4. Wave Packets and uncertainty Principle

4.1 INTRODUCTION AND PRELUDE

Materials also behave as wave - and their associated wavelength depends on momentum but inversely. $\lambda = \frac{h}{p} \Rightarrow p = \cancel{\frac{h\nu}{\lambda}}$

$$\Rightarrow p = \frac{h}{\lambda} = \hbar k \quad \text{as } k = \frac{2\pi}{\lambda}$$

Propagation constant / wave number

Also, $E = \hbar\omega$ $\quad \omega = 2\pi\nu \rightarrow$ Angular frequency

4.2 REPRENTATION OF PARTICLE BY A WAVE PACKET

- How can we construct a wave function that can depict a particle?
- Answer lies in the fact that its amplitude should be sizeable in the neighbourhood of the particle, but should be negligible anywhere else and it must satisfy the Normalisation condition.
- for example - $\Psi(x,t) = Ae^{i(kx-\omega t)}$ cannot be the correct wave function as its Probability density $\equiv P = |\Psi(x,t)|^2 = A^2$ is constant.

  That means particle has constant probability of being found anywhere. And this doesn't make sense.
- Hence, we need to find such amplitude, whose size is considerable in neighbourhood of particle.

Such condition provides that :-

I. Particle can not be represented by single wave function; because amplitude of such wave fn. is Constant

II. Particle can be represented by a wave Packet.

to construct wave packet, we need to consider many waves of different wave numbers and then superimpose them in such manner that — (a). they interferences destructively in far neighbourhood of the particle.

(b) they interferes constructively in close neighbourhood of particle.

SPYQ

Establish why a particle can only be described by wave packet and not a single wave.

Such result can be achieved via means of "Fourier Integrals and Transforms".

Thus let $\psi(x,t)$ be such wave packet —

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \underbrace{A(k)}_{\text{Amplitude.}} \cdot e^{+i(kx-\omega t)}\, dk$$

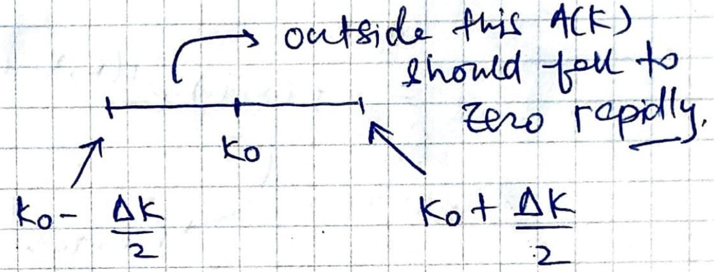
Then by using inverse Fourier Transform one can get Amplitude :-

$A(k) =$

$$A(k)\, e^{-i\omega t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-ikx}\, dx$$

$$\text{or} \quad A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{+i(kx-\omega t)}\, dx$$

Now, we understand thet for the wane packet to represent the particle, the Amplitude must be localized. Thus suppose amplitude is centered around some value $k = k_0$.



Thus we coned rewrite :-

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{k_0-\Delta k/2}^{k_0+\Delta k/2} A(k)\, e^{+i(kx-\omega t)}\, dx \quad \text{—— (I)}$$

Furthermore, we assume thet, ω varies slowly with k ~~iff~~ and hence we expand $\omega(k)$ in a Taylor Series :-

$$\omega(k) = \omega(k_0) + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k=k_0} + \frac{1}{2}(k-k_0)^2 \cdot \left(\frac{d^2\omega}{dk^2}\right)_{k=k_0} + \cdots$$

and as we are considerng k ~~k_0~~ to be close to k_0 :-

we should neglect higher orders of the Taylor expansion.

$$\text{Thus} \rightarrow \quad \omega(k) = \omega(k_0) + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k=k_0} \quad \text{—— (II)}$$

Now lets substitute eq (II) in eq (I) to get :-

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{k_1}^{k_2} A(k) \exp\left[i \left\{ (k-k_0)x - \left(\omega(k_0) + (k-k_0)\frac{d\omega}{dt} \right\} \right] dk$$

$$\Rightarrow \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\Delta k} A(k) \exp\left[i \left\{ (k-k_0)x + k_0 x - \omega_0 t - (k-k_0) t \frac{d\omega}{dk} \right\} \right] dk \quad \text{— (III)}$$

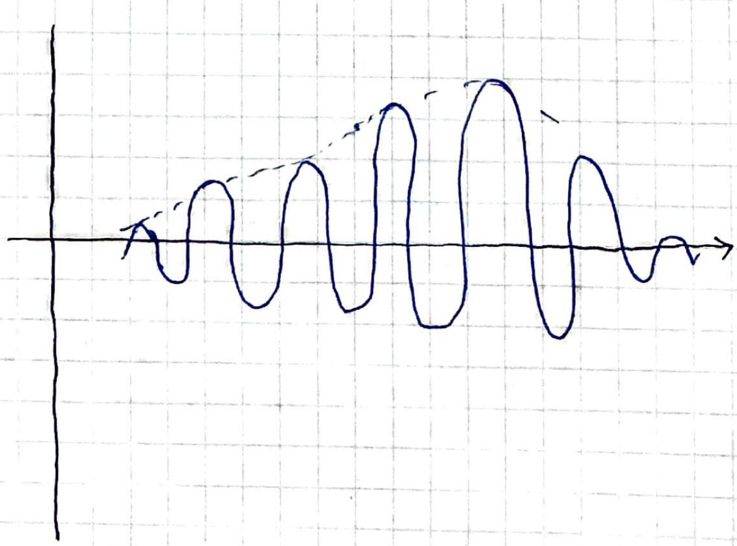
$$= f(x,t)\, e^{i(k_0 x - \omega t)} \quad \text{— (IV)}$$

where,

$$f(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\Delta k} A(k) \exp\left[i \left(x - \frac{d\omega}{dk} \cdot t \right) (k-k_0) \right] dk$$

Eq (IV) reveals that wave function $\psi(x,t)$, do have wavelength $2\pi/k_0$ and frequency $\omega_0/2\pi$, which is modulated by envelope of $f(x,t)$; which further depends on x and t.

This represents a wave packet, which moves with group velocity $V_g = d\omega/dk$.



Also upon close observation one would find that if Δx is spatial extent of wave packet and Δk is wave number range then it is always true that $\Delta x \cdot \Delta k \geq 1$, which resonates tamely with Heisenberg's Uncertainty Principle.

Additional understanding

Recall $\rightarrow$ $p = \hbar k$ and $E = \hbar \omega$

We know group velocity is : $V_g = d\omega / dk$

and hence $V_g = \dfrac{d(\hbar\omega)}{d(\hbar k)} = \dfrac{dE}{dp}$.

this is nothing but familiar classical Hamiltonian expression for velocity of a particle.

- For Non-relativistic free particle of mass, m :

$E = p^2/2m$

or $\dfrac{dE}{dp} = \dfrac{2P}{2m} = V = V_g$

S-PYQ

establish that for both relativistic & non-relativistic case group velocity of a wave packet is equal to particle's velocity.

- For Relativistic case :-

$$E^2 = p^2c^2 + E_0^2$$

$$\Rightarrow 2E\,dE = c^2 \cdot 2P \cdot dp$$

$$\Rightarrow \frac{dE}{dp} = \frac{P \cdot c^2}{E} = \frac{\gamma m v \cdot c^2}{\gamma m c^2}$$

$$\Rightarrow \frac{dE}{dp} = V = V_g.$$

Additionaly. (non-relativistic)

$$\text{Phase velocity } (V_{ph}) = \frac{\omega}{K} = \frac{\hbar\omega}{\hbar k} = \frac{E}{P}$$

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

$$= p/2m$$

$$= v/2.$$

and for relatinistic :-

$$V_{ph} = \frac{E}{P} = \frac{\gamma m c^2}{\gamma m v} = \frac{c^2}{v}$$

Now lets move forward.

4.2.1 <u>wave function in Momentum space</u>

Recall, we have wave function of a group wave representing a particle given by

$$\cancel{\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(p)\, e^{(i/\hbar)}}$$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{i(kx-\omega t)}\, dk.$$

wave function now can be written as :-

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p)\, e^{(i/\hbar)(px-Et)}\, dp. \quad \text{— (VI)}$$

where $A(k)$ has been replaced by "Momentum Amplitude Function".

And if we define $\Rightarrow \Phi(p) = \phi(p).\, e^{-iEt/\hbar}$

then eq (VI) becomes :-

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p,t)\, e^{ipx/\hbar}\, dp$$

And taking inverse fourier transform of $\psi(x,t)$, provides

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-ipx/\hbar}\, dp.$$

and for $t=0$, we get

$$\phi(P) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dp. \qquad \text{(VII)}$$

wave function is momentum space.

Additionally,

$$\int_{-\infty}^{\infty} |\Phi(p,t)|^2 dp = \text{constant} = \int_{-\infty}^{\infty} |\psi(x,t)|^2 dx$$

which is known as Parseval's Theorem.

Now eq (VII) can be written in Three Dimensions too–

$$\psi(r,t) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \Phi(p,t)\, e^{i\vec{p}\cdot\vec{r}/\hbar}\, dp$$

$dp_x \cdot dp_y \cdot dp_z$

volume element in momentum space.

inverse fourier transform

$$\Phi(p,t) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \psi(\vec{r},t) \cdot e^{-i\vec{p}\cdot\vec{r}/\hbar}\, dr.$$

$dx \cdot dy \cdot dz$

4.3 HEISENBERG'S UNCERTAINTY PRINCIPLE

As per classical Mechanics, position & momentum of a particle are independent of each other

↓

Hence, they both can be measured with the arbitrary accuracy simultaneously.

→ But at Atomic Scale this fails.

Recall → Particle is represented by a wave packet.

↓

I. the particle can be found any where in the range where amplitude of the $\psi(x)$ is non-zero.

II. Similarly, momentum could be found any in the region where amplitude of $\phi(p)$ is non-zero.

↓

Thus position of particle and momentum of particle is indeterminete in the range of position & momentum.

↓

IMPORTANT QUESTION ?

upto what ~~possibi~~ precision, one can measure the position & momentum.

Answer → Reciprocity Relation from the last topic. $\Delta x \cdot \Delta k \geq 1$

or $\Delta x \cdot \Delta p \geq \hbar$ —— ①

(by using $p = \hbar k$)

$\Delta x \cdot \Delta p \geq \hbar$ is Heisenberg's uncertainty Relation.

Although the exact statement is $\boxed{\Delta x \cdot \Delta p_x \geq \hbar/2}$

Precision of measurement of x and p are inversely proportional to each other

Additionally position-momentum uncertainty could be used to find energy-time uncertainty.

Recall :-

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

$$\Rightarrow \Delta E = \frac{2p}{2m} \Delta p.$$

$$\Rightarrow \Delta E = (p/m) \cdot \Delta p = \frac{mv}{m} \Delta p = v \Delta p.$$

uncertainty of Δp around p, leads to uncertainty of ΔE about E.

Hence. $\Delta E = v \Delta p$.

Now, we could write v as $v = \frac{\Delta x}{\Delta t}$

So. $$\Delta E = \frac{\Delta x}{\Delta t} . \Delta p.$$

$$\Rightarrow \Delta E \cdot \Delta t = \Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

Hence $\boxed{\Delta E \cdot \Delta t \geq \hbar/2}$ → Energy time H.U.P.

Similarly, angular momentum and angular position uncertainty is $\boxed{\Delta \theta \cdot \Delta L \geq \hbar/2}$

- **General Statement of Uncertainty Principle :-**

It is impossible to simultaneously specify the precise value of both members of certain pairs of dynamical variables of the system.

These values are called Complementary variables and are canonically conjugate to each other in the classical Hamiltonian Sense. The product of the uncertainties in the values of such variables are ~~alte~~ atleast of $\underbrace{\text{order of } \hbar}$.

↳ the smallness of the order reminds that H.U.P is effective only on quantum world

4.4. PRACTICAL IMPLICATIONS OF H.U.P

I. Heisenberg's Gamma Ray Microscope

II. Single Slit Diffraction Experiment

III. Double " Interference Experiment

4.4.1 Heisenberg's Gamma Ray Scope

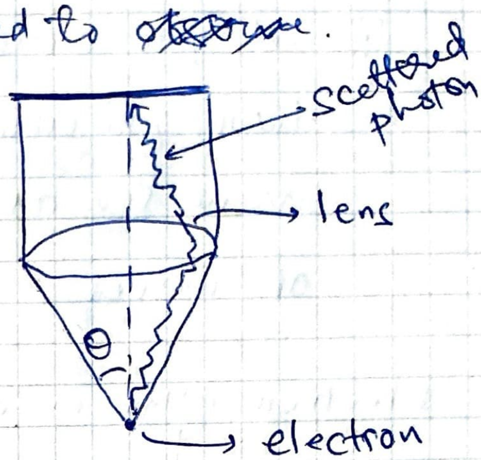
↳ idealized thought by Heisenberg himself.

We are using gamma Ray because it has smallest wavelength ~~as~~ and it will lead to Smallest Resolution & hence Smallest uncertainty in ~~∆~~ x.

That is Abbe Diffraction limit say

$$\text{Resolution} = \frac{\lambda}{2\mu \sin\theta} \quad \Rightarrow \Delta x = \frac{\lambda}{2\sin\theta} \qquad (1)$$

where θ is half angle of maximum cone of the light / gamma ray used to ~~observe~~ observe the electron.



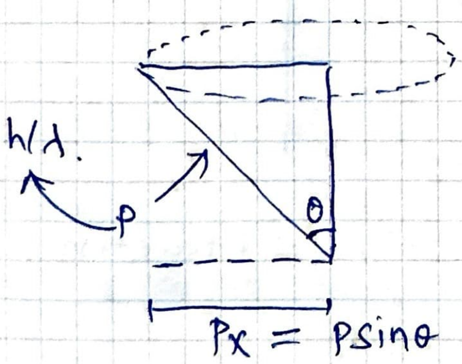
To measure the electron precisely → uncertainty in x should be minimum

↳ hence λ should be minimum.

↳ thus use gamma rays which has minimum wavelength.

But as observation requires gamma ray (made of photon), so we would also take into account the compton effect. [collision in b/w photon & e^-]

Momentum range of photon (within gamma ray) would be from $\underbrace{(-h/\lambda)\sin\theta}_{\text{x-Component of Momentum}}$ to $\underbrace{(+h/\lambda)\sin\theta}_{\text{x-Component of Momentum}}$.



Schematic of Momentum

Thus uncertainty in momentum in x is:-

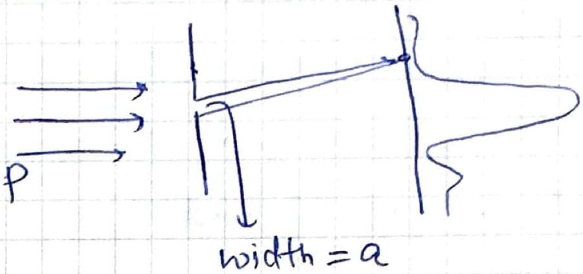
$$\Delta p_x = (2h/\lambda)\sin\theta \quad \text{— (II)}$$

Finally from equation (I) & (II) we get $\boxed{\Delta x \cdot \Delta p_x = h}$

which is H.U.P.

4.4.2 Single slit Diffraction Experiment

? If you could do diffraction using the e^- then you can say e^- do behave as wave too as Diffraction is characteristic of waves.

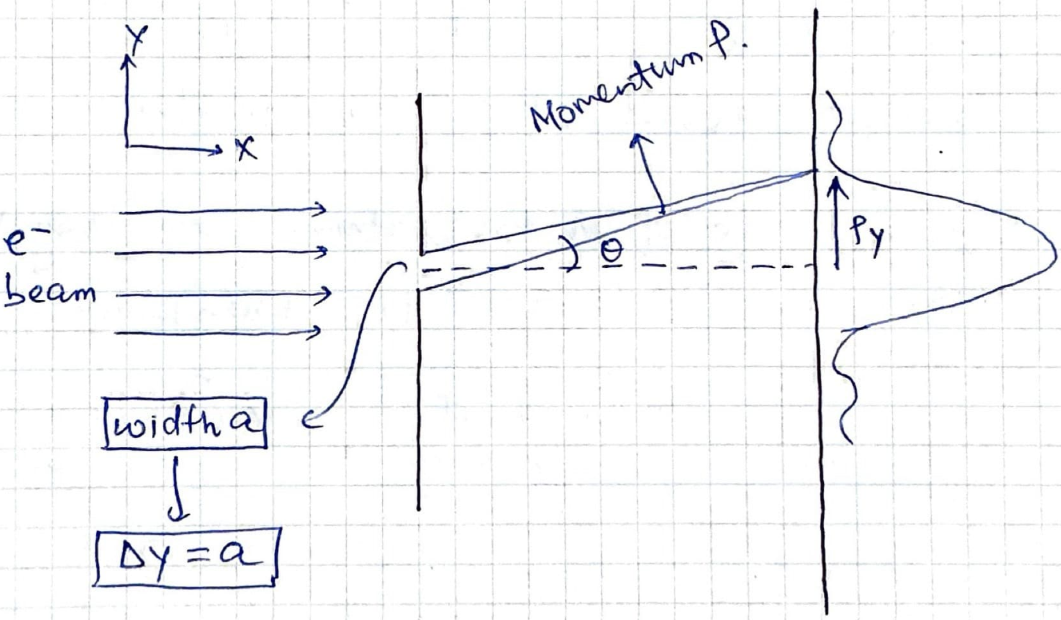


Electron with momentum p

↓

incident on a ~~Diaphraa~~ ~~Diaphr~~ Diaphragm ~~of~~ ~~slit~~ with slit width 'a'.

(additionally smaller the width → greater the knowledge of Y component of the e^-)



Hence, we understand the diffraction experiment.

Thus $\Delta P_y = P \cdot \sin\theta$

$\Delta y = a$

So. $\Delta y \cdot \Delta P_y = a \cdot P \cdot \sin\theta$

$$\Delta y \cdot \Delta P_y = a \cdot \frac{h}{\lambda} \cdot \sin\theta$$

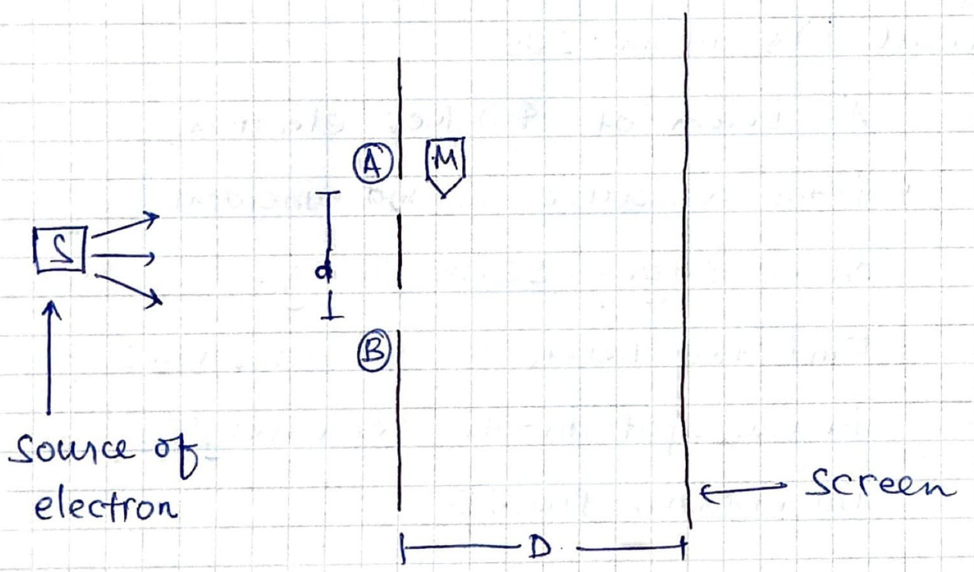
or $\Delta Y \cdot \Delta P_y = a \cdot \frac{h}{\lambda} \cdot \frac{\lambda}{a}$

we used $\sin\theta = \frac{\lambda}{a}$ from theory of diffraction.

Hecnce $\cancel{\Delta Y \cdot \Delta P_y = \hbar}$

$\boxed{\Delta Y \cdot \Delta P_y = h}$ which is H.U.P

4.4.3 Double Slit Interference Experiment



distance b/w Successive Maxima $= \beta = \frac{\lambda D}{d}$

where λ is de Broglie wavelength of the electron.

Now let us put detector M behind ~~slit~~ slit A.
It is a microscope and in order to measure or find through which slit the e^- arrive it should have minimum precision better than $d/2$.

So $\Delta Y < d/2$ —— (i)

Now a/c to H.U.P : $\Delta Y \cdot \Delta P_Y = \hbar$

$\Rightarrow \Delta P_Y = 2\hbar/d$ —— (ii)

And as there is momentum uncertainty in Y-AXIS hence, direction of motion of electron becomes uncertain by $\Delta\theta$ and given by $\Delta\theta = \frac{\Delta P_y}{P}$

or $$\Delta\theta = \frac{\Delta P_y}{P} \geq \frac{2\hbar}{d\,(h/\lambda)} = \frac{\lambda}{\pi d}$$

and this angular uncertainty produces the uncertainty in position of electron.

Recall PYQ from 2017.

PYQ - 2017 A beam of 4.0 keV electrons from a Source is incident on a target 50 cm away. Find the radius of the electron's beam spot due to Heisenberg's uncertainty Principle.

4.5 Bohr complimentarity Principle

Wave and Particle nature of Radiation and Matter are complimentary ~~and~~ ~~hence~~ but exclusive. That is both aspects of wave & particle can not be observed simultaneously. Most direct observation of this is Double-Slit Experiment, where if effort is made to find through which slit the particle appears then interference pattern disappears.

4.6 Consequences of H.U.P

I. finding ground state energy & radius of hydrogen atom

II. Non existence of electrons in Nucleus

III. Zero point energy of ~~hydrogen atom~~ Harmonic oscillator

IV. Broadening of Spectral lines

V. Mass of π- Meson.

4.6.1 Ground State Energy & Radius of the Hydrogen Atom

For ground ~~energy~~ State condition - the energy should be minimum, and energy is Sum of kinetic energy of electron and the potential energy due to electron Proton pair.

Hence $E = K.E + P.E$

$$\Rightarrow E = \frac{p^2}{2m} + \frac{1}{4\pi\epsilon_0} \frac{e.(-e)}{r} \quad \text{——} \quad (I)$$

for this momentum, we could substitute its value from H.U.P

So from H.U.P — we could approxiamete

$\Delta r \simeq r$ (uncertainty in radius would be approxiametely equal to order of radius itself).

$\Delta p \simeq p$ (Same argument for momentum too.)

Hence as per H.U.P: $\boxed{r.p \simeq \hbar}$ —— (II)

Now substituting value of momentum from eq (II) to eq (I),

we get, $E = \dfrac{\hbar^2}{2mr^2} - \dfrac{e^2}{4\pi\epsilon_0 r}$

and condition for ground state is that E should be minimum. Hence -

$$\frac{dE}{dr} = 0 \quad \text{and} \quad \frac{d^2E}{dr} > 0 \text{ (for minima)}$$

$$\Rightarrow \cancel{\frac{\hbar^2}{2m}\left(-2r^{-3}\right)} +$$

$$\Rightarrow \frac{\hbar^2}{2m}\left(-2r^{-3}\right) + \frac{e^2}{4\pi\epsilon_0 r^2} = 0$$

$$\Rightarrow \frac{-\hbar^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2} = 0$$

$$\Rightarrow r = \frac{4\pi\epsilon_0\hbar^2}{me^2} \quad \text{[Bohr Radius]}.$$

$$r = 0.53 \times 10^{-10}\,m \qquad \text{—— (III)}$$

Substituting (III) in (I) we get :-

$E = -13.6$ eV which is ground state energy.

4.6.2 Non-Existence of electrons inside the Nucleus

~~Let us consider Simplest atom (i.e hydrogen atom)~~

We know that the Size of Nucleus is of order of 10^{-14} m. Therefore for an electron to be confined with a nucleus, the uncertainty in its position would not exceed this value.

Hence corresponding uncertainty in Momentum is :-

$$\Delta P_x = \frac{\hbar}{\Delta x} = \frac{1.054 \times 10^{-34} \text{ J.S}}{10^{-14} \text{ m}}$$

$$\Rightarrow \Delta P_x = 1.1 \times 10^{-20} \text{ kg m/s.}$$

And then momentum of such electron must be of same order too.

Calculating
$$KE = PC = (1.1 \times 10^{-20} \text{ kg m/s}) \times (3 \times 10^8 \text{ m/s})$$
$$= 3.3 \times 10^{-12} \text{ J}$$
$$= \frac{3.3 \times 10^{-12}}{1.6 \times 10^{-19}} \text{ eV}$$
$$= 20.6 \text{ MeV}$$

So if electron would be inside the nucleus it must have 20.6 MeV. But when one checks the electrons ~~e~~ emitted from Nuclei in β-decay, then electrons would at most have 2–3 MeV which is way ~~m~~ less then the minimum requirement of 20.6 MeV.

SPYQ Prove that electron can reside within the atom.

4.6.2 Zero point energy of Harmonic Oscillator

Energy of Harmonic Oscillator

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

from H.U.P $\quad P = \frac{\hbar}{2a} \quad$ as $\Delta p \sim p$ $\qquad$ —— (II)

$\Delta x \sim a$

and a is size of area where particle is enclosed.

thus substituting (II) in (I) –

$$E = \frac{\hbar^2}{8ma^2} + \frac{1}{2}m\omega^2 x^2$$

for ground state, energy has to minimum, which would be when $\frac{dE}{da} = 0$ and $\frac{d^2E}{da^2} > 0$

thus $\rightarrow$ $\frac{dE}{da} = 0$

$$\Rightarrow \frac{-2\hbar^2}{8m}\left(\frac{1}{a^3}\right) + m\omega^2 a = 0$$

$$\Rightarrow a = \left[\frac{\hbar}{2m\omega}\right]^{1/2} \qquad \text{—— (III)}$$

for value of a as in eq (I) energy would be minimum.

Hence $\quad E = \frac{\hbar\omega}{2} \quad$ after substituting eq (III) in eq (I).

4.6.3 Broadening of Spectral lines

Example of energy time uncertainty relation

Consider an atom in excited state. It deexites in very short span of time by emitting a photon.

So if 'τ' is lifetime of such state, then energy of such state would be uncertain by amount

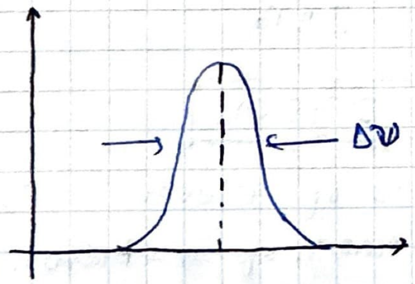
$$\Delta E = \frac{\hbar}{\Delta t} = \frac{\hbar}{\tau} \quad \text{——} \quad (1)$$

$$\Rightarrow h\Delta\nu = \frac{\hbar}{\Delta t} = \frac{\hbar}{\tau}$$

$$\Rightarrow \Delta\nu = \frac{1}{2\pi\tau}$$

This energy width of excited state, will cause frequency of emitted radiation would spread by amount $\boxed{\Delta\nu = 1/2\pi\nu}$

Spectral Broadening



4.6.4 Mass of π-Meson

In 1935 Yukawa Proposed $\rightarrow$ Nuclear forces arises by emission of a particle by one nucleon and absorption other.

Such particle is called pion or π-Meson.

if π - Meson has mass m then its emission would create energy imbalance as per mass energy equivalence.

$$\Delta E = mc^2$$

then corresponding uncertainty in its life time is :

$$\Delta t = \frac{\hbar}{\Delta E} = \frac{\hbar}{mc^2} \quad \text{—— (1)}$$

at speed c, range cover by such π - Meson is given by $r_0 = c \cdot \Delta t = \frac{c\hbar}{mc^2} = \frac{\hbar}{mc}$

or $m = \frac{\hbar}{r_0 c}$

for electron having m_0, we have

$$\frac{m}{m_0} = \frac{1}{2\pi r_0}\left(\frac{h}{m_0 c}\right)$$

$$\Rightarrow \frac{m}{m_0} \approx \frac{\lambda_0}{2\pi r_0}$$

$$\Rightarrow \boxed{m = 275 m_0}$$

↳ mass of electron compared to mass of π - Meson.