WAVE NATUR OF MATTER

1- WAVE BEHAVIOUR OF PARTICLES

The phenomenon of interference and diffractio of light show that light travels in the form of waves. The polarization of light further confirms the wave nature of light by telling that light waves are transverse waves.

The photoelectric effect and compton effect seem to contradict the wave nature of light. These two effect can be explained on the basis of photon theory.

However particle nature and wave nature are complimentary i.e, in one experiment, only one nature can be depicted and both the aspects can't be observed simultane What aspect can be observed depends on the nature of experiment.

For example if we put diffraction grating in the path of light beam, we shall see the wave nature. On the other hand if we use photoelectric effect apparatu we shall observe the particle nature i.e, photons.

Thus no single experiment can be performed in which both the wave aspect and particle aspect are revealed at the same time.

Fig(1)(a) shows a beam of electrons incident on a double slit. The electrons emitted by a hot filament is accelerated by a potential difference (V) to gain some

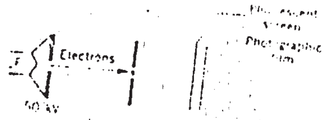


Fig (1)(a)

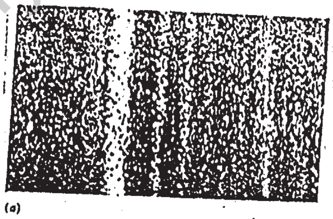
suitable energy. Electron beam after passing through the double slit, strikes a flourescent screen where an interference pattern is formed. This interference pattern is then photographed as shown in fig (1)(b).

Fig(1)b

The deep study of this interference pattern shows that it is similar to the interference pattern obtained with waves. If electrons had no wave properties then we observed bright fringes only in front of two slits on the screen. But bright and dark fringes appear on either sides of the slits which shows that electrons are showing wave properties.

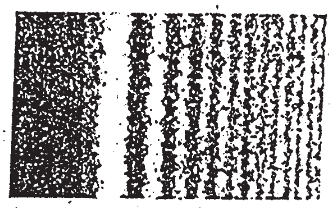
In a similar way neutron beam has also been used in doule slit experiment and the same interference pattern has been observed. It means that wave like properties are not associated with charged particles only but neutral particles can also show wave behaviour.

Fig 2(a) and 2(b) shows the diffration patterns obtained with electron beam and light from a straight edge. Both the patterns are similar.



(a)

Fig 2(a)



(b)

Fig 2(b)

So these experiments give a direct evidance of wave nature of particles.

Sample Pb (1)

(2.1). *In a double slit arrangement used to study intensity pattern of helium atoms passing through the double slit, the slit separation d was 8 μm, and the detector was a distance D = 64 cm from the slits. If the observed spacing between the fringes ω = 8 μm, find the wavelength of helium atoms.*

$$D = 64\,cm = \frac{64}{100}\,m = 0.64\,m$$
$$d = 8\,\mu m = 8 \times 10^{-6}\,m$$
$$\omega = 8\,\mu m = 8 \times 10^{-6}\,m$$

λ = Wave length of He atoms = ?

As fring spacing is given by,

$$\omega = \frac{D\lambda}{d}$$

$$\therefore \lambda = \frac{\omega d}{D}$$

$$= \frac{8\times10^{-6}\times8\times10^{-6}}{0.64}$$

$$= \frac{64}{0.64}\times10^{-12}$$

$$= \frac{64}{64}\times10^{-12}\times100$$

$$\boxed{\lambda = 1\times10^{-10}\,m}$$

2- DE-BROGLIE HYPOTHESIS

According to De-Broglie,

"A wave is associated with a moving particle or a moving particle may behave as a wave."

This wave is called

(i) De-Broglie wave or

(ii) Particle wave or

(iii) Matter wave.

We know that energy of photon by Planck's theory is,

$$E = h\nu \quad \text{——— (i)}$$

where ν is the frequency of radiation.

On the basis of Einstein's theory, this energy is,

$$E = mc^2 \quad \text{——— (ii)}$$

where m is mass of photon and c is velocity of light.

So from (i) and (ii)

$$mc^2 = h\nu$$

$$mc = \frac{h\nu}{c} \qquad \because c = \nu\lambda$$

$$\therefore mc = \frac{h\nu}{\nu\lambda}$$

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

But mc = Mass of photon × velocity of photon.

$\therefore$ mc = Momentum of photon = P

$$\therefore \quad P = \frac{h}{\lambda}$$

$\therefore$ Wave length of photon is,

$$\lambda = \frac{h}{P} \quad \text{——} \quad (A)$$

This equation gives a relation between wave like property 'wave length λ' and particle like property 'momentum P' of photon (radiation).

De-Broglie suggested that the same relation can be written for particle also.

So wave length of particle wave is,

$$\lambda = \frac{h}{mv} \quad \text{——} \quad (B)$$

where mv is the momentum of particle.

This wave length is called De-Broglie wave length. As λ is inversely related to mass of particle. So greater is 'm' shorter is the De-Broglie wave length. Since masses of ordinary objects which we come across in our daily life are larger, so wavelength associated with ordinary objects is too small to be measured. So we cannot study wave like properties of ordinary objects. However electrons, protons and neutron being microscopic in nature, so their wave properties can be studied.

Sample Pb ②

(2.2). Calculate the de Broglie wavelength of (a) a Virus particle of mass 1.0×10^{-15} Kg moving at a speed of 2.0 mm/s and (b) an electron of kinetic energy 120 eV.

$$V = 2\,mm/s = 2 \times 10^{-3}\,m/s$$

(a) $$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.625 \times 10^{-34}}{1.0 \times 10^{-15} \times 2 \times 10^{-3}}$$

$$\lambda = \frac{6.625}{2} \times 10^{-34+3+15}$$

$$\boxed{\lambda = 3.3 \times 10^{-16}\,m}$$

(b) Here $m = 9.1 \times 10^{-31}\,kg$

$$K = 120\,eV = 120 \times 1.6 \times 10^{-19}\,J$$

$$\lambda = \frac{h}{p} \qquad \because K = \frac{1}{2}mv^2$$

$$\lambda = \frac{h}{\sqrt{2Km}} \qquad 2K = mv^2$$

$$2Km = m^2v^2$$

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 120 \times 1.6 \times 10^{-19} \times 9.1 \times 10^{-31}}} \qquad 2Km = p^2$$

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

$$= \frac{6.625 \times 10^{-34}}{\sqrt{3494.4 \times 10^{-50}}}$$

$$= \frac{6.625 \times 10^{-34}}{59.11 \times 10^{-25}}$$

$$= 0.11 \times 10^{-34+25}$$

$$= 0.11 \times 10^{-9}$$

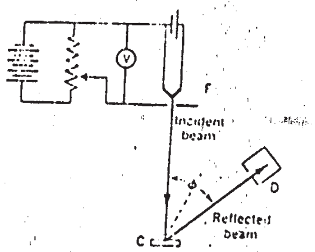
$$\boxed{\lambda = 1.1 \times 10^{-10}\,m}$$

3-TESTING DE-BROGLIE'S HYPOTHESIS

De-Broglie's hypothesis of matter waves was first experimentally verified in 1927 by Davisson and Germer in U.S.A and then by G.P. Thomson in 1929 in England. But we shall discuss Davission and Germer experiment because its explanation is more direct.

DAVISSON-GERMER E ERIMENT

Davission and Germer performed an experiment and proved the De-Broglie's idea of matter waves by proving that electrons could be diffracted like e-m waves. Fig. shows their experimental arrangement.



Electrons from an electron gun are made to fall on a crystal 'C'. The electron gun consists of a hot filament 'f' which produces electrons by thermionic emission. These electrons are then accelerated by a variable potential difference 'V' applied between the filament and anodes in the electron gun. The accelerated beam is collimated by passing it through the slits. In their experiment they used nickle crystal as target.

The beam of electrons is found to be diffracted by the crystal. This can be seen by moving the electron detector 'D' side ways. They observed several positions of maxima and minima for different values of angle ϕ. But the diffraction phenomenon is a wave phenomenon. So very diffraction of electrons shows that they behave as waves.

Let V be the accelerating potential for the electrons then,

$$Ve = KE \text{ of electrons}$$

$$Ve = \frac{1}{2}mv^2$$

$$2Ve = mv^2$$

$$2Vem = m^2v^2$$

$$\text{or} \quad mv = \sqrt{2Vem}$$

So De-Broglie's wave length of electrons is given as,

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{h}{\sqrt{2Vem}} \quad \text{——— } (1)$$

In a particular experiment Davinson and Germer used $V = 54$ volt and observed strong diffracted beam at $\varphi = 50°$.

They found λ by using (1) as,

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 54 \times 1.6 \times 10^{-19} \times 9.1 \times 10^{-31}}}$$

$$= \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 54 \times 1.6 \times 9.1 \times 10^{-50}}}$$

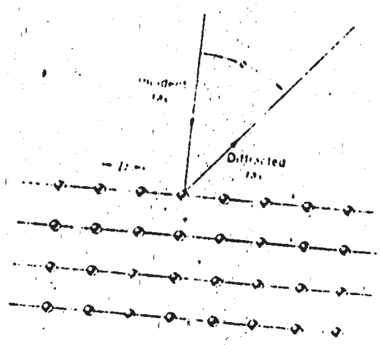
$$= \frac{6.625 \times 10^{-34}}{\sqrt{1572.48} \times 10^{-25}}$$

$$= \frac{6.625 \times 10^{-34+25}}{39.85}$$

$$= 0.167 \times 10^{-9} \, m$$

$$\lambda = 167 \times 10^{-12} \, m$$

$$\boxed{\lambda = 167 \, Pm} \quad \text{——— } (A)$$



Because electrons are diffracted by the crystal as light is diffracted by diffraction grating.

So grating formula can also be used here to find 'λ' as,

$$D \sin \varphi = m\lambda \quad \text{——— } (2)$$

For the Nickle crystal $D = 215$ Pm and $m = 1$ for first order maxima.

$\therefore$ Eq (2) becomes,

$$215 \times 10^{-12} \sin 50^\circ = \lambda$$

$$\lambda = 215 \times 10^{-12} \times 0.766$$

$$\lambda = 164.69 \times 10^{-12} m$$

$$\lambda = 165 \times 10^{-12} m$$

$$\boxed{\lambda = 165\ Pm}$$

It agrees with the value of 'λ' found from De-Broglie's formula $\lambda = \frac{h}{mv}$ given by (A). So we find that De-Broglie's formula is also varified.

So this experiment verifies the De-Broglie's hypothesis of matter waves.

Thus, they proved the diffraction of electrons which was only possible if the electrons were considered as waves because diffraction is purely a wave phenomenon.

4-HEISENBERG UNCERTAINTY PRINCIPLE

After knowing that the dual nature of light and matter, Heisenberg gave a principle known as Uncertainty principle. According to this principle,

"The position and momentum of an electron can not be found accurately at one time."

OR

"It is not possible to determine both the position and the momentum of a particle with unlimited precissions."

Mathematically it is expressed as,

$$\Delta x . \Delta P \simeq h \quad \text{—— (A)}$$

and

$$\Delta E . \Delta t \simeq h \quad \text{—— (B)}$$

Equations (A) & (B) are two forms of U.C.P.

Proof of U.C.P ($\Delta x . \Delta P \simeq h$)

Suppose we want to measure the position and momentum of an election at the same time.

Let x denotes the exact position of the particle. To find its position, we have to see the particle. We may see the particle by (say) a superpowered microscope by using light of some wave length 'λ'. When the photon strikes the election, the photon is scattered. So the scattered photon will enter the microscope and gives the position of the particle. This photon produces an error in the measurement of position. Let ΔX denotes this error or uncertainty in the measurement of position. We know that due to diffraction effects ΔX is of the order of wave length of incident photon i.e,

$$\Delta X \simeq \lambda \quad \text{—— (1)}$$

This equation shows that to decrease the error in position, we should use light of smaller wave length. When the photon strikes the particle and is scattered from it, this changes the momentum of the particle. Let ΔP denotes the error or uncertainty in the measurement of momentum P of the election. The exact value of ΔP can not be predicted, however it cannot be greater than P, the momentum of photon which is $P = \frac{h}{\lambda}$

$$\text{So} \quad \Delta P \simeq \frac{h}{\lambda} \quad \text{——} \; (2)$$

This equation shows that to decrease the error or uncertainty in momentum, we should use light of larger wave length.

So equations (1) and (2) show that if λ is larger, then momentum is measured accurately but position becomes too wrong and vice versa. So both position and momentum of a particle cannot be found accurately at one time.

Multiplying (1) and (2) we get,

$$\Delta P . \Delta x \simeq h \quad \text{——} \; (A)$$

This is one mathematical form of uncertainty principle. It shows that product of uncertainty in position and momentum is nearly equal to Planck's constant.

There is another form of this principle according to which,

$$\Delta E \cdot \Delta t \simeq h \quad \text{——} \; (B)$$

Where ΔE is the error in the measurement of energy in time Δt.

Let us now derive equation (B)

Proof of U.C.P. ($\Delta E \cdot \Delta t \simeq h$)

Suppose we have an ideal machine which counts the peaks of an e-m wave as the wave passes through it. Suppose it counts n peaks in time Δt. Since the machine cannot count a part of the peak. So error Δn in measuring n will be of the order of 1.

So $\Delta n \simeq 1$

If ν denotes the frequency of em wave, then

$$\nu = \frac{n}{\Delta t}$$

$$\Delta \nu = \frac{\Delta n}{\Delta t} \qquad \because \Delta n = 1$$

$$\therefore \Delta \nu = \frac{1}{\Delta t}$$

Now energy E of photon is given by,

$$E = h\nu$$

$$\Delta E = h \Delta \nu$$

$$\because \Delta \nu = \frac{1}{\Delta t}$$

$$\therefore \quad \Delta E = h \frac{1}{\Delta t}$$

$$\text{or} \quad \Delta E \cdot \Delta t = h$$

Which is another form of Heisenberg uncertainty principle. According to it,

"It is not possible to determine both the energy and time coordinate of a particle with unlimited precission."

Consequences:

Let us apply uncertainty principle to the revolving electron. According to this principle,

$$\Delta P \cdot \Delta x = h$$

To measure the position x of electron accurately, ΔP should be very large. But the maximum value of ΔP cannot exceed P.

So, $\Delta P \simeq P$

$\therefore$ The above expression becomes,

$$P \Delta x = h$$

$$\text{or} \quad \Delta x = \frac{h}{P}$$

But $\frac{h}{p} = \lambda$, the wave length of electron.

$$\therefore \quad \Delta x = \lambda$$

If the electron is revolving in 1st orbit then,

$$\lambda = 2\pi r$$

$$\therefore \quad \Delta x = 2\pi r$$

It means the minimum error in the position of electron is of the order of circumference of the first orbit i.e, minimum value of Δx is greater than radius of the orbit. Hence it is impossible to know the exact position of the electron in the orbit. So an electron has no place inside the nucleus. The consequences that arise are,

(i) The detailed picture of the atom as given by Bohr's Theory can't be varified by experiments.

(ii) An electron has no place inside the nucleus.

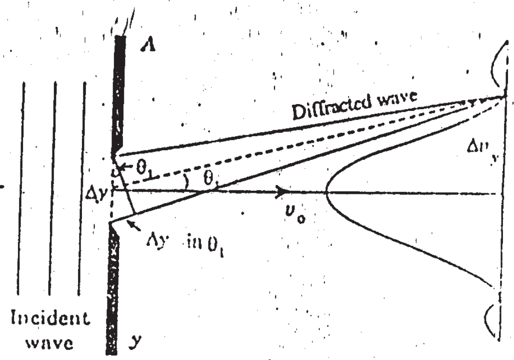
(iii) Newtonian mechanics fails to describe the motion of electrons in an atom. It can however be used fairly well to explain the motion of bodies of macroscopic size.

5- The uncertainty Principle and Single Slit Diffraction

Consider a beam of electrons of speed V_0 moving from left to right as shown in fig. (i).

We want to measure simultaneously exact precision 'y' and the velocity component V_y for an electron in this beam. But we will see that U.C.P will hinder their measurements.

To measure 'y' we stop the beam by a screen A having a slit of width 'Δy'. If the election passes through the slit, then we can find its vertical position 'y' accurately. The accuracy in measuring 'y' can be increased by decreasing the width of the slit. Because wave is associated with a moving election. So electron beam after passing gets diffracted as shown in the fig. So a diffraction pattern is obtained on the screen B placed perpendicular to the direction of incident beam. This pattern consists of a central maxima and alternate minima and maxima above and below this central maxima.



Fig(1)

Now by U.C.P, there have uncertainity Δy in the measurement of 'y'.

Similarly there is an uncertainity ΔV_y in the measurement of $f\ V_y$.

Now first minima of diffraction pattern is given by,

$$\frac{\Delta y}{2}\sin\theta = \frac{\lambda}{2}$$

$$\Delta y \sin\theta = \lambda$$

then $\quad \Delta y\, \theta = \lambda$

If θ is v.v small

$$\sin\theta \simeq \theta$$

$$\therefore \quad \theta \approx \frac{\lambda}{\Delta y} \quad \text{—(a)}$$

Also $\quad \theta \approx \dfrac{\Delta V_y}{V_0} \quad$ —(b)

Combining (a) & (b) we get,

$$\frac{\lambda}{\Delta y} \approx \frac{\Delta V_y}{V_0}$$

$$\Delta V_y \cdot \Delta y \approx \lambda V_0$$

As De Broglie wave length is given by,

$$\lambda = \frac{h}{mV_0}$$

$$\therefore \Delta V_y \cdot \Delta y \approx \frac{h}{mV_0} V_0$$

$$\Delta V_y \cdot \Delta y \approx \frac{h}{m}$$

$$\Delta (mV_y) \Delta y \approx h$$

$$\Delta P_y \cdot \Delta y \approx h$$

Which is the U.C. principle.

According to it, the product of uncertainty in y-component of momentum and vertical position of electron is nearly equal to planck's constant.

If we want to know the exact vertical position of electron, then slit spacing should be decreased. But by decreasing the slit spacing, the diffraction pattern expands and ΔP_y increases.

And if we want to decrease ΔP_y, the slit spacing should be increased. By doing this ΔP_y decreases but vertical position of electron becomes too wrong.

So if we try to increase our information about one variable, the other become, too wrong & vice versa.

So U.C.P is a statement of our ability to simultaneously determine certain properties of particle.

6- WAVE FUNCTION

It is a variable quantity which characterizes the De-Broglie's wave. It is denoted by 'ψ'. It depends upon space co-ordinates x, y, z as well as time 't'. So ψ is a function of x, y, z and t i.e,

$$\psi = \psi(x, y, z, t)$$

The value of the wave function associated with a moving body at a certain point (x, y, z) in space and time t is related to the probability of finding the body there at that time. ψ itself is not an observable quantity. ψ itself has no physical significance but the square of ψ i.e, $|\psi|^2$ has physical significance. $|\psi|^2$ is called probability density of the particles presence at a certain point at a certain time. So wave function ψ is that quantity whose square gives the probability of finding the particle at a certain point at a certain time. A large value of $|\psi|^2$ means the strong probability of the body presence, while a small value of $|\psi|^2$ means the small probability of its presence. As long as $|\psi|^2$ is not $=0$ somewhere, there is a definite chance of detecting the particle however small it may be. The wave function is a complex quantity. So it can be written as,

$$\psi = (A + iB)$$

However its square is always a real quantity. The square of ψ is obtained by the product of wave function ψ with its complex conjugate ψ^* as,

$$|\Psi|^2 = \Psi\Psi^* = (A+iB)(A-iB)$$

$$|\Psi|^2 = A^2 + B^2$$ which is a real quantity.

A, B are real unknown constants.

So probability density is always real quantity.

Normalization condition of Wave function

If the probability of finding the particle is 100% Then integral

$$\int \Psi^2 dV = 1 \quad \text{—— (i)}$$

is called normalization condition, where integral is taken over all space.

If $\int \Psi^2 dV = 0$ then particle does not exist.

If $\int \Psi^2 dV = \infty$ Then the particle is everywhere present simultaneously.

Properties of Ψ :-

(i) It is single valued i.e, have one value at a particular place and time.

(ii) Ψ and its partial derivatives $\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\Psi}{\partial z}$ are continuous.

(iii) $|\Psi|^2$ can't be -ve or complex, so its integral must be a finite quantity.

SCHRODINGER EQUATION

(i) Time Dependent Form:

The equation of a wave moving along x-axis with velocity 'V' is given by.

$$y = Ae^{-i\omega(t - \frac{x}{V})}$$

But in quantum mechanics, the wave function Ψ corresponds to the displacement 'y' of wave motion in a string. So putting $y = \Psi$ we get,

$$\Psi = Ae^{-i\omega(t - \frac{x}{V})}$$

$\because \omega = 2\pi\nu$ and $V = \nu\lambda$

$$\therefore \quad \Psi = Ae^{-i2\pi\nu(t - \frac{x}{\nu\lambda})}$$

$$\Psi = Ae^{-i2\pi(t\nu - \frac{x}{\lambda})}$$

$$\Psi = Ae^{-\frac{2i\pi}{h}(h\nu t - \frac{h}{\lambda}x)}$$

If E, P are energy and momentum of the particle then,

$$E = h\nu \quad \text{and} \quad P = \frac{h}{\lambda}$$

$$\therefore \quad \Psi = Ae^{-\frac{2i\pi}{h}(Et - Px)}$$

$$\Psi = Ae^{-i\frac{2\pi}{h}(Et - Px)}$$

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

$$\therefore \quad \Psi = Ae^{-i/\hbar(Et - Px)} \quad \text{—— (1)}$$

$\because \frac{1}{\hbar} = \frac{2\pi}{h}$

This wave equation is equivalent to the equation of motion of a free particle having total energy E and momentum P along x-axis.

Now

$$\frac{\partial \Psi}{\partial x} = \frac{iP}{\hbar} Ae^{-i/\hbar(Et-Px)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \left(\frac{iP}{\hbar}\right)^2 Ae^{-i/\hbar(Et-Px)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \left(\frac{iP}{\hbar}\right)^2 \Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{P^2}{\hbar^2}\Psi \quad \text{——— (a)}$$

From (1) we get,

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} Ae^{-i/\hbar(Et-Px)}$$

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar}\Psi \quad \text{——— (b)}$$

For small speeds $(V << C)$, the total energy E of the bound particle is the sum of K.E and potential energy V where V is a function of position and time.

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

$$E = \frac{1}{2}mv^2 + V$$

$$E = \frac{1}{2m}m^2v^2 + V$$

$$E = \frac{P^2}{2m} + V$$

Multiplying both sides of this equation by the wave function Ψ, we get,

$$E\Psi = \frac{P^2}{2m}\Psi + V\Psi$$

From (a) $P^2\Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$

From (b) $E\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}$

$\therefore$ The above expression becomes,

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

or $$\boxed{\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - V\Psi} \quad \text{——— (2)}$$

This is time dependent form of Schrodinger equation in one dimension.

In three dimensions, this equation becomes,

$$\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m}\left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}\right) - V\Psi$$

But $$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = \nabla^2\Psi.$$

$$\therefore \quad \boxed{\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\Psi - V\Psi} \quad \text{——— (3)}$$

This is time dependent form of Schrodinger equation in three dimensions.

In this equation ∇^2 is called Laplacian operator.

OPERATOR:-

"An operator is a mathematical instruction that tells us what operation to carry out on the quantity that follows it."

NOTE:-

It is to be noted that equations (2) & (3) are schrodinger equations for bound particles. For free particles put $V=0$ in these equations to get the equations for particles.

(ii) Time Independent Form:

In so many cases, the potential energy of a particle does not depend upon time and hence potential energy changes with position of the particle only.

As we know that,

$$\Psi = Ae^{-i/\hbar(Et - Px)}$$

$$\Psi = Ae^{-\frac{iE}{\hbar}t} \cdot e^{\frac{iPx}{\hbar}}$$

Putting $Ae^{\frac{iPx}{\hbar}} = \psi$ we get,

$$\Psi = \psi e^{-\frac{iEt}{\hbar}} \quad \text{—— (1)}$$

From (1)

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar}\psi e^{-\frac{iEt}{\hbar}} \quad \text{—— (a)}$$

$$\frac{\partial \Psi}{\partial x} = \frac{\partial \psi}{\partial x} e^{-\frac{iEt}{\hbar}}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial x^2} e^{-\frac{iEt}{\hbar}} \quad \text{—— (b)}$$

As we know that time dependent equation is given by,

$$\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - V\Psi$$

Putting (a) & (b) in this equation we get,

$$\frac{\hbar}{i}\left(-\frac{iE}{\hbar}\psi e^{-\frac{iEt}{\hbar}}\right) = \frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} e^{-\frac{iEt}{\hbar}}\right) - V\Psi$$

From (1) $\Psi = \psi e^{-\frac{iEt}{\hbar}}$

$$\frac{\hbar}{i}\left(-\frac{iE}{\hbar}\psi e^{-\frac{iEt}{\hbar}}\right) = \frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} e^{-\frac{iEt}{\hbar}}\right) - V\psi e^{-\frac{iEt}{\hbar}}$$

$$\therefore \quad \frac{\hbar}{i}\left(-\frac{iE}{\hbar}\psi\right) = \frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2}\right) - V\psi$$

or

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

or

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

∴ The above expression becomes,

$$-\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

or
$$\boxed{\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V\Psi} \quad \text{—— (2)}$$

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$$\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) - V\Psi$$

But $\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} = \nabla^2\Psi$

$$\therefore \quad \boxed{\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\Psi - V\Psi} \quad \text{—— (3)}$$

This is time dependent form of Schrodinger equation in three dimensions.

In this equation ∇^2 is called Laplacian operator.

OPERATOR:-

"An operator is a mathematical instruction that tells us what operation to carry out on the quantity that follows it."

NOTE:-

It is to be noted that equations (2) & (3) are schrodinger equations for bound particles. For free particles put $V=0$ in these equations to get the equations for particles.

(ii) Time Independent Form:

In so many cases, the potential energy of a particle does not depend upon time and hence potential

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

or

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

This is time independent S-equation in one dimension. In three dimensions this equation becomes,

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

or

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

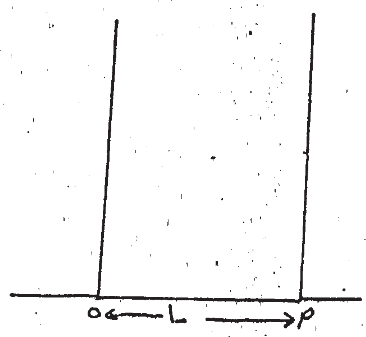
This is Time independent S-equation in three dimensions.

APPLICATIONS OF SHRODINGER WAVE EQUATION

1) Motion of particle in a potential well.
(OR)
Motion of particle in one dimensional box

Consider a particle of mass 'm' moving freely along x-axis in a potential well of length OP=L as shown. The potential energy of the particle remains zero at all points with in the box and is infinity at x=0 and x=L. So the particle can not penetrate the walls of well and so can move only inside the wall.

The motion of such particle can be studied by using time independent S.W. equation in one dimension. i.e.



$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{—— } (1)$$

Since inside the box, the particle moves freely. So V=0 i.e there is no force acting on the particle.

$\therefore$ Expression (1) becomes.

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

$\partial \rightarrow d$
$\because \psi$ is a func of x only.

or $$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$\partial \to d$
$\because \psi$ is fn. of x only.

put $$\frac{2m}{\hbar^2}E = K^2$$

$$\therefore \frac{d^2\psi}{dx^2} + K^2\psi = 0 \quad \text{—— (2)}$$

It is a linear, homogeneous and 2nd order differential equation. It can be written as.

$$D^2 + K^2 = 0$$
$$D^2 = -K^2$$
$$D^2 = i^2K^2$$
$$D = \pm iK$$

The solution of (2) is

$$\psi = A_1 e^{iKx} + A_2 e^{-iKx}$$

$$\psi = A_1(\cos kx + i\sin kx) + A_2(\cos kx - i\sin kx)$$

$$\psi = (A_1 + A_2)\cos kx + i(A_1 - A_2)\sin kx$$

$$\psi = A\cos Kx + B\sin kx \quad \text{—— (3)}$$ where $A = A_1 + A_2$, $B = i(A_1 - A_2)$

Here A and B are constants and can also be evaluated by using boundry conditions.

(i) $\psi(x) = 0$ at $x = 0$
(ii) $\psi(x) = 0$ at $x = L$

Using 1st boundry condition in (3) we get

$$0 = A\cos 0 + B\sin 0$$

$$\Rightarrow A = 0$$

$\therefore$ Eq. (3) becomes

$$\psi = B\sin kx \quad \text{—— (4)}$$

using 2nd b.c in (4)

$$\Rightarrow B \sin KL = 0$$

$\Rightarrow$ either $B = 0$ or $\sin KL = 0$

As $B \neq 0$ because otherwise the particle would not exists within the box.

$$\therefore \sin KL = 0$$

$$\Rightarrow KL = n\pi$$

$$K = \frac{n\pi}{L} \quad \text{———} \quad (5)$$

So eq (4) becomes

$$\psi = B \sin\left(\frac{n\pi}{L}x\right) \text{———} (6)$$

Now the constant B is still to be determined. For calculating 'B' we use normalization condition which gives maximum probability of finding the particle from $0 \to L$ along x-axis

i.e

$$\int_0^L \psi^2 dx = 1$$

$$\int_0^L B^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \quad \text{using (6) we get}$$

$$B^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \quad \text{———} \quad (i)$$

Put $\frac{n\pi}{L}x = \phi$ ——— (a)

$$\frac{n\pi}{L} dx = d\phi$$

$$\therefore dx = \frac{L}{n\pi} d\phi$$

[From (a) when $x = 0$, $\phi = 0$
and when $x = L$ $\phi = n\pi$]

$\therefore$ Expression (i) becomes

$$B^2 \int_0^{n\pi} (\sin^2\phi)\left(\frac{L\,d\phi}{n\pi}\right) = 1$$

By multiplying and dividing by 2 we get

$$\frac{B^2}{2}\int_0^{n\pi}(2\sin^2\phi)\left(\frac{L\,d\phi}{n\pi}\right) = 1$$

$$\frac{B^2 L}{2n\pi}\int_0^{n\pi} 2\sin^2\phi\, d\phi = 1$$

But $\int_0^{n\pi} 2\sin^2\phi = n\pi$

$$\therefore \quad \frac{B^2 L}{2n\pi}\times n\pi = 1$$

$$\frac{B^2 L}{2} = 1$$

$$B^2 = \frac{2}{L}$$

$$B = \sqrt{\frac{2}{L}}$$

Putting the value of B in eq (6) we get

$$\psi = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi}{L}x\right) \text{———} (7)$$

This is the solution of S.W. equation. This eq. contains all the informations about the particle.

ENERGY OF THE PARTICLE

The energy of the particle within the potential well is kinetic only because $P.E = V = 0$

Now we shall show that energy of particle is quantized as follows.

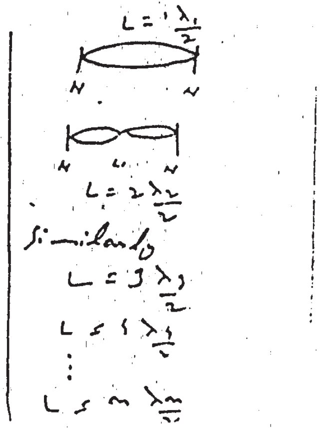
From De-Broglie's relation, we have

$$\lambda_n = \frac{h}{P_n}$$

$$\therefore \quad P_n = \frac{h}{\lambda_n} \text{———} (a)$$

as $L = n\dfrac{\lambda_n}{2}$

$$\therefore \quad \lambda_n = \frac{2L}{n}$$



$\therefore$ Expression (a) becomes

$$P_n = \frac{nh}{2L} \quad \text{——} \quad (b)$$

Now K.E is given by

$$E_n = \frac{1}{2} m v_n^2$$

$$E_n = \frac{1}{2} \frac{m^2 v_n^2}{m}$$

$$E_n = \frac{P_n^2}{2m}$$

using (b) we get

$$E_n = \left(\frac{nh}{2L}\right)^2 \cdot \frac{1}{2m}$$

$$E_n = \frac{n^2 h^2}{4L^2} \cdot \frac{1}{2m}$$

$$E_n = n^2 \left(\frac{h^2}{8mL^2}\right)$$

where $n = 1, 2, 3, \ldots$ is quantum number.

So we find that energy of particle with in the potential well is quantized.

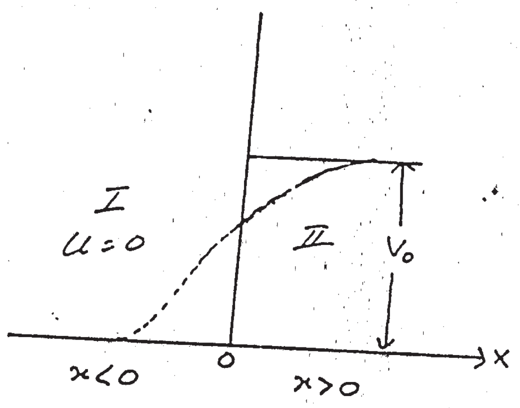
Q:- How will you apply S.W. eq To study the motion of a particle in a Potential well (in one dimensional box)? Show that the particle possesses discrete values of energy in the potential well?

POTENTIAL STEP

Suppose a particle is moving in a region in which the potential energy is as shown in fig. This situation is called potential step.

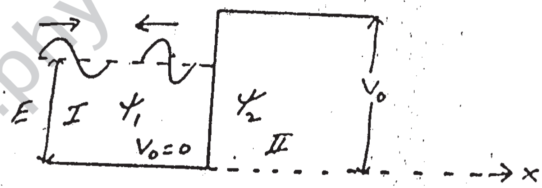
The potential energy is zero for $x<0$ and has a constant value V_0 for $x>0$.

So in region I, the entire energy of the particle is K.E and in region II the particle has partly K.E and partly P.E.



Consider a stream of particles each of mass 'm' moving along x-axis having only K.E and no potential energy.

We shall consider two cases.



1:- When $(E<V_0)$

According to time independent S.W. eq in one dimension along x-axis, we have

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V_0)\,\psi = 0$$

for region (I),

Put $\psi = \psi_1$, $V_0 = 0$ and $\frac{\partial^2 \psi}{\partial x^2} = \frac{d^2\psi}{dx^2}$

$$\therefore \quad \frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2} E\,\psi_1 = 0$$

Put $\frac{2m}{\hbar^2} E = K_1^2$

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0$$

Its solution is

$$\psi_1 = A_1 e^{iK_1 x} + B_1 e^{-iK_1 x} \quad \text{——} \quad (1)$$

for region II

Put $\psi = \psi_2$

$$\therefore \frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0$$

Put $\frac{2m}{\hbar^2}(V_0 - E) = K_2^2$

$$\frac{d^2\psi_2}{dx^2} - K_2^2\psi_2 = 0$$

Its solution is

$$\psi_2 = A_2 e^{K_2 x} + B_2 e^{-K_2 x} \quad \text{——} \quad (2)$$

In equation (1) the term $A_1 e^{iK_1 x}$ represents the incident particle and $B_1 e^{-iK_1 x}$ represents the reflected particle.

In equation (2) the term $A_2 e^{K_2 x}$ represents increasing wave and $B_2 e^{-K_2 x}$ represents decreasing wave. But the term $A_2 e^{K_2 x}$ is not acceptable because the probability of finding the particle in region II is very small. So the term $A_2 e^{K_2 x}$ is neglected.

$\therefore$ eq (2) becomes.

$$\psi_2 = B_2 e^{-K_2 x} \quad \text{——} \quad (3)$$

Due to -ve exponential the particle can not go deep into region II.

DETERMINATION OF CONSTANTS (A_1, B_1, B_2)

The constants A_1, B_1, B_2 can be determined by using boundry conditions.

$$\begin{cases} \text{(i)} \quad \text{At } x=0 \quad \psi_1 = \psi_2 \\ \text{(ii)} \quad \text{At } x=0 \quad \dfrac{d\psi_1}{dx} = \dfrac{d\psi_2}{dx} \end{cases}$$

using these boundry conditions in ① and ③ we get

(using Ist b.c) $\quad A_1 + B_1 = B_2$ —— ④

Since $\dfrac{d\psi_1}{dx} = A i K_1 e^{iK_1x} - B_1 i K_1 e^{-iK_1x}$

$$\frac{d\psi_1}{dx} = iK_1 (A_1 e^{iK_1x} - B_1 e^{-iK_1x})$$

and $\dfrac{d\psi_2}{dx} = -B_2 K_2 e^{-K_2x}$

(using 2nd b.c) $\quad \dfrac{d\psi_1}{dx} = \dfrac{d\psi_2}{dx}$ at $x=0$

$$\therefore iK_1(A_1e^{iK_1x} - B_1e^{-iK_1x}) = -B_2K_2e^{-K_2x}$$

$$iK_1(A_1 - B_1) = -B_2K_2$$

or $\quad A_1 - B_1 = \dfrac{-B_2K_2}{iK_1}$ —— ⑤

Adding ④ and ⑤ we get

$$2A_1 = B_2\left(1 - \frac{K_2}{iK_1}\right)$$

$$2A_1 = B_2\left(\frac{iK_1 - K_2}{iK_1}\right)$$

$$B_2 = \frac{2A_1 iK_1}{iK_1 - K_2} \quad \text{—— (a)}$$

Now subtracting ④ and ⑤ we get

$$2B_1 = B_2\left(1 + \frac{K_2}{iK_1}\right)$$

Putting the values of B_2 from (a) we get

$$2B_1 = \frac{2A_1 iK_1}{iK_1 - K_2}\left(1 + \frac{K_2}{iK_1}\right)$$

$$2B_1 = \frac{2A_1 iK_1}{iK_1 - K_2}\left(\frac{iK_1 + K_2}{iK_1}\right)$$

$$2B_1 = 2A_1\left(\frac{iK_1 + K_2}{iK_1 - K_2}\right)$$

$$B_1 = A_1\left(\frac{iK_1 + K_2}{iK_1 - K_2}\right) \quad \text{——— (b)}$$

Putting the values of B_1 and B_2 in eq ① and eq ③ we get

$$\psi_1 = A_1 e^{iK_1 x} + \left(\frac{iK_1 + K_2}{iK_1 - K_2}\right) A_1 e^{-iK_1 x}$$

$$\psi_1 = A_1\left(e^{iK_1 x} + \frac{iK_1 + K_2}{iK_1 - K_2} e^{-iK_1 x}\right) \quad \text{——— (6)}$$

$$\psi_1 = A_1 e^{iK_1 x} + B_1 e^{-iK_1 x} \quad \text{— (1)}$$

and

$$\psi_2 = \frac{2iK_1 A_1}{iK_1 - K_2} e^{-K_2 x}$$

$$\psi_2 = A_1 \frac{2iK_1}{iK_1 - K_2} e^{-K_2 x} \quad \text{——— (7)}$$

$$\psi_2 = B_2 e^{-K_2 x} \quad \text{— (3)}$$

REFLECTION CO-EFFICIENT (R)

It is defined as

"The ratio of the amplitude of the reflected wave to the amplitude of the incident wave."

i.e

$$R_1 = \frac{|B_1|^2}{|A_1|^2}.$$

$$|B_1|^2 = \left(\frac{iK_1 + K_2}{iK_1 - K_2} A_1\right)^2 \quad \text{from (b)}$$

Now $|B_1|^2 = B_1 B_1^*$

$$|B_1|^2 = \frac{iK_1 + K_2}{iK_1 - K_2} \times \frac{-iK_1 + K_2}{-iK_1 - K_2} |A_1|^2$$

$$|B_1|^2 = \frac{iK_1 + K_2}{-(-iK_1 + K_2)} \times \frac{-iK_1 + K_2}{-(iK_1 + K_2)} |A_1|^2$$

$$|B_1|^2 = |A_1|^2$$

$$\therefore \quad R = \frac{|B_1|^2}{|A_1|^2} = \frac{|A_1|^2}{|A_1|^2} = 1$$

$$R = 1$$

This means that incident and reflected waves have same intensity. This means that all the particles with $E < V_0$ are reflected back.

TRANSMISSION CO-EFFICIENT (T)

It is defined as

"The ratio of the amplitude of the transmitted wave to the amplitude of the incident wave".

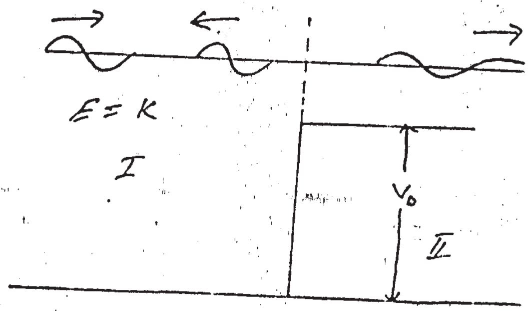
i.e $$T = \frac{|A_2|^2}{|A_1|^2} = \frac{0}{|A_1|^2} \quad \therefore A_2 = 0$$

$$T = 0$$

So when $E < V_0$, no wave is transmitted

Case (ii) When $(E > V_0)$

According to time independent S.W. equation in one dimension along x-axis, we have



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

for region I put $\psi = \psi_1$ and $V_0 = 0$

$$\therefore \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

put $\frac{2mE}{\hbar^2} = K_1^2$

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0$$

Its solution is

$$\psi_1 = A_1 e^{iK_1x} + B_1 e^{-iK_1x} \quad \text{——} \quad (1)$$

for region II $E > V_0$; $\psi = \psi_2$

$\therefore$ S.W. equ. becomes

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

Now put $\frac{2m}{\hbar^2}(E - V_0) = K_2^2$

$$\therefore \frac{d^2\psi_2}{dx^2} + K_2^2\psi_2 = 0$$

Its solution is

$$\psi_2 = A_2 e^{iK_2x} + B_2 e^{-iK_2x} \quad \text{——} \quad (2)$$

In eq. (1) the term $A_1 e^{iK_1x}$ represents incident particles and the term $B_1 e^{-iK_1x}$ represents reflected particles. In eq. (2) the term $A_2 e^{iK_2x}$ represents incident particles while the term $B_2 e^{-iK_2x}$ shows reflected particles.

Since, in region II, in this case there is no reflected beam and all the particles are going towards right. So 2nd term of eq is neglected

$$\therefore \quad \psi_2 = A_2 e^{iK_2 x} \quad \text{——} \quad (3)$$

DETERMINATION OF CONSTANTS

Using boundry conditions

$$\begin{cases} \text{i) At } x=0 & \psi_1 = \psi_2 \\ \text{ii) At } x=0 & \dfrac{d\psi_1}{dx} = \dfrac{d\psi_2}{dx} \end{cases}$$

using the boundry conditions in (1) and (3)

using Ist boundry condition:-

$$A_1 + B_1 = A_2 \quad \text{——} \quad (4)$$

Since

$$\frac{d\psi_1}{dx} = A_1 iK_1 e^{iK_1 x} - B_1 iK_1 e^{-iK_1 x}$$

$$\frac{d\psi_1}{dx} = iK_1 (A_1 e^{iK_1 x} - B_1 e^{-iK_1 x}).$$

and

$$\frac{d\psi_2}{dx} = iK_2 A_2 e^{iK_2 x}$$

using 2nd boundry condition:-

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad \text{at} \quad x=0$$

$$iK_1 (A_1 - B_1) = iK_2 A_2$$

$$A_1 - B_1 = \frac{K_2 A_2}{K_1} \quad \text{——} \quad (5)$$

Adding (4) and (5) we get

$$2A_1 = A_2 \left(1 + \frac{K_2}{K_1}\right)$$

$$2A_1 = A_2 \left(\frac{K_1 + K_2}{K_1}\right)$$

$$A_2 = \frac{2A_1 K_1}{K_1 + K_2} \quad \text{——} \quad (a).$$

Now subtracting (4) and (5) we get

$$2B_1 = A_2\left(1 - \frac{K_2}{K_1}\right)$$

$$2B_1 = A_2\left(\frac{K_1 - K_2}{K_1}\right)$$

Putting the value of A_2 from (a) we get

$$2B_1 = \frac{2K_1A_1}{K_1 + K_2}\left(\frac{K_1 - K_2}{K_1}\right)$$

$$B_1 = A_1\left(\frac{K_1 - K_2}{K_1 + K_2}\right) \text{ —— (b)}$$

The fact that $B_1 \neq 0$ indicates that some particles are reflected at $x = 0$ which is contradicted by classical physics according to which all the particles with $E > V_0$ should go to the IInd region.

Putting the values of B_1 and A_2 in ① and ③ we get

$$\psi_1 = A_1e^{iK_1x} + \frac{K_1 - K_2}{K_1 + K_2}A_1e^{-iK_2x}$$

$$\psi_1 = A_1e^{iK_1x} + B_1e^{-iK_1x} \text{ —— ①}$$

$$\psi_1 = A_1\left[e^{iK_1x} + \left(\frac{K_1 - K_2}{K_1 + K_2}\right)e^{-iK_2x}\right] \text{ —— ⑥}$$

and

$$\psi_2 = \frac{2A_1K_1}{K_1 + K_2}e^{iK_2x} \text{ —— ⑦}$$

$$\psi_2 = A_2e^{iK_2x} \text{ —— ③}$$

REFLECTION CO-EFFICIENT

$$R = \frac{|B_1|^2}{|A_1|^2} = \left(\frac{K_1 - K_2}{K_1 + K_2}\right)^2 A_1^2 \Big/ A_1^2$$

$$R = \left(\frac{K_1 - K_2}{K_1 + K_2}\right)^2$$

TRANSMISSION CO-EFFICIENT

$$T = \frac{|A_2|^2}{|A_1|^2}$$

$$T = \left(\frac{2A_1K_1}{K_1+K_2}\right)^2 \Big/ |A_1|^2$$

$$T = \left(\frac{2K_1}{K_1+K_2}\right)^2 \cdot \frac{A_1^2}{A_1^2}$$

$$T = \frac{4K_1^2}{(K_1+K_2)^2}$$

Q: What do you mean by potential well step? A stream of particles are impinging on a step of height V_0. If E is the energy of particle, discuss their behaviour when $E<V_0$ & $E>V_0$.

(OR) Give the step potential solution of Schrodingers equation?

SEPARATION OF TIME DEPENDENT AND SPACE DEPENDENT PARTS OF S.W. EQ.

We know solve the time dependent S.W. equ. and by a mathmatical technique called separation of variables.

We assume a solution of the form

$$\Psi(r,t) = \psi(r)\,\phi(t) = \psi\phi \quad \text{——} \quad (A)$$

Putting it in S.W. equ. we get

$$\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\Psi - V\Psi$$

or
$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

or
$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial \Psi}{\partial t} \text{ ——— } (A')$$

$\because$ from (A) $\Psi = \psi\phi$

$$-\frac{\hbar^2}{2m}\nabla^2(\psi\phi) + V(\psi\phi) = i\hbar\frac{\partial(\psi\phi)}{\partial t}$$

Now ∇^2 operates only on space part and ϕ is function of time only.

$$\therefore \quad -\frac{\hbar^2}{2m}\phi\nabla^2\psi + V\psi\phi = i\hbar\,\psi\frac{\partial\phi}{\partial t}$$

Dividing both sides by the product $\psi\phi$, we get

$$-\frac{\hbar^2}{2m}\frac{\nabla^2\psi}{\psi} + V = \frac{i\hbar}{\phi}\frac{\partial\phi}{\partial t} \text{ ——— } (B)$$

The L.H.S of (B) is a function of space co-ordinates only and R.H.S is a function of time only.

Putting L.H.S = R.H.S = E called separation constants.

$$\therefore \quad -\frac{\hbar^2}{2m}\frac{\nabla^2\psi}{\psi} + V = E \text{ ——— } (C)$$

and
$$\frac{i\hbar}{\phi}\frac{\partial\phi}{\partial t} = E \text{ ——— } (D)$$

Here E = Total energy of the system.

Eq. (C) can be written as.

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

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

Multiplying throughout by $\frac{2m}{\hbar^2}\psi$

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{——— } (1)$$

which is time independent S.W. eqn.

Now eq. D can be written as

$$\frac{i\hbar}{\phi}\frac{d\phi}{t} = E$$

or
$$\frac{d\phi}{\phi} = \frac{E}{i\hbar}\,dt$$

$$\frac{d\phi}{\phi} = -\frac{iE}{\hbar}\,dt$$

Integrating both sides

$$\ln\phi = -\frac{iE}{\hbar}t + K$$

The constant of integration depends upon initial conditions and can be put $=0$

$$\ln\phi = -\frac{iE}{\hbar}t$$

or
$$\phi = e^{-\frac{iE}{\hbar}t}$$

So eq. (A) becomes

$$\Psi(r,t) = \psi(r)\,e^{\frac{-iEt}{\hbar}}$$

where ψ is a solution of eq. (A')

Thus the and time dependent parts of the S.W. equation are thus separated out.

Q:- Given S.W. equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}.$$

depends not on ψ and time dependent
part only when time independent ψ by
and depends on ψ and time
dependent part

Postulates of Quantum Mechanics

Quantum Mechanics:- When we deal with any small object of atomic size we use quantum mechanics. It is a new type of mechanics based on the wave nature of particles.

Quantum mechanics is based upon the following postulates.

First Postulate:- According to this postulate the state of a system is completely specified by a function ψ which is a function of space and time co-ordinates. This function is called wave function. The wave function should be single valued, finite and continuous. By the 2nd part of 1st postulate states that the product of the wave function ψ is i.e.

$$\psi\psi^* \, dx\,dy\,dz = \psi\psi^* \, d\tau \quad \text{—— (1)}$$

Separate out its and time dependent parts. (OR) Write down time dependent S.W. eq. and separate out its and time dependent parts.

POSTULATES OF QUANTUM MECHANICS

Quantum Mechanics:-

When we deal with very small objects e.g electrons, then we use quantum mechanics. It is a new type of mechanics based on the wave nature of particles.

Quantum mechanics is based upon the following postulates.

First Postulate:-

(a) According to this postulate the state of a system is completely specified by a function Ψ which is a function of space and time co-ordinates. This function is called wave function. This wave function Ψ should be single valued, finite and continuous.

(b) The 2nd part of Ist postulate states that the nature of the wave function Ψ is s.t

$$\Psi \Psi^* dxdydz = \Psi \Psi^* d\tau \quad \text{——} \quad (1)$$

should represent the probability of finding the particle in a volume $d\tau$.

If we consider a volume which encloses a particle then

$$\int \Psi \Psi^* d\tau = 1 \qquad \text{——— (2)}$$

This shows that the probability of finding a single particle in the volume should be 100%.

Second Postulate:-

According to this postulate certain measurable quantities can be represented as mathematical operator O. The physical ~~properties~~ properties of the variable can be deduced from the mathematical properties of operator O.

Third Postulate:-

According to this postulate the average value $\langle O \rangle$ of the variable represented by the operator is given by the expression

$$\langle O \rangle = \int \Psi^* O \Psi \, d\tau$$

PROBABILITY DENSITY

"The term probability density represents the probability of finding the particles/photons at certain points."

If we consider a string of length 'L' fixed at both the ends; then standing waves can be set up only if its length is integral multiple of $\lambda/2$ i.e

$$L = n\,\lambda_n/2$$

$$\text{or} \quad \lambda_n = \frac{2L}{n} \quad \text{where } n = 1, 2, 3, \ldots$$

In terms of angular wave number.

$$K = \frac{2\pi}{\lambda}$$

$$K_n = \frac{2\pi}{\lambda_n}$$

$$K_n = \frac{2\pi}{2L} \times n$$

$$K_n = \frac{\pi n}{L}$$

The amplitude of standing wave is

$$y_n = y_{max} \sin K_n x$$

$$y_n = y_{max} \sin\left(\frac{n\pi}{L}\right) x$$

Like standing waves in a string; standing e.m. waves can be set up in a cavity. At the ends of cavity where the reflection of the waves takes place from the conducting material, the electric field becomes zero.

So $E = 0$ at $x = 0$, $x = L$

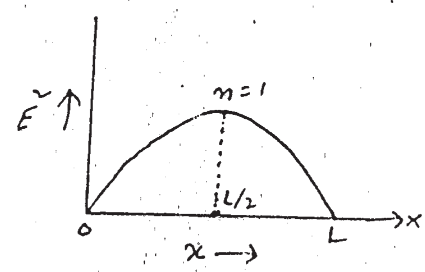
The amplitude of oscillating electric field is

$$E_n = E_{max} \operatorname{Sin} K_n x$$

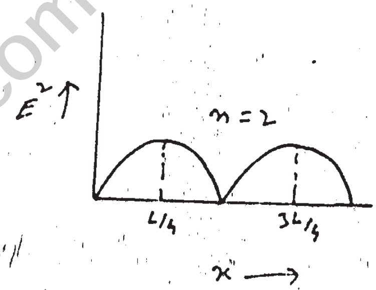
$$E_n = E_{max} \operatorname{Sin}\left(\frac{n\pi}{L}\right) x$$

Fig. shows graph between E_n^2 and x.

We find that for $n=1$ density of photons is maximum at $x = L/2$ and minimum at $x=0$ (near the walls).



For $n=2$, the density of photons is maximum at $x = L/4$ and $x = \frac{3}{4}L$ and minimum at $x=0$ and $x = L/2$.



For a single photon, we do not use the term density of photons but instead we say that "The square of electric field amplitude at a certain point gives probability to find the photon at that point."

It should be noted that we do not consider the actual location of photon, but instead its probability to be found in a certain location.

BARRIER TUNNELING

"The penetration of classically impenetrable barriers by electrons is called Barrier Tunneling".

Consider a barrier of height 'U' and width 'L' in fig (i). An electron of energy 'E' is approaching the barrier from left.

As $E<U$, so classically the electron would be reflected and would retrace their origional path. However by Quantum mechanics there is a finite chance that the electrons penetrate the barrier and continue their motion towards right.

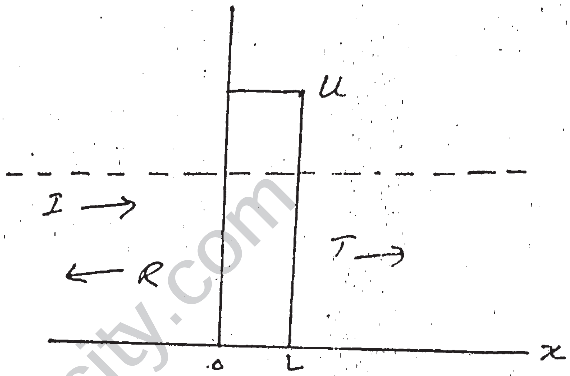


Fig (i)

To explain the situation, we use the terms R and T called reflection co-efficient and transmission coefficient respectively. Now $R+T=1$ i.e if $T=0.05$ then $R=1-0.05=0.95$ i.e if no. of incident electrons is 100, then (5) electrons will penetrate and 95 electrons will go back.

Fig (ii) shows the probability density $P(x)$ verses 'x'.

To the left of the barrier, the reflected wave has smaller amplitude than the incident wave which interfere without total cancellation at any point.

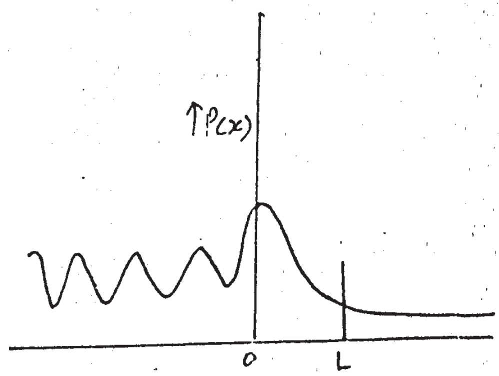


Fig (ii)

Within the barrier the wave decays exponentially. On the far side of barrier, the wave amplitude is reduced and this wave of reduced amplitude gives uniform probability density.

According to S.W. equation (time independent) along x-axis

$$\frac{d^2\psi}{dx^2} - \frac{8\pi^2 m}{h^2}(U-E)\psi = 0 \qquad x>0$$

or $$\frac{d\psi^2}{dx^2} - K^2\psi = 0 \qquad \text{where} \quad K = \sqrt{\frac{8\pi^2 m}{h^2}(U-E)}$$

It can be shown that.

$$T = e^{-2KL}$$

This formula is an ~~approxi~~ approximation and holds when $T \ll 1$.

The value of T depends upon L, m, U. T decreases if L increases or U increases or m increases. So T becomes very small if mass of the particles become larger.

EXAMPLES OF BARRIER TUNNELING

The phenomenon of Barrier Tunneling is very important and has many practical applications.

1:- Consider a bare copper wire cut into two piece and then two ends are twisted together. The will still conduct electricity inspite of an insulating layer of CuO. The electrons get throug this thin layer by Barrier Tunneling.

2:- Thermonuclear fussion reaction is source of energy in the sun. When two nuclie come close to each other, they are slowed down due to mutual repulsion. So there is a coulomb barrier in between them. So the protons of the two nuclie have ability to tunnel through this coulomb barrier.

3:- i.e emission of α-particles by radioactive nuclei and fission of a heavy nucleus into two parts is due to Barrier Tunneling.

4:- Tunneling diode is a practical application of Barrier Tunneling. In tunnel diode the

the electrons tunnel through the device by controlling the height of barrier.

5:- In a scanning tunneling microscope, the tip of the needle moves up and down on the surface of sample under investigation. Electrons from the sample tunnel through the gap b/w the sample and the needle.

Q:- How will you apply the S.W. eq. to study of a free particle?

We want to calculate wave function of a free particle i.e a particle to no forces.

According to S.W (Time indep.) eq along x-axis

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad \text{———} \quad (1)$$

Putting $\frac{2m}{\hbar^2}E = K^2$

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0$$

It is a linear, homogeneous and 2nd order differential equation.

Its solution is of the form

$$\psi = A e^{\pm ikx} \text{ ——— (a)}$$

where A is a constant.

The time dependent wave function for the particle is given by

$$\phi = e^{-\frac{iEt}{\hbar}} \text{ ——— (b)}$$

$$\Psi = \psi \phi$$

So from (a) and (b)

$$= A e^{\pm ikx} \cdot e^{-\frac{iEt}{\hbar}}$$

$$\Psi = A e^{i(\pm kx - Et/\hbar)}$$

$\because$ $E = h\nu$ and $\hbar = \frac{h}{2\pi}$

$$\Psi = A e^{i(\pm kx - \omega t)} \text{ ——— (2)}$$

$\because \frac{E}{\hbar} = \frac{h\nu 2\pi}{h}$
$= 2\pi\nu = \omega$

Eq. (2) can be separated into two parts

$$\Psi = A e^{i(kx - \omega t)} \text{ ——— (3)}$$

and

$$\Psi = A e^{-i(kx + \omega t)} \text{ ——— (4)}$$

where +ve sign indicates the motion of wave function for along + x-axis and -ve sign for the reverse direction.

Sample problem (7)

PROBLEM (2.8). *The rest mass of newly discovered particle was measured to be 3097 MeV. This particle was expected to decay into particles of smaller mass. What is the mean time interval between production and decay for these short lived particles. The uncertainty in energy was 0.063 MeV.*

Sol :- $\Delta t = ?$

$$\Delta E = 0.063 \text{ Mev} = 0.063 \times 10^{6} \times 1.6 \times 10^{-19} \text{ J}$$

As $\Delta E \Delta t = \hbar$

$$\Delta t = \frac{\hbar}{\Delta E} \qquad \hbar = \frac{h}{2\pi}$$

$$\Delta t = \frac{h}{2\pi \Delta E}$$

$$= \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 0.063 \times 10^{6} \times 1.6 \times 10^{-19}}$$

$$\Delta t = 1.1 \times 10^{-20} \text{ Sec.}$$

Sample problem (8)

PROBLEM (2.3). *Consider an electron confined by electrical forces to an infinitely deep potential well of depth 100 pm. What are the energies of its three allowed lowest states and of the state with n = 15 ?*

Sol :- $E_1 = ?$, $E_2 = ?$, $E_3 = ?$, $E_{15} = ?$

$$L = 100 \text{ pm} = 10^{2} \times 10^{-12} = 10^{-10} \text{ m}$$

From the relation

$$E_n = \frac{n^2 h^2}{8 m L^2}$$

Put $n = 1, 2, 3, 15$ we get.

$$E_1 = \frac{(1)^2 * (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2}$$

$$= 6.03 \times 10^{-18} \text{ J}$$

$$= \frac{6.03 \times 10^{-18}}{1.6 \times 10^{-19}} = 37.7 \text{ ev}$$

$$E_2 = 2 \times 2 \times 37.7 = 151 \text{ ev}$$

$$E_3 = 3 \times 3 \times 37.7 = 339 \text{ ev}$$

$$E_{15} = 15 \times 15 \times 37.7 = 8480 \text{ ev}$$

Sample problem (9)

PROBLEM (). *Consider a 1 μ gm speck of dust moving back and forth between two rigid walls separated by 0.1 mm. It moves so slowly that it takes 100 s for the particle to cross the gap. What quantum number describes this motion ?*

Sol :-

$m = 1 \mu gm = 1 \times 10^{-6} \times 10^{-3}$ kg $= 1 \times 10^{-9}$ kg

$L = 0.1$ mm $= 0.1 \times 10^{-3}$ m

$t = 100$ Sec

$n = ?$

As the energy of particle is

$$E = \frac{1}{2} m v^2$$

$$= \frac{1}{2} m \left(\frac{L}{t}\right)^2$$

$$= \frac{1}{2} \times 10^{-9} \times \left(\frac{0.1 \times 10^{-3}}{100}\right)^2$$

$$E = \frac{1}{2} \times 10^{-9} \times (10^{-6})^2$$

$$E = 0.5 \times 10^{-21} J$$

$$E = 5 \times 10^{-22} J$$

By the relation

$$E_n = \frac{n^2 h^2}{8 m L^2}$$

$$n^2 = \frac{8 m L^2}{h^2} E_n$$

$$n^2 = \frac{L^2}{h^2} 8 \times 10^{-9} \times 5 \times 10^{-22}$$

$$n = \frac{L}{h} \sqrt{40 \times 10^{-9} \times 10^{-22}}$$

$$n = 3 \times 10^{14}$$

This is very large number. It is impossible to distinguish b/w $n = 3 \times 10^{14}$ and $n = 3 \times 10^{14} + 1$. So the quantized nature of this motion will not reveal itself.

Sample problem (11)

PROBLEM ([redacted]). *An electron is trapped in an infinitely deep well of width L. If the electron is in its ground state, what fraction of its time does it spend in the central third of the well ?*

<u>Sol</u>:- The position probability density in the nth state is

$$P_n(x) = \left[\sqrt{\frac{2}{L}}\ \operatorname{Sin}\left(\frac{n\pi x}{L}\right)\right]^2$$

for ground state $n=1$

$$P_1(x) = \frac{2}{L}\operatorname{Sin}^2\left(\frac{\pi x}{L}\right)$$

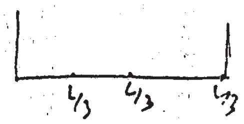
The integral of the quantity over the entire well is unity.

$$\therefore \int_0^L P_1(x)\,dx = 1$$

$$\int_0^L \frac{2}{L}\operatorname{Sin}^2\left(\frac{\pi x}{L}\right) = 1$$

The required function is given by

$$f = \int_{L/3}^{2L/3} P_1(x)\,dx$$



$$\frac{L}{3}+\frac{L}{3}+\frac{L}{3} = L$$

$$= \int_{L/3}^{2L/3} \frac{2}{L}\operatorname{Sin}^2\left(\frac{\pi x}{L}\right)dx$$

$$=$$

$$= \frac{2}{L}\int_{L/3}^{2L/3} \sin^2\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{1}{L}\int_{L/3}^{2L/3} 2\sin^2\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{1}{L}\int_{L/3}^{2L/3} \left(1-\cos\frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{L}\left[x - \frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/3}^{2L/3}$$

$$f = 0.61$$

So the electron spends 61% of its time in the central third of the trap and about 19.5% in each of the outer two thirds. $[0.195 + 0.61 + 0.195] = 1$.

The End.