Engineering Physics (BT-201)
B.Tech. I Year
CO - 01
Unit I - QUANTUM PHYSICS

By

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OUTLINE

- WAVE PARTICLE DUALITY
- GROUP AND PARTICLE VELOCITIES
- UNCERTAINTY PRINCIPLE
- ELEMENTARY PROOF AND APPLICATIONS (Uncertainty Principle)
- COMPTON SCATTERING
- ENERGY AND MOMENTUM OPERATORS
- TIME DEPENDENT AND TIME INDEPENDENT SCHRÖDINGER WAVE EQUATION
- ONE DIMENSIONAL SQUARE POTENTIAL WELL

QUANTUM MECHANICS

We know that classical mechanics can successfully explain the motion of astronomical bodies (such as stars, planets satellites etc.) means Newton's law of motion, as well as macroscopic bodies (such as motion under). Except this motion of charged particles in e.m. fields, elastic vibrations in solids, propagation of sound waves in glass etc. can also be explained successfully by classical mechanics, but some phenomenon like black body radiation, photo-electric effect, Compton effect, specific heat of solids at low temperature, stability of atoms, emission and absorption of light etc. could not be explained, which is explained by quantum mechanics.

Wave particle duality or dual nature of light

Light obeys the phenomena of interference, diffraction, polarization, photoelectric effect, Compton Effect etc. The phenomena of interference, diffraction and polarization can be explained by assuming that light is a form of wave. By the wave theory of light, it has been proved that light possesses a wave nature. However, some other phenomena like photoelectric effect, Compton Effect and discrete emission and radiation can be explained only with the help of the quantum theory of light. According to the quantum theory, light radiation travels in the form of energy bundles called quanta of energy hv, where v is the frequency of radiation. Hence according to the quantum theory, light possesses a corpuscular (particle) nature. Therefore, sometimes light obeys the wave theory and sometimes the corpuscular theory, Hence, light has dual nature.

DE-BROGLIE HYPOTHESIS OR DE-BROGLIE MATTER WAVES

Louis De-Broglie suggested that the dual nature is not only of light, but each moving material particle has the dual nature. He assumed a wave should be with each moving particle, (all micro particles) which is called the matter waves. Although these waves can travel through vaccum like e.m. waves, but these are different from
e.m. waves, because these waves associated with all types of charged and neutral particles.

PROOF OF DE-BROGLIE WAVES

According to Plank's quantum theory light is in form of small bundles of energy ($h\upsilon$) called quanta or photons.

If we consider a photon (quantum) to be a wave of frequency υ then its energy

$E=h\upsilon$ ……..*(i)* Or $E=hc/\lambda$ [i.e. $c=\upsilon\lambda$]

Where c = velocity of light (or photon) in vaccum

λ = wavelength of photon or radiation

h = Plank's constant = 6.625×10^{-34} J-sec

Now if we consider photon as a particle of mass m, then from Einstein's mass-energy equivalence (or theory of relativity) energy of photon

$E= mc^2$……….*(ii)* from eq.(i) & (ii) $mc^2 = h\upsilon = hc/\lambda$

or $mc = h/\lambda$

or $\lambda = h/mc$ [i.e. $p = mc$]

or $\lambda = h/p$…………*(a)* where λ is a De-Broglie wavelength.

Thus this is an evidence of De-Broglie nature of radiation (photon) the wavelength (λ) to particle like nature of radiation (photon) the momentum (p). It means this equation shows dual nature of light.

We know that the kinetic energy of the particle

$$E = \frac{1}{2}(mv^2) = \frac{1}{2}(m^2v^2/m) = P^2/2m$$

$$\text{or } P^2 = 2mE$$

$$\text{or } P = \sqrt{(2mE)}$$

So, De-Broglie wavelength $\lambda = h/\sqrt{2mE}$..........*(b)*

According to kinetic theory of gases the average kinetic energy of the material particle

$$\frac{1}{2}(mv^2) = 3/2kT$$

$$\text{Or } m^2v^2 = 3mkT$$

$$\text{Or } P^2 = 3mkT$$

$$\text{Or } P = \sqrt{3mkT}$$

So De-Broglie wavelength $\lambda = h/\sqrt{3mkT}$............*(c)*

where k = Boltzmann's constant = 1.38×10^{-23} J/K

T = Absolute temperature

If an particle accelerated through a potential difference of V volts, then

Work done by electric field = increase (gain) in kinetic energy

$$\text{or } qV = \frac{1}{2} mv^2$$

$$\text{or } mqV = \frac{1}{2} m^2v^2$$

$$\text{or } 2mqV = m^2v^2 = P^2$$

$$\text{or } \sqrt{2mqV} = P$$

So, De-Broglie wavelength $\lambda = h/\sqrt{2mqV}$

In case of electron wavelength of wave associated with the moving electron

$$\lambda = h/\sqrt{2meV}$$

$$\text{or } \lambda = \sqrt{(150/V)}\ \text{Å} = 12.27/\sqrt{V}\ \text{Å}.$$

PROPERTIES OF DE-BROGLIE WAVES

1. We know that the wavelength of matter waves (de-Broglie waves) associated by a moving particle is $\lambda = h/mv$

   It means $\lambda \alpha (1/m)$ and $\lambda \alpha (1/v)$.

   For a particle at rest means $v = 0$ so $\lambda = \infty$ and if $v = \infty$ then $\lambda = 0$. Here $\lambda = 0$ means that the matter waves are generated only when the particles are in motion.

2. Matter waves are independent of charge because it generated by any moving particle.

3. Energy of particle is given by $E=hv$ or $v=E/h$, where v is the frequency of wave.

   We know that $E= mc^2$, where c is the velocity of light.

   So we can write $v= mc^2/h$……………….(1)

   We know that wavelength of a wave associated with the particle of mass m, moving with velocity v is, $\lambda = h / mv$ …………………..…(2)

   If de-Broglie's wave velocity (phase velocity) is v_p, then

   $v_p = v\lambda$

   or $v_p = mc^2/h * h / mv$

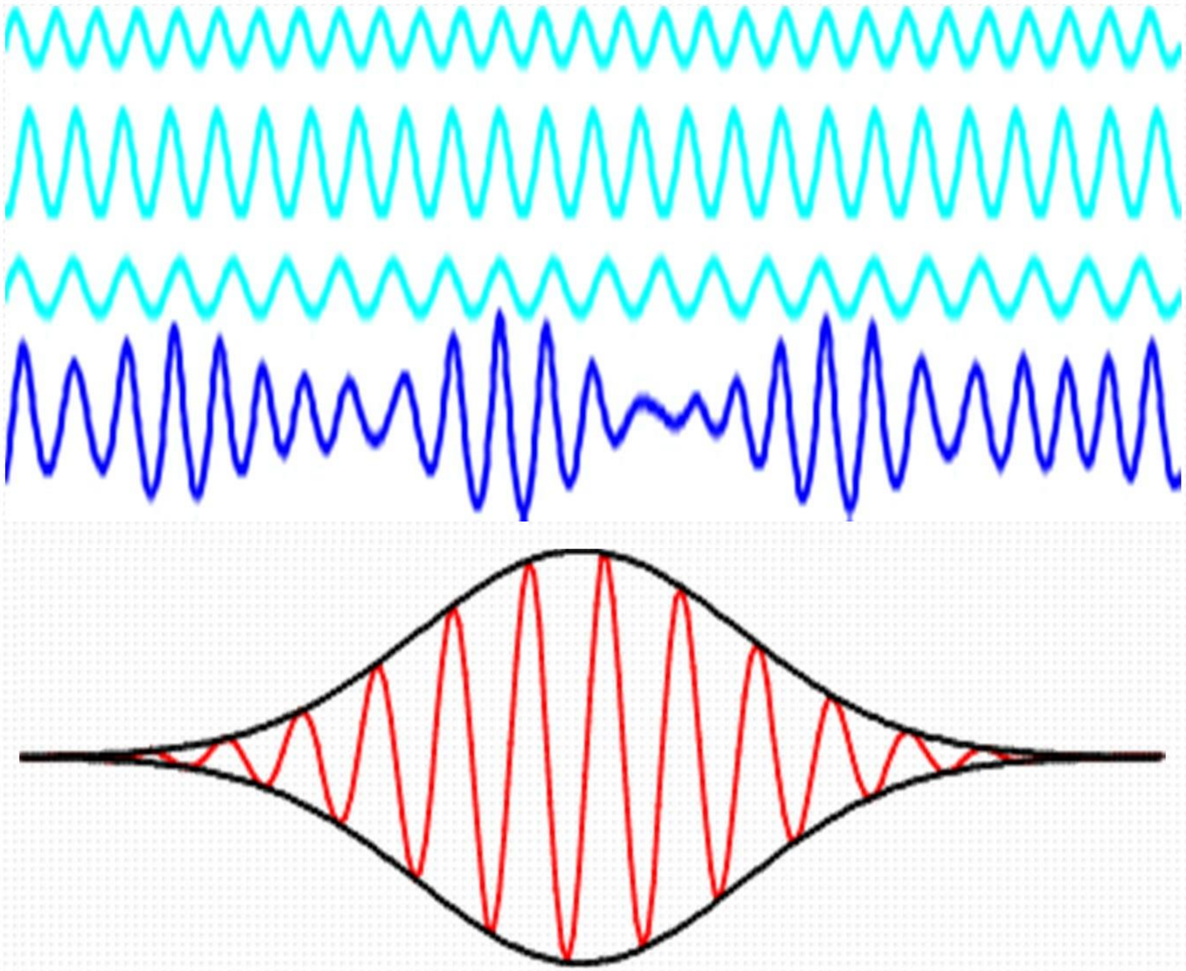
   or $v_p = c^2/v$

- From Einstein's theory of velocity, the speed of light is maximum speed that can be attained by a particle in nature.
- Thus from equation $v_p = c^2/v$, the velocity of de-Broglie's wave associated with the particle would travel faster than the particle itself,
- Hence it is evident that a particle will not equivalent
  to a single wave, but equivalent to a group of wave, called wave packet or wave group.

Wave- Packet or Relation B/W group velocity and phase velocity

- A wave packet consist of a group of several waves of slightly different velocities & wavelength and formed by the superposition of waves situated on and around the center wavelength given by the de-Broglie formula.
- The amplitude and phase of the component waves are such that they interfere constructively in limited region where the particle is found and outside this region they interfere destructively, so amplitude falls to zero rapidly.
- Thus when several waves of slightly different wavelength travel along a straight line in one direction. The resultant waves obtained due to their superposition in form of group of waves which is called the wave packet.

Wave-Packet



The velocity of component or constituents waves of a wave packet is called phase velocity and the velocity of the wave packet is called the group velocity.

Consider the wave group arise from the combination of two waves that have the same amplitude A, but differ by an amount $O\omega$ in angular frequency and an amount OK in wave number. These two waves can be represented as,

$y_1 = A \cos(\omega t - kx)$

$y_2 = A\cos[(\omega + O\omega)t - (k + Ok)x]$

Where $\omega = 2\pi\upsilon$ is angular frequency & $k = 2\pi/\lambda$ is wave number (propagation constant)

The motion of wave packet or the displacement equation of wave packet obtained due to their superposition will be at any point 'x' and time 't'.

CONT..

$Y = y_1 + y_2$

or $Y = A\,[\cos(\omega t - kx) + \cos\{(\omega + O\omega)t - (k + Ok)x\}]$

or $Y = 2A\cos\dfrac{(\omega t - kx) + \{(\omega + O\omega)t - (k + Ok)x\}}{2} . \cos\dfrac{[(\omega t - kx) - \{(\omega + O\omega)t - \{(k + Ok)x\}]}{2}$

[Because cosC + cosD = 2cos {C+D}/2. Cos{C-D}/2]

Or, $Y = \dfrac{2A\cos[(\omega t - Kx + \omega t + O\omega t - Kx - OKx)]}{2} \times \dfrac{\cos[(\omega t + O\omega t - Kx - OKx - \omega t + Kx)]}{2}$

Or, $Y = \dfrac{2A\cos[2(\omega t - Kx) + (O\omega t - OKx)]}{2} \times \dfrac{\cos(O\omega t - OKx)}{2}$

Or, $Y = \dfrac{2A\cos\,[(2\omega + O\omega)\,t - (2K + OK)x]}{2} \times \dfrac{\cos(O\omega t - OKx)}{2}$

Because $O\omega << \omega$ and $OK << K$, so we can write $2\omega + O\omega = 2\omega$ and $2K + OK = 2K$

CONT..

Or, $Y= 2A\cos[(2\omega t-2Kx)/2 \times \cos(O\omega t-OKx)/2]$

$$Y= 2A\cos(\omega t-Kx) \times \cos(O\omega t-OKx)/2$$

Or, $Y= 2A\cos(O\omega t-OKx)/2 \times \cos(\omega t-Kx)$

This equation represents a wave of angular frequency 'ω' & propagation constant 'K'. The amplitude of this wave is $2A\cos(O\omega t-OKx)/2$
The velocity of group wave (vg) is the velocity with which the maximum amplitude moves and maximum amplitude will be '2A' i.e.,
$2A\cos(O\omega t-OKx)/2 = 2A$

It means $\cos(O\omega t-OKx)/2 = 0$ means $O\omega t-OKx = 0$

Or $O\omega t=OKx$, or $(O\omega/OK)t = x$

Because we know that $x/t= v$ (distance/ time = velocity). So in case of wave packet group velocity $v_g = \frac{dx}{dt} = \frac{d}{dt}\frac{O\omega t}{OK} = O\omega / OK$

Or, we can write $v_g = \frac{d\omega}{dK}$ ----------------------------(1)

Because when $= \lim_{OK‹\ 0} \left(\frac{O\omega/2}{OK/2}\right)$

Because the displacement equation of a wave y= A cos (ωt-Kx)

So, phase or wave velocity v_p =dx/dt

So, A will be maximum when cos (ωt-Kx)=1 Or, ωt-Kx=0 or x= ωt/K

So, phase velocity $v_p = \frac{dx}{dt} = \frac{d}{dt}\frac{\omega t}{K}$ or $v_p = \omega/K$ ---------------------------(2)

So, from equation (1) $v_g = d\omega/dK$

Means $v_g = \frac{d}{dK}(Kv_p)$ $\quad\because v_p = \omega/K$

or $v_g = v_p \times 1 + K \,.\, dv_p/dK$

or $v_g = v_p + (2\pi/\lambda) \,.\, dv_p/d(2\pi/\lambda)$

or $v_g = v_p - (2\pi/\lambda) \,.\, \frac{dv_p}{(2\pi/\lambda^2)d\lambda}$ $\quad\because d(1/x) = -(1/x)dx$

or $v_g = v_p - \frac{\lambda . dv_p}{d\lambda}$

Thus group velocity (v_g) depends on the phase velocity (v_p) and variation of phase velocity with the wavelength ($dv_p/ d\lambda$).

DIFFERENT CASES

<u>In the non-dispersive medium</u>: If $dv_p/ d\lambda = 0$ i.e., the medium is such that in it the phase velocity doesn't depend on the wavelength then,

$$v_p = v_g$$

i.e., the group velocity and phase velocity are equal. Such a medium is which the $v_p = v_g$ is called non-dispersive medium. For example; $v_p = v_g$ for electromagnetic wave in vacuum and elastic wave in a homogenous medium.

<u>In the dispersive medium</u>: In a dispersion medium $dv_p/ d\lambda$ is positive and $v_g < v_p$. For example; v_g of electromagnetic wave in a dielectric substance is less than v_p .

But if the value of $dv_p/ d\lambda$ is negative in a dispersive medium , then $v_p > v_g$. For example; in electric conductors the group velocity v_g is more than the phase velocity v_p.

Relationship between group velocity & phase velocity for the De-Broglie wave associated with a particle of rest mass (m_o) moving with a velocity v).

➢ (Relativistic Case)

Because we know that angular frequency ,

$\omega = 2\pi\upsilon = 2\pi.(mc^2/h)$ [$.\dot{}.$ E= m = hυ or υ = mc^2/h]

Or $\omega = \frac{2nn_0c^2}{h\sqrt{1-\frac{v^2}{c^2}}}$------------(1) $\left[.\dot{}. \quad n = \frac{n_0}{\sqrt{1-\frac{v^2}{c^2}}} \right]$

And propagation constant K = $2\pi/\lambda = 2\pi.(m\upsilon/h)$ [$.\dot{}.$ λ=h/p=h/mv]

$K = \frac{2nn_0v}{h\sqrt{1-\frac{v^2}{c^2}}}$ ------------(2)

So phase velocity $v_p = \omega/K = c^2/v$, and

Graph velocity $v_g = \dfrac{d\omega}{dK} = \dfrac{d\omega/dv}{dK/dv}$

Now $\dfrac{dm}{dv} = \dfrac{d}{dv}\left[\dfrac{2nn_0c^2}{h\sqrt{1-\frac{v^2}{c^2}}}\right]$ or $\dfrac{d}{dv}\left[\dfrac{2nn_0c^2}{h}\left(1-\dfrac{v^2}{c^2}\right)^{-\frac{1}{2}}\right]$

$\dfrac{dm}{dv} = \dfrac{2nn_0c^2}{h}\left[\dfrac{d}{dv}\left(1-\dfrac{v^2}{c^2}\right)^{-\frac{1}{2}}\right]$ After Differentiation

$\dfrac{dm}{dv} = \dfrac{2nn_0c^2}{h}\left[\dfrac{v}{c^2}\left(1-\dfrac{v^2}{c^2}\right)^{-\frac{3}{2}}\right]$ Similary for $\dfrac{dK}{dv} = \dfrac{2nn_0}{h}\left[\left(1-\dfrac{v^2}{c^2}\right)^{-\frac{3}{2}}\right]$

So we can write Graph velocity $v_g = \frac{dm}{dK} = \frac{dm}{dv} / \frac{dK}{dv} = v$

$$v_p = \frac{c^2}{v_g}$$

So, the De – Broglie wave group associated with a moving body travels with the same velocity as the moving particle. It is evident that a material particle in motion is equivalent to a group of waves or a wave packet.

Relation between Vp and Vg for a non- relative free particle (Non-relativistic case)

Suppose v_g & v_p represents the group and phase velocity respectively for a non-relativistic free particle of mass 'm'.

Let 'λ' is the De- Broglie wavelength and 'υ' is the frequency of the wave then, the phase velocity, $v_p = \upsilon\lambda$--------------------(1)

According to De-Broglie hypothesis, $\lambda = h/mv_g^2$,----------------------(2)

Total energy, E= kinetic energy = $mv_g^2/2$
[Because potential energy of freely moving particle is constant]
Also E= $h\upsilon$. Or, $\upsilon = E/h = mv_g^2/2h$ -----------------------(3)
So from equation (1), (2) and(3),
Because phase velocity $v_p = \upsilon.\lambda = mv_g^2/2h \times h/mv_g^2$

$$v_p = v_g/2$$

Hence for a non- relativistic free particle the phase velocity is half of the group velocity.

Heisenberg's Uncertainty Principle

"It is impossible to determine simultaneously the position and momentum of the particle with any desired accuracy."

This definition is known as Heisenberg's uncertainty principle.

- This limitation is critical when dealing with small particles such as electrons.
- But it does not matter for ordinary-sized objects such as cars or airplanes.
- To locate an electron, you might strike it with a photon.
- The electron has such a small mass that striking it with a photon affects its motion in a way that cannot be predicted accurately.
- The very act of measuring the position of the electron changes its momentum, making its momentum uncertain.

Werner Heisenber
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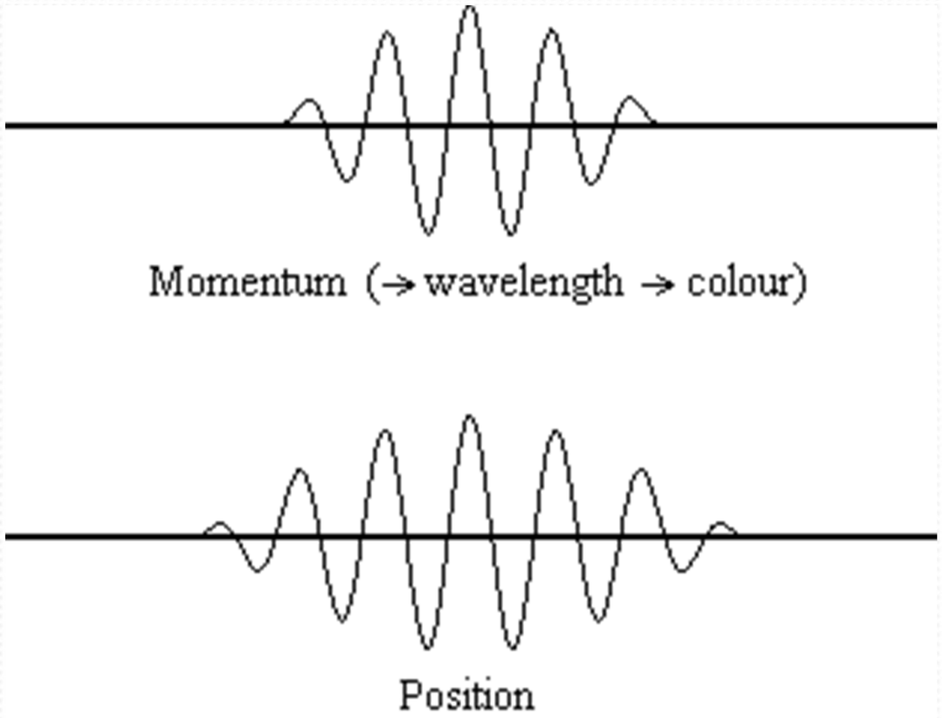
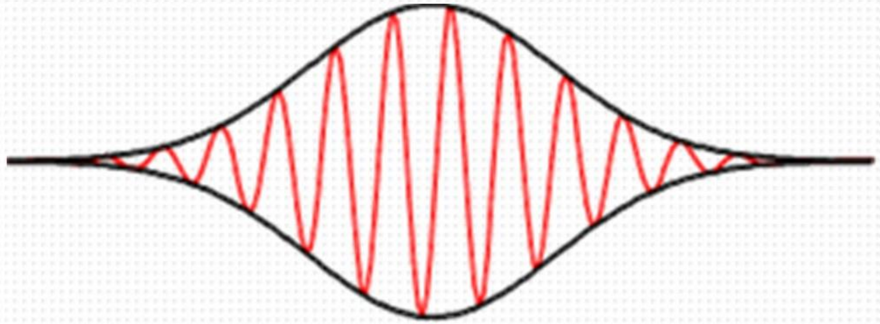
If we want accuracy in position, we must use short wavelength photons because the best resolution we can get is about the wavelength of the radiation used. Short wavelength radiation implies high frequency, high energy photons. When these collide with the electrons, they transfer more momentum to the target. If we use longer wavelength, i.e less energetic photons, we compromise resolution and position.



Proof of Heisenberg's principle

1. Position and Momentum uncertainty:-

Heisenberg's principle can be proved by assuming that a particle in motion is equal to wave group and $v_g = v$. We know that a moving particle is equal to a wave group rather than a particle. It means there is limit for the measurement of particle properties.



Let a particle surrounded by a wave group. Let this wave group arises from the combination of two waves that have same amplitude A but differ by an amount $\Delta\omega$ in angular frequency and an amount Δk in propagation constant.

These two waves can be represented as :-

$y_1 = A\cos(\omega t - kx)$

and $y_2 = A\cos[(\omega + \Delta\omega)t - (k + \Delta k)x]$

The displacement of wave group at any time & at any point x will be.

$Y = y_1 + y_2$

or $Y = A\,[\cos(\omega t - kx) + \cos\{(\omega + O\omega)t - (k + Ok)x\}]$

or $Y = 2A\cos\left[\dfrac{(\omega t - kx) + \{(\omega + O\omega)t - (k + Ok)x\}}{2}\right] . \cos\left[\dfrac{(\omega t - kx) - \{(\omega + O\omega)t - \{(k + Ok)x\}}{2}\right]$

[Because $\cos C + \cos D = 2\cos\{C+d\}/2 .\ \mathrm{Cos}\{C-D\}/2$]

Or, $Y = 2A\cos\dfrac{[(2\omega + O\omega)t - (2K + OK)x]}{2} \times \cos(O\omega t - OKx)/2$

Because $O\omega << \omega$ and $OK << K$, so we can write $2\omega + O\omega = 2\omega$ and $2K + OK = 2K$

Or, $Y = 2A\cos(O\omega t - OKx)/2 \times \cos(\omega t - Kx)$

This equation represents a wave (wave packet) of angular frequency 'ω' & propagation constant 'K'. The amplitude of this wave is
$2A \cos(O\omega t\text{-}OKx)/2$

Because the particle is moving with a velocity equal to the velocity of wave packet so the position of the particle can be anywhere in the wave packet so we can say the uncertainty in the position of the particle equals to the length of wave packet. Means distance between two consecutive modes. Node is formed when amplitude =0, means

$$2A \cos(O\omega t\text{-}OKx)/2 = 0$$

$$\text{Or} \qquad \cos(O\omega t\text{-}OKx)/2 = 0$$

It is possible when $(O\omega t\text{-}OKx)/2 = \pi/2, 3\pi/2, 5\pi/2,\ldots$

At a particular time 't' at positions x_1 and x_2,

(Oωt-OK x_1)/2 = π/2 -------------------- (1)

(Oωt-OK x_2)/2 = 3π/2 ------------------ (2)

From equations (1) and (2), we can write

OK/2.(x_2- x_1) = π

If the error in the measurement of the position of the particle is (x_2- x_1) = Ox, then

OK. Ox = 2π ------------------ (3)

If Op is error in the measurement of the momentum of the particle and OK in propagation constant then,

OK= 2π/Oλ = (2π.Op)/h So from Equation (3) we can write,

(2π.Op)/h. Ox = 2π Or Op. Ox = h Or Op. Ox ≥ ħ/2π

It means that if we make simultaneous measurement of two quantities namely position and momentum of the particle the product of the fundamental errors is approximately equal to Plank's constant.

Application of Uncertainty principle

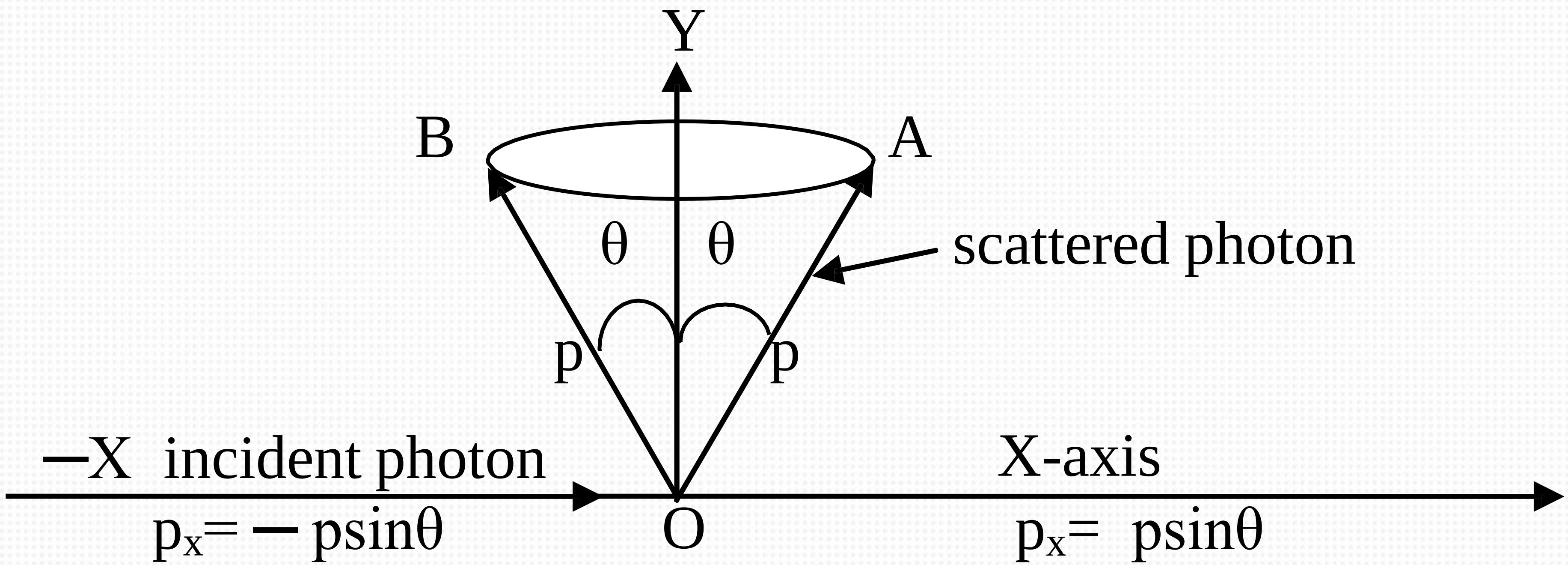
Determination of position of α-particle by γ-ray microscope:

For the determination of position of an particle (electron), it should be targeted (illuminated) by light (photons).From physical optics it is known that the exactness of position increase with decrease in wavelength of light. So uncertainty in position 'Ox', so we take γ-rays microscope to be small, wavelength 'λ' should be small. We know that from the theory of resolving power, the minimum distance between two objects x_1 and x_2 to be seen clearly or the uncertainty in the position is

$(x_2 - x_1) = Ox = \lambda/2\sin\theta$ -------------------------(1)

Where λ is wavelength of γ-rays and θ is semi-vertical angle of the cone of the objective with the object.

Suppose γ-rays incident on a stationary electron at O. The scattered γ-rays to be seen by the microscope which reaches through the objective of the microscope AB. The γ-rays consist of photons of energy $h\upsilon$ and momentum $h\upsilon/c$. Due to collision of photons with electron there will be a transfer of momentum from photon to electron. Therefore change in momentum of photon which will reach the objective of microscope.


Y
B
A
θ
θ
scattered photon
p
p
—X incident photon
X-axis
O
$p_x = -\,p\sin\theta$
$p_x = p\sin\theta$

So the momentum of photon in the direction of motion of electron will be p sinθ and in the direction opposite of motion of electron will be psin(-θ).

Total change in momentum Op = psinθ − psin(-θ)

Op = psinθ + psinθ

Op = 2psinθ ---------------------- (2)

From equation (1) (2), we get

Op.Ox = λ/2sinθ. 2psinθ

Or Op.Ox = h/p2sinθ.

2psinθ Or Op.Ox = h

Or Op.Ox ≥ ħ/2π

Thus in the determination of position of a particle by γ-ray microscope the product of uncertainty in position and uncertainty in momentum is of the order of h. It is in accordance with Heisenberg's Uncertainty principle.

2. Diffraction of an electron beam by a single slit: Consider an electron beam travelling in X-direction which is incident on a narrow slit AB. Since the electron beam has a wave behavior, so we get diffraction pattern on the screen. Because it is quite uncertain to say that from which place of the slit the electron passes. If the width of the slit is Oy, the maximum uncertainty in the position of electron screen = Oy (in Y-direction)

Obviously narrow the slit less the uncertainty in position. But according to the theory of diffraction at a single slit, for half angular width of principal maxima

$Oy.\sin\theta = \lambda$ for the wave of wavelength λ.

Or $\sin\theta = \lambda/Oy$

So maximum uncertainty in the position of electron is,

$Oy = \lambda/\sin\theta$ ....(1)

If the wavelength of wave associated with electron is λ, then from de-Broglie $\lambda = h/p$.

The momentum of electron in parallel to the slit (i.e. in Y- direction) can have any value between $p\sin\theta$ and $p\sin(-\theta)$ because the diffracted electron can be found anywhere within the principle maxima (angular spread from $-\theta$ to $+\theta$).

Therefore uncertainty in momentum in direction parallel to the slit

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

$\Delta p_y = 2(h/p).\sin\theta$ ....(2)

From (1) and (2), we get

$\Delta p_y.\ Oy = \lambda/\sin\theta.2(h/p).\sin\theta = 2h \geq \hbar$

3. Non-existence of electron in nucleus: From Rutherford's experiment we know that size of nucleus is equal to 10^{-14}meter. If electron exists in the nucleus then uncertainty in position of electron is Ox is the same as the size of nucleus. It means

$$Ox = 10^{-14}\text{meter.}$$

So minimum uncertainty in momentum $Op_{min} = h/Ox = 6.625\times10^{-34}$j.sec.

10^{-14}meter

$$\text{Or } Op_{min} = 6.625\times10^{-34}\text{kg.m}^2/\text{sec}^2\text{.sec} = 6.625\times10^{-20}\text{kg.m/sec} \quad 10^{-14}\text{meter}$$

For electron of minimum momentum inside the nucleus minimum energy $OE_{min} = (p^2c^2 + m_oc^4)^{1/2}$

$OE_{min} = [(3.31\times10^{-20})^2(3\times10^8)^2+(9.1\times10^{-31})^2\,(3\times10^8)^4]^{1/2}$

$$OE_{min} = [(10.95\times10^{-40})(9\times10^{16})+(82.81\times10^{-61})(9\times10^{32})]^{1/2}$$

$$OE_{min} = [(98.55\times10^{-24})+(414.05\times10^{-29})]^{1/2}$$

Because second term is much smaller than first in above equation, so we can neglect it.

$$OE_{min} = 9.93\times10^{-12}\text{ joule}$$

$$\text{Or } OE_{min} = 9.93\times10^{-12}\text{ eV} \quad 1.6\times10^{-19}$$

$$\text{Or } OE_{min} = \quad 9.93\times10^{-12}\text{ MeV} \quad 1.6\times10^{-19}\times10^{6}$$

$$\text{Or } OE_{min} = 52.26\text{ MeV}$$

Because maximum kinetic energy of a β- particle emitted from radioactive nuclei is of the order of 4 MeV.

Conditions For Acceptable Wave Function

Because $\psi^*\psi = |\psi|^2$ = a real quantity. Thus it is clear that $|\psi|^2$ is a real quantity and is a measure of probability density. Hence probability of finding the particle in a small volume dv = $|\psi|^2 dv = |\psi|^2 dxdydz$ Since total probability of finding the particle in any position is unity.

$$\text{So } \int_{-\infty}^{+\infty} |\psi|^2 dv = 1 \text{ or } \int_{-\infty}^{+\infty} \psi^*\psi dv = 1$$

This condition is known as normalization condition. The function satisfied the condition is called normalized wave function.

So ψ must be normalized, single valued because at any instant t there can be only one probability for the particle to be at a point; ψ must be finite and continuous.

Expectation Value: -

$$\text{The expectation value of a quantity } \langle f(r) \rangle = \frac{\iiint \psi^* f(r)\, \psi dv}{\iiint \psi^*\, \psi dv}$$

-

$$\langle f(r) \rangle = \frac{\iiint f(r)|\psi|^2 dv}{\iiint |\psi|^2 dv}$$

If the wave function is normalized then $\iiint f(r)|\psi|^2 dv = 1$, so

$$\langle f(r) \rangle = \iiint f(r)|\psi|^2 dv$$

Schrodinger's Wave Equation

It is a differential equation of the de-Broglie waves associated with the particle and describes the motion of particle.

If a wave function associated with a particle which is moving with velocity v in +ve direction, then displacement of wave is given by

$$\psi = Ae^{-i\omega(t - x/v)} \quad \text{.........................(1)}$$

$$= Ae^{-i(\omega t - x.2\pi\upsilon/\upsilon\lambda)} \quad \text{(Because } v = \upsilon\lambda \text{ and } \omega = \text{)}$$

$$= Ae^{-i(\omega t - x.2\pi/\lambda)}$$

$$= Ae^{-i(\omega t - k.x)} \quad \text{(Because } 2\pi/\lambda\text{)}$$

$$= Ae^{-i\,2\pi(\upsilon t - x/\lambda)}$$

$$= Ae^{-i\,2\pi(Et/h - xP/h)} \quad \text{(Because } E = h\upsilon \text{ and } \lambda = h/p\text{)}$$

$$= Ae^{-i\,2\pi/h\,(Et - P.x)}$$

$$= Ae^{-i/\hbar\,(Et - P.x)} \quad \text{.........................(2)}$$

This is a wave equation for a freely moving particle. Now differentiating equation (2) with respect to get

$$\partial\psi/\partial t = -(iE/\hbar).\,Ae^{-i/\hbar\,(Et - P.x)}$$

$$\partial\psi/\partial t = -(iE/\hbar).\,\Psi \quad \text{(Because } \psi = Ae^{-i/\hbar\,(Et - P.x)}\text{)}$$

$$\partial\psi/\partial t = -(i/\hbar).E\psi$$

or $E\psi = (i\hbar)\,\partial\psi/\partial t$ ....(3)

So energy operator $E = (i\hbar).\partial/\partial t$ ....(4)
Now partially differentiating equation (2) with respect to x, we get

$\partial\psi/\partial x = (iP/\hbar).\, Ae^{-i/\hbar\,(Et - P.x)}$

$\partial\psi/\partial x = (iP/\hbar).\Psi$ (Because $\psi = Ae^{-i/\hbar\,(Et - P.x)}$)

or $P\psi = (\hbar/i).\partial\psi/\partial x$

or $P\psi = (-i\hbar).\partial\psi/\partial x$ ....(5)

So momentum operator $P = (-i\hbar).\partial/\partial x$ ....(6) We know that total energy of the particle

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

` $E = mv^2/2 + V$ or $E = p^2/2m + V$

Total energy in terms of wave function or operating wave function on above equation, $E\psi = (p^2/2m)\,\psi + V\psi$ ....(7)

Putting the value of E & P from equation (4) & (6) we get, $[(i\hbar).\partial/\partial t\,]\psi = [(-i\hbar).\partial/\partial x\,]^2\psi/2m + V\psi$

$(i\hbar).\partial\psi/\partial t = [(\hbar^2/-1).\partial^2/\partial x^2\,]\psi/2m + V\psi$

$(i\hbar).\partial\psi/\partial t = (\hbar^2/-2m).\partial^2\psi/\partial x^2 + V\psi$

$(i\hbar).\partial\psi/\partial t = -(\hbar^2/2m).\partial^2\psi/\partial x^2 + V\psi$

This is Schrodinger time dependent equation for one dimension. For three dimensional case, $(i\hbar).\partial\psi/\partial t = -\,(\hbar^2/2m).[\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2]\,\psi + V\psi$

or $(i\hbar).\partial\psi/\partial t = -\,(\hbar^2/2m).\quad\psi + V\psi$ (Where $\quad = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$)

For free moving particle V = 0 so we can
write, $(i\hbar).\partial\psi/\partial t = -(\hbar^2/2m).$
ψ
Now putting the value of P from equation (4) to equation (7) we get,

$$E\psi = -(\hbar^2/2m).\partial^2\psi/\partial x^2 + V\psi$$

$$\text{or } (\hbar^2/2m).\partial^2\psi/\partial x^2 + (E - V)\psi = 0$$

$$\text{or } \partial^2\psi/\partial x^2 + (2m/\hbar^2).(E - V)\psi = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(8)$$

This is Schrodinger time independent equation for one dimension. For three dimensional case, $[\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2]\psi + (2m/\hbar^2).(E - V)\psi = 0$

$$\psi + (2m/\hbar^2).(E - V)\psi = 0$$

For free moving particle V = 0 so we can write,

$$\psi + (2m/\hbar^2).E\psi = 0$$

Q. Show that the function $\psi = Axe^{(-x^2/2)}$ is the eigen function of the operator A


Thank You!