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

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

or $P^2=2mE$

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

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

Or $m^2v^2 = 3mkT$

Or $P^2 = 3mkT$

Or $P = \sqrt{3mkT}$

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

where k = Boltzmann's constant = $1.38X10^{-23}$ 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

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

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

or $2mqV = m^2v^2 = P^2$

or $\sqrt{2mqV} = P$

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

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

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

or $\lambda = \sqrt{(150/V)}$ Å$= 12.27/\sqrt{V}$ 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 $E=h\nu$ or $\nu=E/h$, where ν is the frequency of wave.

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

   So we can write $\nu= mc^2/h$……………….(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

   $v_p= \nu\lambda$

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

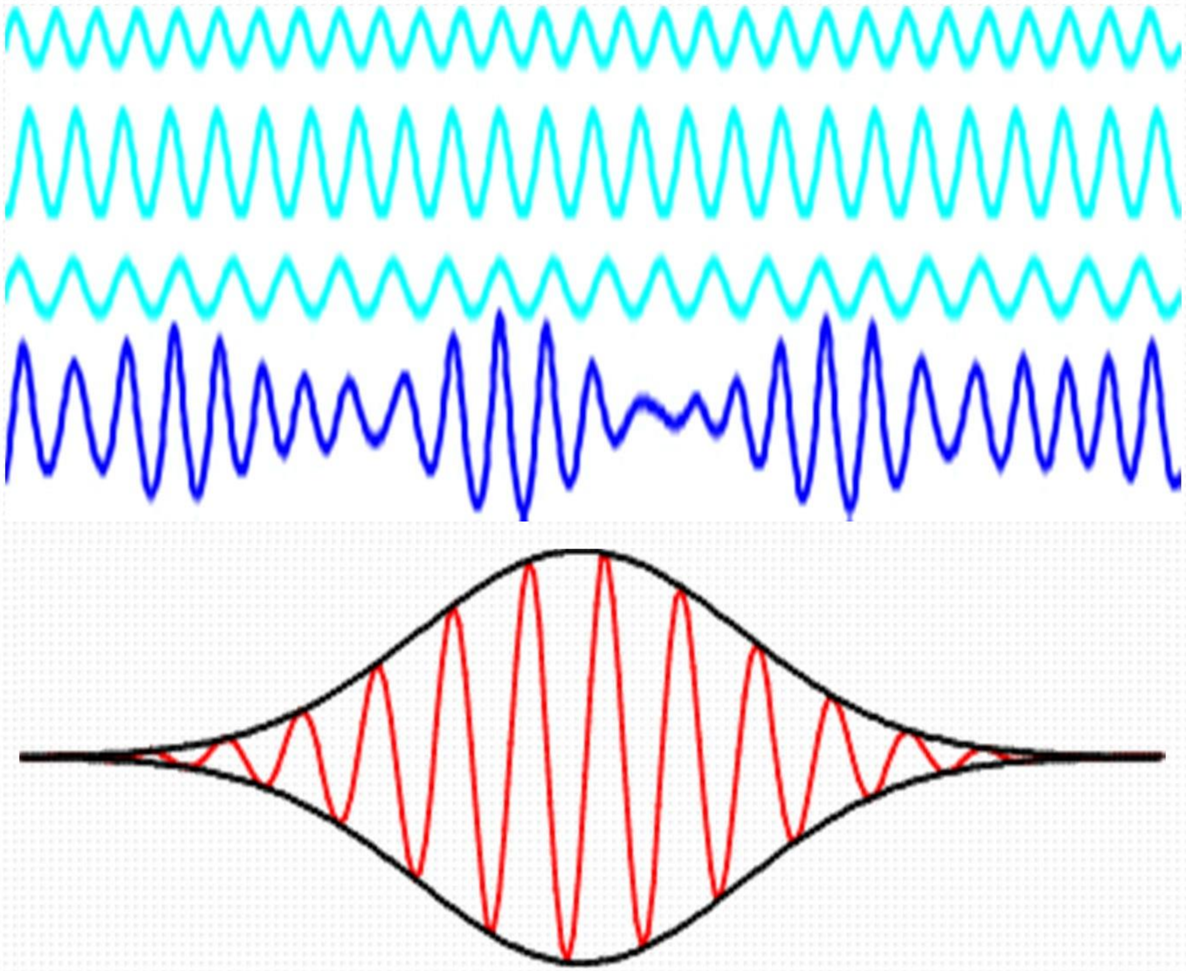
   or $v_p = c^2/ v$

- 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



Heisenberg's Uncertainty Principle

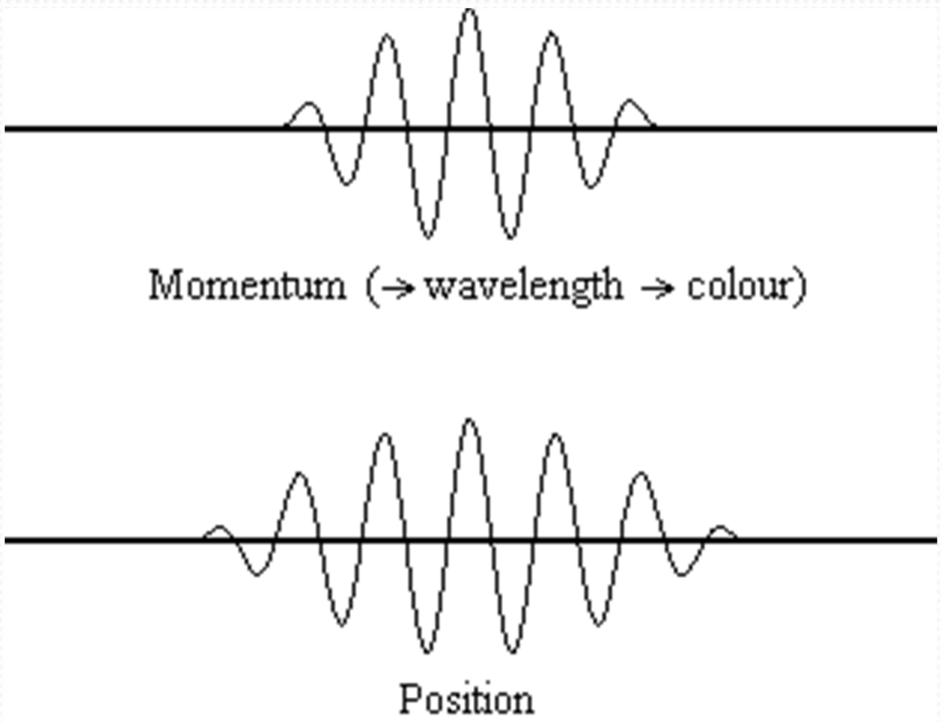
"It is impossible to determine simultaneously the position and momentum of the particle with any desired accuracy."

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 Heisenberg

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.



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 = $|\psi|^2dv = |\psi|^2dxdydz$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: -

The expectation value of a quantity

$$< f(r) > = \frac{\iiint \psi^* f(r) \psi dv}{\iiint \psi^* \psi dv}$$

-

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

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

$$< f(r) > = \iiint f(r)|\psi|^2 dv$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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