[UNIT-2]

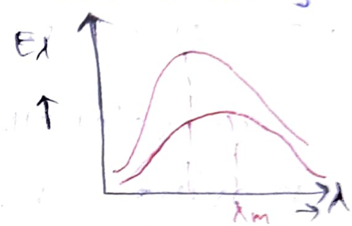
De - Broglie Hypothesis -

EM - Spectrum: γ-rays $\rightarrow$ Hartizan or (Radio waves).

Nature of Radiation (Light) & Matter.

Wave nature
1. Reflection
2. Refraction
3. Interference
4. Diffraction
5. Polarisation

Particle Nature
→ Black Body radiation



$\boxed{\lambda_m \cdot T = \text{Constant}}$

→ Photo electric effect
→ Compton - effect

Note:— ① Planck's Radiation formula -

$$\boxed{E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{d\lambda}{e^{hc/\lambda KT} - 1}}$$

② Photo electric effect confirms presence of Energy in photon.

③ Compton Effect → Presence of momentum with the photon.

④ ~~A~~ If there is no mass but there is some energy or momentum we can call it particle.

* De-Broglie Hypothesis (matter wave Concept) :-

Matter and radiation both exhibit the dual character i.e, particle and wave character. So, In order to establish a correlation b/w these two entirely different characters, Prof. Louis de Broglie proposed that "There is associated a wave with each moving material particle".

OR,

A moving particle under certain circumstances presents the wave nature.

The wavelength of the wave associated with moving material particle (de-Broglie wavelength) is given by -

$$\boxed{\lambda = \frac{h}{mv}} \quad \text{--- (1)}$$

If electron encirculing in H-atom presents the wave (character) nature, then the circumference of the orbit of H-atom -

$$\boxed{2\pi r = n\lambda} \quad \text{--- (2)}$$

and ~~the~~ Bohr's Postulate -

$$\boxed{mvr = \frac{nh}{2\pi}} \quad \text{--- (3)}$$

From (2) + (3)

$$\boxed{\lambda = h/mv}$$

→ Different form of De-Broglie wavelength -

* Non relativistic case - (In terms of K.E) -

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

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

$$\boxed{\lambda = \frac{h}{\sqrt{2mE_K}}}$$

In terms of ~~electric~~ acc. potential -

$$E_K = qV$$

$$\boxed{\lambda = \frac{h}{\sqrt{2mqV}}}$$

* Relativistic case -

In terms of K.E -

$$E^2 = p^2c^2 + m_0^2c^4$$

$$p^2c^2 = E^2 - m_0^2c^4$$

$$p^2c^2 = (E_K + m_0c^2)^2 - m_0^2c^4$$

$$p^2c^2 = E_K[E_K + 2m_0c^2]$$

$$P = \frac{\sqrt{E_K(E_m + 2m_0c^2)}}{c}$$

$$\boxed{\lambda = \frac{hc}{\sqrt{E_K(E_K + 2m_0c^2)}}}$$

* In terms of acc. potential

$$E_K = qV$$

$$\boxed{\lambda = \frac{hc}{\sqrt{qV(qV + 2m_0c^2)}}}$$

* De - Broglie wave velocity (w) :-

Once we associate a wave with ~~velocity~~ moving material particle, it may have some velocity which is known as de-Broglie wave velocity.

$$w = \nu\lambda$$

$$= \left(\frac{E}{h}\right) \times \left(\frac{h}{p}\right)$$

$$w = \frac{E}{p} = \frac{mc^2}{mv}$$

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

In relativistic mechanics

$v <<< c \Rightarrow w >>> c$

which is not acceptable w.r.t overall result.

Schrodinger's Explanation :-

$\omega >>> c$

To resolve the above controversial result Schrodinger suggested that there may be associated a no. of waves weather than a single ~~to~~ particle with a moving material particle. He imagined the situation as the production of beats in sound where more than one wave superpose eachother to give rise to a resultant wave and we recieve the sounds in regular intervals.

For mathematical simplycity Schrodinger assumed two waves having slightly difference in angular frequency and propogation vector. which give rise to resultant wave

The eq^n of first wave constituting -

$$Y_1 = A\cos(\omega t - kx) \quad \text{--- (1)}$$

Similarly eq^n of other wave -

$$Y_2 = A\cos[(\omega + d\omega)t - (k + dk)x] \quad \text{--- (2)}$$

Therefore the eq^n of resultant wave or the wave group -

$$Y = Y_1 + Y_2 \quad \text{--- (3)}$$

$$Y = A\cos(\omega t - kx) + A\cos[(\omega + d\omega)t - (k + dk)x$$

$$Y = 2A\cos\frac{1}{2}[(2\omega + d\omega)t - (2K + dK)x] \cdot \cos\frac{1}{2}(d\omega t - dKx)$$

$\because$ $\omega >> d\omega$ and $K >> dK$ then,

$2\omega + d\omega = 2\omega$, $2K + dK = 2K$

$$\boxed{Y = 2A\cos(\omega t - Kx)\cos\left[\frac{d\omega}{2}t - \frac{dK}{2}x\right]} \quad \text{--- (4)}$$

This is the eqn of resultant wave or wave group.

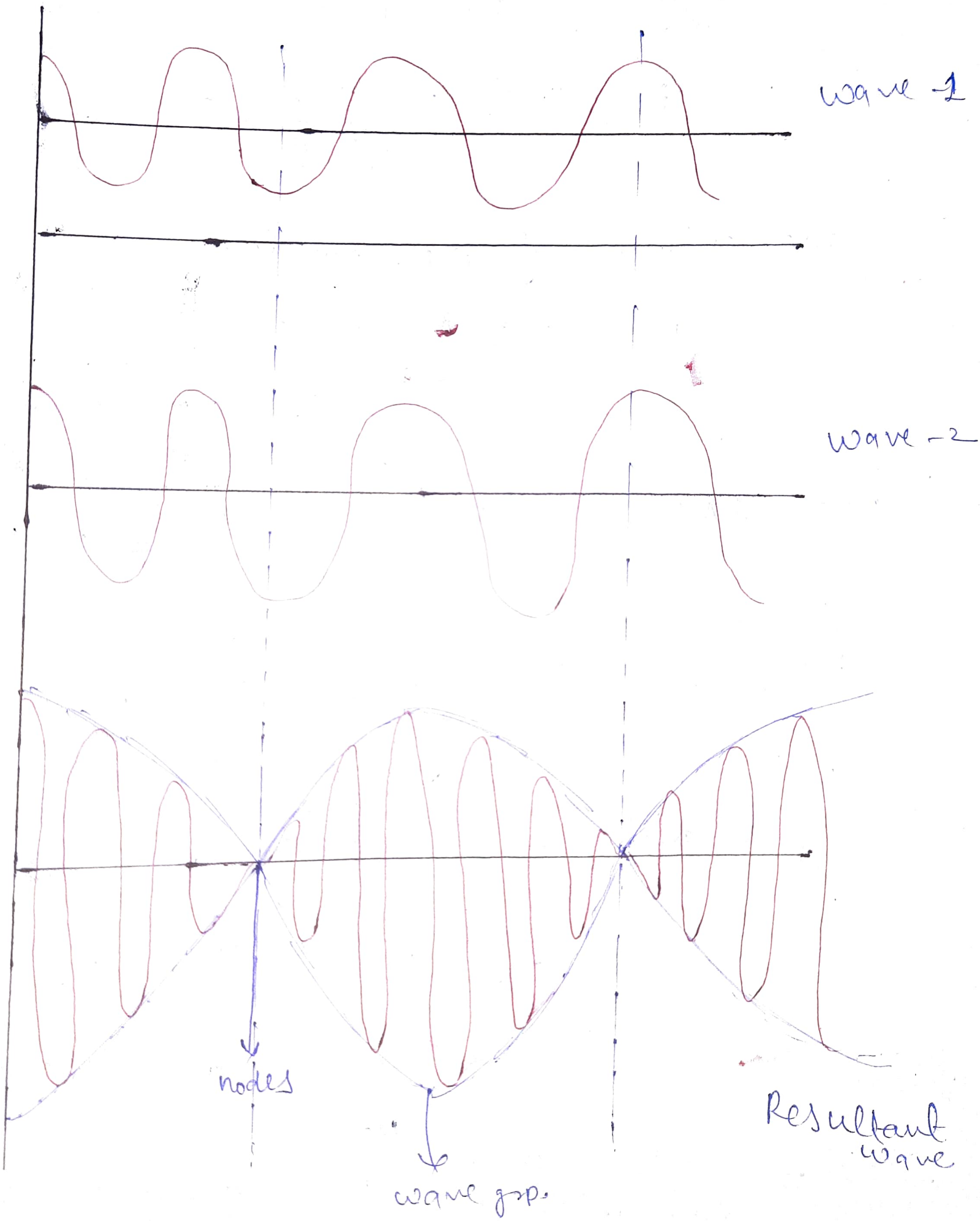
The eqn of resultant wave contains the original wave having angular freq ω and propogation vector K superimposed upon a modulation having angular ~~freq~~ freq $\frac{d\omega}{2}$ and propogation vector $\frac{dK}{2}$, the effect of which is to produce the successive wave groups.

He defined the phase velocity as — the ratio of angular freq and propogation vector of the original wave, which comes out equal to

$$\text{(phase velocity) } U_p = \frac{\omega}{K} = 2\pi\nu \times \frac{\lambda}{2\pi} = w \text{ (wave velocity)}$$

$$\text{Group velocity } V_g = \frac{d\omega/2}{dK/2} = \frac{d\omega}{dK}$$

* Graphical representation of wave group-



* Velocity of wave group : (V_g) –

The energy of the particle –

$$E = mc^2 = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} c^2 \quad \text{--- (1)}$$

The momentum of the particle –

$$P = mv = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}} \quad \text{--- (2)}$$

$$\omega = 2\pi\nu = \frac{2\pi E}{h} = \frac{2\pi}{h} \frac{m_0 c^2}{\sqrt{1-v^2/c^2}} \quad \text{--- (3)}$$

$$k = \frac{2\pi}{\lambda} = \frac{2\pi P}{h} = \frac{2\pi}{h} \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}} \quad \text{--- (4)}$$

Group velocity –

$$V_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} \quad \text{--- (5)}$$

from (3)

$$\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h\left[1-\frac{v^2}{c^2}\right]^{3/2}}$$

from (4)

$$\frac{dk}{dv} = \frac{2\pi m_0}{h\left[1-v^2/c^2\right]^{3/2}}$$

Hence,

$$V_g = \frac{d\omega/dv}{dk/dv}$$

putting values –

$$\boxed{V_g = v}$$

Therefore a moving material particle is associated with the wave grp which moves with the same velocity as that of the particle.

OR,

Microscopic moving material particle present itself as a wave group.

* Experimental confirmation of Matter waves –

* Electron microscope
* Davisson – Germer Experiment
* G.P Thomson Experiment

→ Davisson – Germer experiment :- –

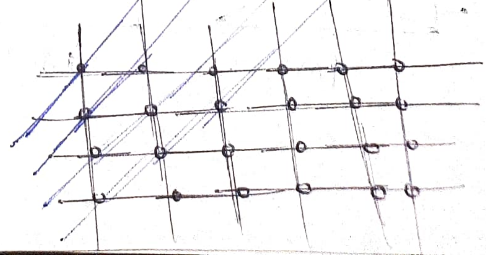
Suppose an electron is accelerated by 100 volt, wavelength associated with this electron –

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.64 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 100}}$$

$$\lambda =$$

Therefore we need such a slit system in which slit spacing should be of this order.

* slit system → Nickel crystal (spacing = 1.23 A°)

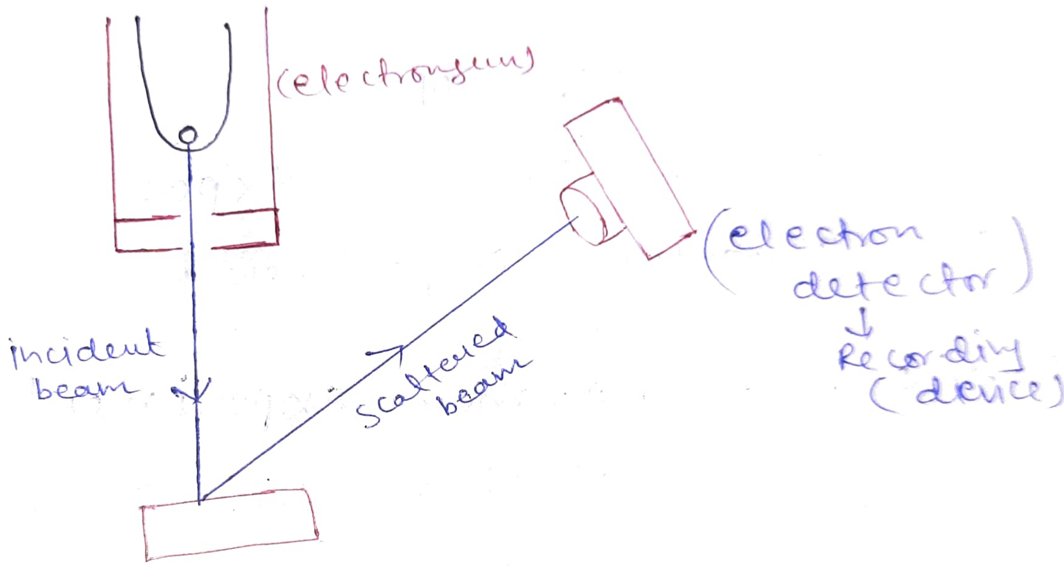


Major components:

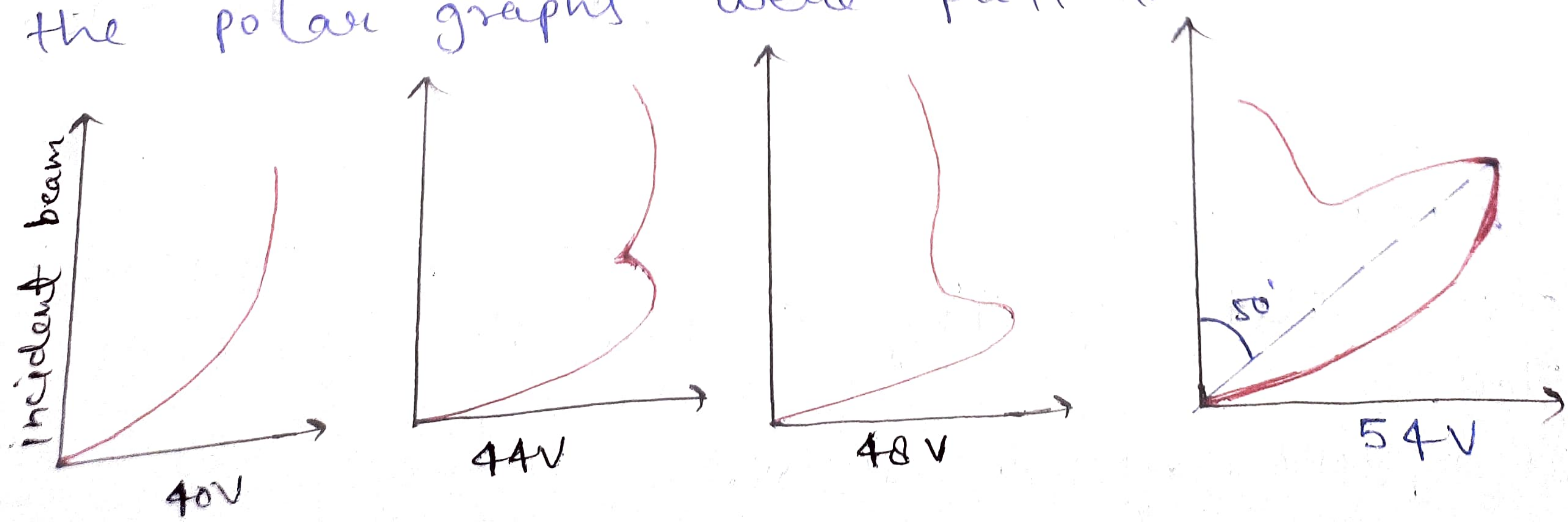
(a) Electron Guns → To produce electron beam, collimate and accelerate the electron beam.

(b) Slit system → upon which fine beam of electrons is allowed to incident (Nickel crystal)

(c) Recording device → Scattered intensity into current.



The experiment was performed at different voltages begning from 40 V to 100 V. and the polar graphs were plotted.



If the electron is behaving (presenting) wave nature it must undergo differaction similar to x-radiations and therefore, one can use Bragg's eqn under this situation.

$$\boxed{2d\sin\underbrace{\theta}_{\text{glancing angle.}} = n\lambda}$$

* where d is interplanar (slit) separation
↓
(interatomic distance)

* n is order of diffraction

Considering 1st order differaction -

$$2 \times 1.23\ A^\circ \times \sin 65^\circ = \lambda$$

$$\boxed{\lambda = 1.65\ A^\circ}$$

Considering de-Broglie formula -

$$\lambda = \frac{h}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 54}}$$

$$\boxed{\lambda = 1.66\ A^\circ}$$

Hence wave nature of material parti is experimentally confirmed.

* Heisenberg's Uncertainity Principal :-

* Dual nature of matter and radiation is responsible for this.

→

$$\Delta P \cdot \Delta x \geq \frac{\hbar}{2}$$ (Momentum - Position) uncertainity

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

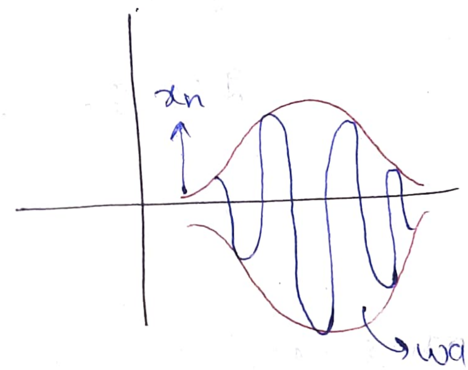
$$\Delta J \cdot \Delta \theta \geq \frac{\hbar}{2}$$ (Ang. momentum - Position) uncertainity

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$ (Energy-time Un--)

→ Derivation of uncertainity principle -

eq^n of wave group -

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



at nodes $y = 0$

$$\cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] = 0$$

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_n = (2n+1)\pi/2 \quad \text{--- (i)}$$

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_{(n+1)} = (2n+3)\pi/2 \quad \text{--- (ii)}$$

(ii) - (i)

$$\frac{\Delta k}{2}\left[x_n - x_{n+1}\right] = \pi$$

$$\frac{\Delta k}{2} \times \Delta x = \pi$$

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

$$\because \quad k = \frac{2\pi}{\lambda} = \frac{2\pi}{h} \times p$$

$$\Delta k = \frac{2\pi}{h} \times \Delta p$$

So

$$\boxed{\Delta p \cdot \Delta x = h}$$

→ Energy - time uncertainity

Kinetic Energy -

$$K = \frac{p^2}{2m}, \quad \Delta E = \frac{2p\Delta p}{2m} = \frac{p}{m}\Delta p$$

$$p = mv = m\frac{\Delta x}{\Delta t} \Rightarrow \frac{p}{m} = \frac{\Delta x}{\Delta t}$$

$$\Delta E = \frac{\Delta x}{\Delta t} \cdot \Delta p$$

$$\boxed{\Delta E \cdot \Delta t = \Delta x \cdot \Delta p = h}$$

* Consequences of Uncertainity Principle:-

→ Ground state energy and radius of H-atom

Total energy of H- atom -

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} \quad \text{---(i)} \qquad [E = K.E + P.E]$$

Error -

$$\Delta E = \frac{(\Delta p)^2}{2m} - \frac{e^2}{4\pi\varepsilon_0(\Delta r)} \quad \text{---(ii)}$$

Using uncertainity principal –

$$\Delta p \cdot \Delta x \simeq \hbar$$

* $\Delta p \cdot \Delta r \simeq \hbar$

$$\Delta p = \frac{\hbar}{\Delta r}$$

Assuming $\Delta p \approx p$, $\Delta r \approx r$

$$\Rightarrow \quad p = \frac{\hbar}{r}$$

Putting in (i)

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} \quad \text{--- (iii)}$$

for lowest energy state –

$$\frac{dE}{dr} = 0$$

$$-\frac{2\hbar^2}{2mr^3} + \frac{e^2}{4\pi\varepsilon_0 r^2} = 0 \quad \text{--- (iv)}$$

$$\therefore r = r_0 = \frac{4\pi\varepsilon_0 (\hbar)^2}{me^2}$$

on substituting ε_0, h, m & e we find –

$$\boxed{r_0 = 0.53 \text{Å}}$$

This is popularly known as radius of the Bohr's first orbit of H- atom.

(iii) + (iv)

$$E = \frac{-me^4}{2\hbar^2 (4\pi\epsilon_0)^2} - \frac{\hbar^2}{2mr_0^2}$$

On substituting of the values of $\hbar$, m, r_0 in the above we get

$$\boxed{E = -13.6 \text{ eV}}$$

This is the lowest energy state of Bohr-atom and is named as ground state energy.

→ Zero point energy of Harmonic oscillator :-

Total Energy of Harmonic oscillator-

$$E = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad \text{—— (i)}$$

$$\Delta E = \frac{(\Delta p)^2}{2m} + \frac{1}{2} m\omega^2 (\Delta x)^2 \quad \text{—— (ii)}$$

using uncertainity principle-

$$\Delta p \cdot \Delta x \simeq \hbar$$

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

assuming $\Delta E \simeq E$, $\Delta x \simeq x$, $\Delta p \simeq p$

for lowest energy-

$$\frac{dE}{dx} = 0$$

$$\therefore E = \frac{\hbar^2}{2mx^2} + \frac{1}{2} m\omega^2 x^2 \quad \text{—— (iii)}$$

$\frac{dE}{dx} = \frac{-2\hbar^2}{2m x^3} + \frac{1}{2} m\omega^2 \times 2x = 0$ ... uncertain by

$$x = \left[\frac{\hbar}{m\omega}\right]^{1/2}$$

putting in (iii)

$$E_{min} = \frac{\hbar^2 \times m\omega}{2m \times \hbar} + \frac{1}{2} m\omega^2 \frac{\hbar}{m\omega}$$

$$\boxed{E_{min} = \hbar\omega_0}$$

$\omega_0 \rightarrow$ frequency in ground state

This is known as zero-point energy. Therefore, contrary to the classical prediction, the quantum mechanical oscillator exibit a minimum non-zero value of energy as given ~~below~~ above. This result is entirely different with the well known classical result.

→ Non-existance of electron in Nucleus:-

Assume that electron, can reside in the Nucleus.

Nuclear diameter $\approx 10^{-14}$ m

By uncertainity principal—

$$\Delta p \cdot \Delta x \simeq \hbar$$

Assume that $\Delta p \simeq p$, $\Delta x \simeq x$

so,

$$p \approx \frac{\hbar}{x} = \frac{1.05 \times 10^{-34}}{10^{-14}\ m} = 1.05 \times 10^{-20}\ kg\,m\,s^{-1}$$

An electron whose momentum is uncertain by this much order of magnitude must have energy many times of this value. Using relativistic momentum energy relation –

$$E^2 = p^2c^2 + m_0^2c^4$$

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

$$E = \sqrt{(1.05\times10^{-20})^2 \cdot (3\times10^8)^2 + (9.1\times10^{-31})^2(3\times10^8)^4}$$

neglecting $m_0^2c^4$ for simplicity –

$$E = 1.05\times10^{-20} \times 3\times10^8$$

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

$$E \approx 20.6\,\text{MeV}$$

after assuming $m_0^2c^4$

$$E > 20.6\,\text{MeV}$$

Experimentally using β-ray expt $\approx$ 2-3 MeV.

This means electron can't reside in nucleus

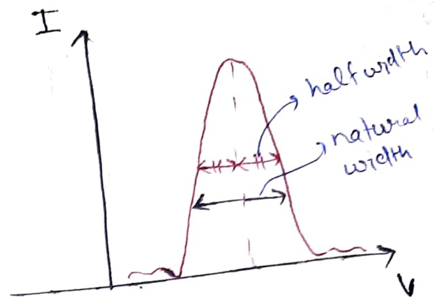
→ Finite width of the spectral lines :-
Using Energy - time uncertainty relation-

$$\Delta E \cdot \Delta t \simeq \hbar$$

$$\hbar \cdot \Delta\nu \cdot \Delta t \simeq \hbar$$

$$\Delta\nu \doteq \frac{1}{\Delta t} = \frac{1}{10^{-8}}$$

$$\Delta\nu \approx 10^{8} \text{ Hz}$$



⇒ Spectral line can never be infinitely sharp.

* Bohr's Atomic Model and Uncertainity principal-

From the first postulate of Bohr's orbit-

$$\Delta E = 0$$

By U.P -

$$\Delta E \cdot \Delta t \approx \hbar$$

$$\Delta t \approx \infty$$

But actually it is 10^{-8}.

Therefore Bohr's model is not consitent from the point of view of the Uncertainity principal.

* Wave function (ψ) and its physical signification

→ Basic postulates of Quantum Mechanics -(Wave Mechanics):-

When we associate a wave with a material particle this definately indicate that certain physical quantity will be varying in space and time. For example- variation of pressure in space and time gives rise to the propogation of mechanical waves.

Similarly the variation of Electric field vector and magnetic field vector in space and time leads the Electromagnetic wave propogation.

So, if the microscopic material particle exhibit as a wave (Matter wave) it must have then some wave eq^n. In which some physical quantity will definately be there which will vary in space and time. that variable quantity corresponding the matter wave is known as wave function (ψ). This 'ψ' alone has no physical significance since it is linked with the probability of finding particle, and the probability can never be negative. It is either 0 or 1. But square of modulus $(|\psi|)^2$ will always be +ve and therefore it is known as probability density. If it is considered over the unit volume of space.

$(|\psi|)^2 \propto$ Prob. of finding particle in a given region at a given instant.

$\int_{-\infty} |\psi|^2 \, dv = 1$ → ~~prob.~~ Certainty of finding the particle in a given region at a given instant.

In many situations the wave function is a complex quantity – i.e –

$$\psi = \cancel{at}\ a + ib \quad , \quad \psi^* = a - ib$$

$$\psi \cdot \psi^* = a^2 + b^2 = \text{a real quanity}.$$

$$\int_{-\infty}^{\infty} \psi_{(x,t)} \, \psi^*_{(x,t)} \, dv = 1$$ → wave function is said to be normalised.

$= 0$ → Absence of particle in a given region at a given instant (wave functions is said to be orthogonal).

→ Basic requirments of ψ :–

1. For values of (x, y, z) ; ψ should be single valued.
2. For all values of (x, y, z) , ψ should be continuoy.
3. For all values of (x, y, z) , ψ should be finite.
4. For all values of (x, y, z), $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial y}$, $\frac{\partial \psi}{\partial z}$ (partial derivative) must ~~be~~ exist and cont.
5. If ~~f~~ ψ is not normalised, then it is to multiplied ~~Allotted~~ by a constant 'A'.

$$\int_{-\infty}^{\infty} A\,\Psi_{(x,t)} \cdot A\,\Psi^*_{(x,t)}\, dv = 1.$$

$$A^2 \cdot \int_{-\infty}^{\infty} \Psi(x,t) \cdot \Psi^*_{(x,t)}\, dv = 1$$

$$\Rightarrow \boxed{A^2 = \frac{1}{\int_{-\infty}^{\infty} \Psi_{(x,t)} \cdot \Psi^*_{(x,t)}\, dv}}$$

* Schrodinger's wave eqn :-

Differential eqn of wave motion –

$$\boxed{\frac{d^2 y}{dx^2} = \frac{1}{u^2}\frac{d^2 y}{dt^2}}$$

$$\boxed{y = A\, e^{-i\omega(t - x/v)}}$$

Similarly –

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{u^2}\frac{\partial^2 \psi}{\partial t^2}} \quad \text{— (1)}$$

$$\Rightarrow \Psi(x,t) = A e^{-i\omega(t - x/v)}$$

$$\Rightarrow \Psi(x,t) = A e^{-2\pi i(\nu t - \nu x/v)}$$

$$\boxed{\Psi(x,t) = A e^{-2\pi i(\nu t - x/\lambda)}} \quad \text{--- (ii)}$$

Using $\lambda = h/p = \frac{2\pi\hbar}{2\pi p} = \frac{2\pi\hbar}{p}$

$E = h\nu = \frac{2\pi h}{2\pi}\nu = 2\pi\hbar\nu \Rightarrow$ } de-Broglie Concept

$\Rightarrow \nu = E/2\pi\hbar$

$$\boxed{\Psi(x,t) = A\, e^{-\frac{i}{\hbar}(Et - Px)}} \quad \text{--- (3)}$$

Total energy of the particle –

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

on operating this by $\Psi(x,t)$ –

$$E\,\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t) + V\,\Psi(x,t)$$

on differentiating partially eq (3) w.r.t t –

$$\frac{\partial \Psi(x,t)}{\partial t} = -\frac{iE}{\hbar}\Psi(x,t)$$

$$\Rightarrow \boxed{E}\,\Psi(x,t) = \boxed{-\frac{\hbar}{i}\frac{\partial}{\partial t}}\Psi(x,t)$$