Rightarrow \frac{hc}{m_0c^2}(1-\cos\phi) = \frac{1}{\nu'} - \frac{1}{\nu}$$

$$\Rightarrow \frac{h}{m_0c}(1-\cos\phi) = \frac{c}{\nu'} - \frac{c}{\nu}.$$

We know, $\nu = \frac{c}{\lambda} \Rightarrow \lambda = \frac{c}{\nu}$

$$\Rightarrow \lambda' - \lambda = \frac{h}{m_0c}(1-\cos\phi)$$

∴ The compton shift, $\boxed{\Delta\lambda = \frac{h}{m_0c}(1-\cos\phi).}$

Compton shift at $\phi = 90^\circ$, $\Delta\lambda = 0.511$ MeV.

* de-Broglie Principle :-

→ According to "photoelectric effect" & "compton effect", Light contains particle nature.

→ But according to "de-Broglie", Every moving particle contains wave Nature.

$$E = mc^2, \quad E = h\nu$$

$$\Rightarrow mc^2 = h\nu = \frac{hc}{\lambda}$$

$$\Rightarrow \frac{h}{\lambda} = mc$$

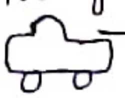
$$\Rightarrow \boxed{\lambda = \frac{h}{mc}} \text{ (or) } \boxed{\lambda = \frac{h}{p}}$$

λ → wave; mc → particle

→ According to de-Broglie, every moving particle contains "wavenature" & velocity.

→ Every moving particle means both micro & Macro particles.

Macro	Micro
1000 kg → 10 m/s	e^- → 1×10^6 m/s
$\lambda = \frac{h}{mv} = \frac{6.625 \times 10^{-34}}{1000 \times 10}$	$\lambda = \frac{6.625 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^6}$
$\therefore \lambda \cong 10^{-37}$ m.	$\therefore \lambda \cong 10^{-10}$ m.



→ From the above scenarios, we concluded that De-Broglie's waves will be occurred/seen by us in "Micro-level only".

→ de-Broglie waves are also called matter waves

→ "$\lambda = \frac{h}{p}$" is called de-Broglie's wavelength.

* Matter Waves :-

① These are not Mechanical waves. [∵ travels through vaccum].

② These are not Electromagnetic waves. Because for electromagnetic waves they requires charge.

* De-Broglie wavelength:-

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

$$\because p = \sqrt{2mE}$$

case-1 :- For Thermal.

$$E = \frac{3}{2} K \cdot T$$

$$\therefore \boxed{\lambda = \frac{h}{\sqrt{2m \times \frac{3}{2} K \cdot T}} = \frac{h}{\sqrt{3m K \cdot T}}}$$

case-2 :- For $\bar{e}$ $V_{\text{Potential}}$.

$$\Rightarrow \lambda_e = \frac{h}{\sqrt{2 m_e eV}} \quad [\because U = eV].$$

$$\Rightarrow \boxed{\lambda_e = \frac{1.227}{\sqrt{V}} \text{ n.m}} \quad \text{(or)} \quad \boxed{\lambda_e = \frac{12.27}{\sqrt{V}} \mathring{A}}.$$

* Conclusions (or) Relations of de-Broglie wavelength:-

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

② $\lambda \propto \frac{1}{\sqrt{V}}$

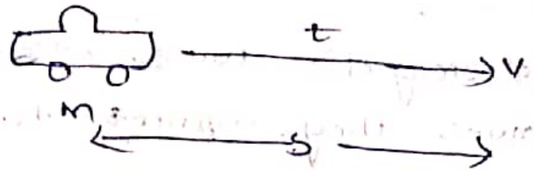
③ $\lambda \propto \frac{1}{m}$.

Ex:- Proton, $\bar{e}$ $\Rightarrow$ Same speed

$$\lambda_e > \lambda_p \quad [\because m_e > m_p]$$

* Heisenberg Uncertainity Principle :-

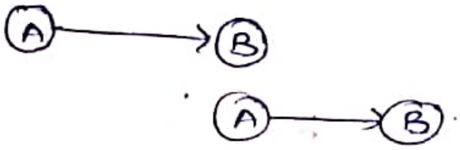
→ Let us discuss about certainity.



We can calculate 'position' [Distance] and 'Momentum' [velocity] at a particular time.
This is called 'certainity'.

→ In Laser experiment (or) Young's double slit experiment, if we decrease the slit width then Fringe width increases.

→



Momentum of A transferred to momentum of B

Accurately we are unable to calculate 'momentum' & 'position' simultaneously.

→ This principle says that "It is impossible to measure both position & momentum of a particle at the same time exactly."

→ Let Δp be change in momentum & Δx be change in position

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

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

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

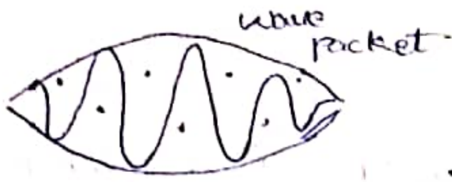
$$\Delta x \cdot \Delta p \simeq \frac{\hbar}{2}$$

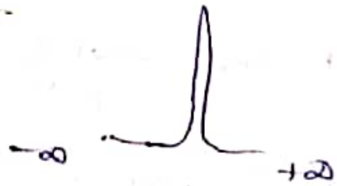
Here. Δx, Δp are canonically conjugates.

→ The terms whose product is in Joule/seconds units are called 'canonically conjugates.'

* Note:- Heisenberg Uncertainity:-

→ Let us consider a wave packet like this





↓ Here we cannot find the position of particle

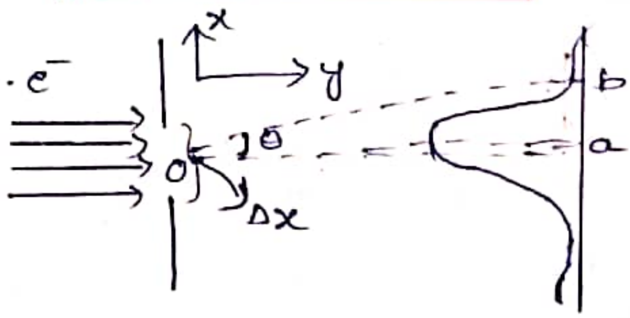
↓ Here we cannot find the velocity of particle

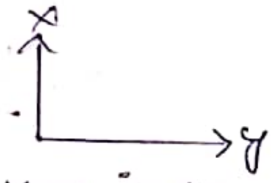
→ Heisenberg said for any canonical conjugates ie it is impossible to find the position & momentum of the body simultaneously at orbitary precision

Ex:- x and P_x ; t and E ; θ and L } canonically conjugate variables.

→ He gave uncertainity principle as

$$\boxed{\Delta x \cdot \Delta P_x = \frac{h}{2\pi} = \hbar}$$





$v = 0$ in x-direction at slit width

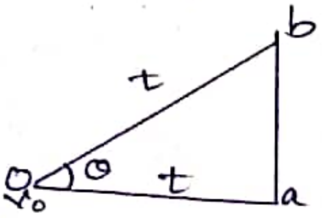
$\Delta x \sin\theta = \lambda$ [Δx = slit width]

$\Rightarrow \sin\theta = \frac{\lambda}{\Delta x}$ [$b \sin\theta = n\lambda$]

If θ is small

$\Rightarrow \theta = \frac{\lambda}{\Delta x}$ [$\sin\theta \simeq \theta$] $\longrightarrow$ (i)

From figure, $\tan\theta = \frac{ab}{oa}$.



$\Rightarrow oa = v_0 t$ Let $v_{xb} = \frac{ab}{t}$

$\Rightarrow ab = v_{xb} t$

Now, $\tan\theta = \frac{ab}{oa} = \frac{V_{xb}t}{V_0 t}$

If θ is small

$\Rightarrow \theta = \frac{V_{xb}\cancel{t}}{V_0 \cancel{t}}$

$\Rightarrow \theta = \frac{V_{xb}}{V_0}$ [velocity in x'-direction] → (2)

From (1) & (2) equations

$\Rightarrow \frac{\lambda}{\Delta x} = \frac{V_{xb}}{V_0}$.

We can write $\frac{\lambda}{\Delta x} = \frac{h}{p\Delta x} = \frac{h}{mV_0 \Delta x}$

$\Rightarrow \frac{h}{mV_0\Delta x} = \frac{V_{xb}}{V_0}$.

We can write $V_{xb} = \Delta V$

$\Rightarrow \frac{h}{m\cancel{V_0}\Delta x} = \frac{\Delta V}{\cancel{V_0}}$

$\Rightarrow \Delta x(\Delta V \cdot m) = h$

$\therefore \boxed{\Delta x \cdot \Delta P = h}$

Note :-

(1) $\Delta x \, \Delta P_x \geq \hbar$

$\Delta y \, \Delta P_y \geq \hbar$

$\Delta z \, \Delta P_z \geq \hbar$

(2) $\Delta t \, \Delta E \geq \hbar$

(3) $\Delta\theta \, \Delta L \geq \hbar$.

Uncertainities.

Advantages of Heisenberg uncertainity:

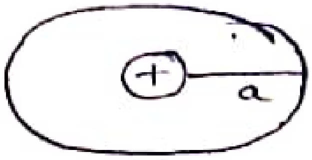
(or)

Applications:-

(1) "Groundstate energy and radius of Hydrogen atom":-

We know that $E = K.E + P.E.$

$$\Rightarrow E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 a}$$ [where a = radius of 1st orbital]



Here uncertainity in the position [a].

$$\Rightarrow \Delta x \cdot \Delta P_x \cong \hbar \qquad [\hbar \rightarrow h\ bar].$$

$$\Rightarrow a \cdot \Delta P = \hbar$$

$\therefore$ uncertainity in momentum, $\boxed{\Delta P = \frac{\hbar}{a}}$

$$\therefore E = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\varepsilon_0 a}.$$

For "ground state", the energy 'e' has to be 'minimum'.

$$\Rightarrow \frac{dE}{da} = 0 = \frac{-\hbar^2}{m a_0^3} + \frac{e^2}{4\pi\varepsilon_0 a_0^2}.$$

$$\therefore \boxed{a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \simeq 0.5\ A^\circ.}$$

Radius of Groundstate of Hydrogen atom.

$$\text{Now, } E = \frac{-me^4}{(4\pi\varepsilon_0)^2 2\hbar^2} = \frac{-me^4}{8\varepsilon_0^2 \hbar^2}.$$

$$\therefore \boxed{E_G = \frac{-me^4}{8\varepsilon_0^2\hbar^2}}$$

* Wave Function :- (ψ)

→ 'Wave function' (ψ) determines the total information of a particle like 'Momentum', 'Energy', 'position' etc---.

Properties of 'ψ' :-

① 'ψ' must be a finite value.

Ex: ① $\int_0^\infty e^{-x}\,dx = \left[-e^{-x}\right]_0^\infty = -\left[e^{-\infty} - e^0\right]$

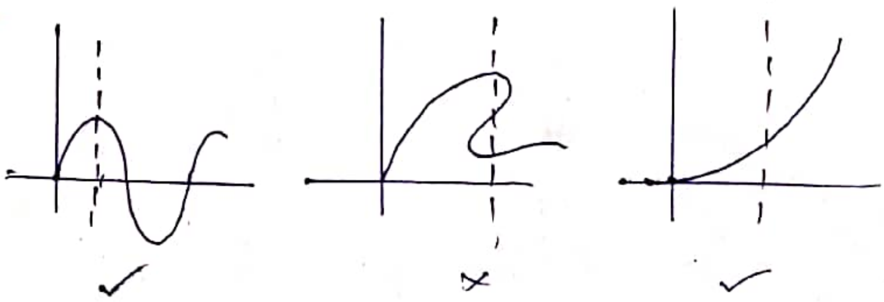
$= -[0-1] = -1$

② 'Summation' [Σ] is discontinuous, so the obtained ψ is not valid [∵ Infinite].

③ $\int_0^\infty x^5\,dx = \infty$ — This function also Invalid.

② 'ψ' must be single valued. [There will be an Identical solution].

Ex :-



③ 'ψ' must be continuous.

④ 'First derivative' $\left[\frac{\partial\psi}{\partial x}\right]$ of ψ also must be 'continuous'.

Note :-

→ For 'finite', 'single valued', 'continuous' wave functio[n] [ψ] only describes the 'parameters' of a particle.

* Triple Integral :-

→ when a particle escapes from the Nucleus then it must be in triple integral [Entire universe]

$$\boxed{\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \psi\psi^* \, dx\,dy\,dz = 1.}$$

Here, $\psi\psi^* = |\psi|^2 = P$ [probability of finding e^-]

We can write as $dx\,dy\,dz = d\tau$ (or) dv. sometimes.

* Operators :-

→ There are mainly 2 operators in quantum mechanics. They are.

(1) Momentum operator.

(2) Energy operator.

→ In Quantum Mechanics, Energies are two types

(i) Legrangian energy.

(ii) Hamiltonian energy. $\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right] = \hat{H}$

(a) Momentum & Energy operators :-

→ We have, $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V.$

By Applying it to Energy operator

$$\Rightarrow \hat{E}\psi = \hat{H}\psi$$

$$\Rightarrow \left[\frac{\hat{p}^2}{2m} + \hat{V}\right]\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}\right]\psi$$

$$\Rightarrow \frac{\hat{p}^2\psi}{2m} + \cancel{\hat{V}\psi} = \frac{-\hbar^2}{2m}\nabla^2\psi + \cancel{\hat{V}\psi}$$

$$\Rightarrow \hat{p}^2\psi = -\hbar^2\nabla^2\psi$$

$$\Rightarrow \hat{p}^2\psi = \frac{\hbar^2\nabla^2\psi}{i^2}$$

$\therefore \boxed{\hat{p} = \frac{\hbar}{i}\nabla}$ → Momentum operator. (or) $\boxed{\hat{p} = -i\hbar\nabla}$

* Expectation value $\langle \hat{O} \rangle$:-

$$\boxed{\hat{O} = \iiint_{-\infty}^{+\infty} \frac{\langle \psi^* | \hat{O} | \psi \rangle}{\langle \psi^* | \psi \rangle} \, d\tau}$$

- Here $\langle \; | \; | \; \rangle$ — $\langle$ Bra, $\rangle$ ket.

* Normalization :-

→ Ex:-

$$\iiint_{-\infty}^{+\infty} \psi^* \psi \, d\tau = N$$

where, 'N' is otherthan '1'.

Generally probability doesnot exceed 1. so,

$$\Rightarrow \frac{1}{N} \iiint_{-\infty}^{+\infty} \psi^* \psi \, d\tau = \frac{N}{N}$$

$$\Rightarrow \iiint_{-\infty}^{+\infty} \left(\frac{\psi^*}{\sqrt{N}}\right)\left(\frac{\psi}{\sqrt{N}}\right) d\tau = 1.$$

→ This process is called 'Normalization'.

* Schrodinger Time Independent Wave Equation :-

1-D

→ General 1-D wave equation,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \psi}{\partial t^2}.$$

Solution :- $\psi(x,t) = e^{i(kx - \omega t)}$ ⟶ (1)

$$\Rightarrow \frac{\partial \psi}{\partial x} = ? \quad \& \quad \frac{\partial \psi^2}{\partial x^2} = ?$$

We know, $E = h\nu$

$$\Rightarrow E = h\nu \times \frac{2\pi}{2\pi} = \hbar\omega \quad \left[\because \hbar = \frac{h}{2\pi}, \; \omega = \nu 2\pi\right]$$

$$\Rightarrow E = \hbar\omega.$$

We have momentum, $p = \frac{h}{\lambda}$

$\Rightarrow p = \frac{h}{\lambda} \times \frac{2\pi}{2\pi}$ [multiply & divide by 2π]

$\Rightarrow p = \hbar k$. $\left[\because \hbar = \frac{h}{2\pi},\ k = \frac{2\pi}{\lambda}\right]$

Substitute E & P values in eq^n (1)

$\Rightarrow \psi = e^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)}$ $\left[\because \begin{matrix} p = \hbar k, \\ E = \hbar\omega \end{matrix}\right]$.

Here, p, E are canonical conjugates

$\Rightarrow \psi = e^{\frac{i}{\hbar}(px - Et)}$

$\Rightarrow \psi = e^{\frac{i}{\hbar}(px - Et)} \longrightarrow (2)$.

Differentiate eq^n (2) w.r. to 'x'

$\Rightarrow \frac{\partial\psi}{\partial x} = \frac{ip}{\hbar} e^{\frac{i}{\hbar}(px - Et)}$

Again differentiate w.r. to 'x'

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

$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = \left(\frac{i^2 p^2}{\hbar^2}\right) e^{\frac{i}{\hbar}(px - Et)}$.

$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = \frac{-p^2}{\hbar^2}\psi \longrightarrow (3)$ [$\because$ From eq^n (2) & $i^2 = -1$].

Now, Differentiate eq^n (2) w.r. to 't'

$\Rightarrow \frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar} e^{\frac{i}{\hbar}(px - Et)}$

$\Rightarrow \frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar}\psi \longrightarrow (4)$ [$\because$ From (2)]

We know "E = K.E + P.E"

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

operate 'ψ' on both sides.

$\Rightarrow E\psi = \frac{p^2\psi}{2m} + V\psi \longrightarrow (5)$

substitute eq^n(3) in eq^n(5)

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

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

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

$$\Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0.}$$

∴ This is the "schrodinger Time Independent wave equation in 1-D."

In 3-D:-

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

$$\Rightarrow \boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0.}$$

∴ This is the "schrodinger Time Independent wave equation in 3-D"

* Energy operator:-

Now from eq^n(4),

$$\Rightarrow \frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar}\psi$$

$$\Rightarrow \frac{\partial\psi}{\partial t} = \frac{-iE}{\hbar} \times \frac{i}{i}\psi$$

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

$$\Rightarrow \hat{E} = i\hbar\frac{\partial}{\partial t}.$$

∴ Energy operator $\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$

* Schrodinger Time Dependent wave equation:-

1-D

→ consider equations (3), (4) & (5).

Substitute eq^n (3) & (4) in eq^n (5).

$$\text{eq}^n (5) \Rightarrow E\psi = \frac{p^2\psi}{2m} + V\psi$$

$$\Rightarrow E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad [\because \text{Eq}^n (3)].$$

$$\Rightarrow i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad [\text{From energy operator}]$$

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

$$\Rightarrow E\psi = H\psi \quad [\because \text{Hamaltonian energy-1D}]$$

$\therefore$ $\boxed{E\psi \text{ (or) } i\hbar\frac{\partial\psi}{\partial t} = H\psi}$ is the "Schrodinger Time Dedependent wave equation" in 1-D.

3-D:-

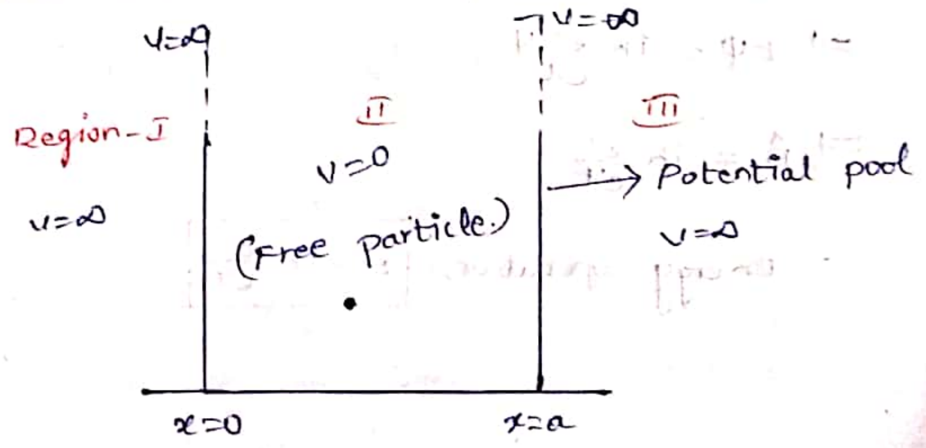
→ "Schrodinger Time Dedependent wave equation in 3-D" is $\boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2\nabla^2\psi}{2m} + V\psi}$

* Particle in 1-D Box:-

(or)

Application of Schrodinger Equation:- [Time Independent]

→ Let us take one particle in a box [Infinite]



→ According to De Broglie, if there is a particle there is a wave.

→ In Region-I & III, No chance to the existence of a particle [$\because v=\infty$].

→ particle presents in Region-II only.

$v(x)=0$, $0<x<a$. [Reg-II]

$v(x)=\infty$, $x\leq 0$ and $x\geq a$.

} potential expressions → ①

→ Wave functions,

$\psi(x)=0$, [In Region-I & III].

At Boundaries, [No particle at Boundaries],

$\Rightarrow \psi(x)=0$. at $x=0$

$\psi(x)=0$ at $x=a$.

} → ②

→ According to schrodinger wave equation [Time Independent].

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\psi=0. \longrightarrow ③$$

For Region-II, $V(x)=0$

Substitute $V(x)=0$ in eqn ③

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

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}E\psi=0. \longrightarrow ④$$

We know, $k=\frac{p}{\hbar}=\frac{\sqrt{2mE}}{\hbar}$

$$\Rightarrow k^2=\frac{2mE}{\hbar^2}$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}+k^2\psi=0. \longrightarrow ⑤$$

This is the "second order differential equation".

General solution, $\psi(x)=A\sin kx+B\cos kx \longrightarrow ⑥$

Apply Boundary conditions to eq^n ⑥

(i) $\psi(x)=0$ at $x=0$ $\Rightarrow \psi(0)=0$

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

$\Rightarrow \psi(0) = B = 0$

$\Rightarrow B=0$.

substitute $B=0$ in eq^n ⑥

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

$\Rightarrow \psi(x) = A\sin kx$. $\longrightarrow$ ⑦

(ii) $\psi(x)=0$ at $x=a$ $\Rightarrow \psi(a)=0$.

Applying $\psi(a)=0$ to eq^n ⑦

$\Rightarrow \psi(a) = A\sin ka = 0$

$\Rightarrow A\sin ka = 0$. [Here $A\neq 0$, otherwise there is no particle in box]

So, $\sin ka = 0$

$\Rightarrow \sin ka = \sin(n\pi)$.

$\Rightarrow ka = n\pi$

$\Rightarrow k = \frac{n\pi}{a}$. $\longrightarrow$ ⑧

From eq^{n}s ⑦ & ⑧

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

$\Rightarrow \int_0^a \psi^*(x)\,\psi(x)\,dx = 1$.

$\Rightarrow \int_0^a A^2\sin^2\left(\frac{n\pi x}{a}\right)dx = 1$. [$\because$ No complex conjugate, so both are same].

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

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

$$\Rightarrow \frac{A^2}{2}\int_0^a 1 - \int_0^a \cos\frac{2n\pi}{a}. = 1$$

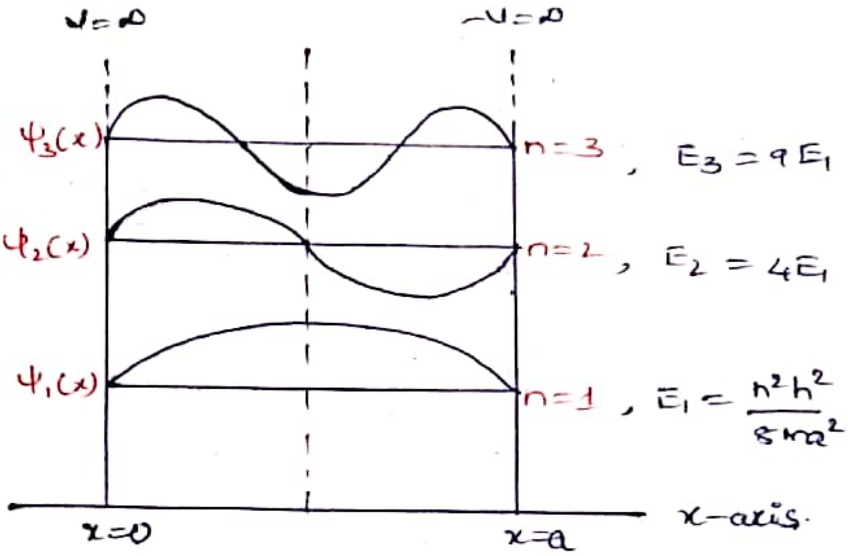
$$\Rightarrow \frac{A^2}{2}(a) - 0 = 1$$

$$\Rightarrow \frac{A^2}{2} = \frac{1}{a}$$

$$\Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\therefore \boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)}$$ → wave function for region II

Graph:-



Energy:-

We have, $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

We know, $k = \frac{n\pi}{a}$ $\Rightarrow k^2 = \frac{n^2\pi^2}{a^2}$

$$\Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}} \quad (\text{or}) \quad \boxed{E_n = \frac{n^2h^2}{8ma^2}} \quad \left[\because \hbar = \frac{h^2}{2\pi}\right].$$

Note:-

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

Momentum:-

$$P = \hbar K = \hbar\left(\frac{n\pi}{a}\right)$$

$$\Rightarrow \boxed{P_n = \frac{n\pi\hbar}{a}} \quad (\text{or}) \quad \boxed{P_n = \frac{nh}{2a}}$$