

## THE WAVE NATURE OF MATTER

### 50.1 Wave Behavior of Particles

The electromagnetic radiations like light, X-rays etc., can produce the phenomenon of interference, diffraction and polarization due to their wave nature. But under certain circumstances they can produce photoelectric effect and Compton Effect which is the evidence of their particle nature. It means that electromagnetic radiations have dual nature; wave as well as particle nature.

In a similar way the particles like electrons, neutrons and protons etc. must have dual nature. If the beam of electrons accelerated through a known potential difference 'V', is made to fall on a double slit and after passing through the double slit, they are allowed to strike on a fluorescent screen. It has been observed that pattern obtained on the screen is similar to the pattern of interference of light.

If the double slit is replaced by a circular aperture, then the diffraction pattern of electrons is similar to that of light was observed. The diffraction of electrons, similar to that of light, can also be observed by using a straight line edge. So the wave nature of particles like electrons, protons, neutrons, even atoms and molecules have been observed experimentally.

### 50.2 Double Slit Experiment

In Double slit experiment, a filament produces a spray of electrons which are accelerated through a potential difference of 50 kV. After passing through double slit, the electrons produce a visible interference pattern fluorescent screen, which can be photographed.

### 50.3 De Broglie Wavelength

In 1924, Louis De Broglie proposed that a particle must also behave like wave, in the similar way, wave behave like particles. According to quantum theory of light, the energy  $E$  of a photon is:

$$E = h\nu \quad \text{-----} \quad (1)$$

Where  $h$  is the Plank's constant and  $\nu$  is the energy of photon.

According to Einstein, the energy  $E$  corresponding to the mass  $m$  to a particle is described as:

$$E = mc^2 \quad \text{-----} \quad (2)$$

Where  $c$  is speed of electromagnetic radiations.

Comparing equation (1) and (2), we get:

$$mc^2 = hv$$

$$mc = \frac{hv}{c}$$

$$p = \frac{hv}{c}$$

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

Here  $\lambda$  is the wavelength of wave associated with moving particle. Such waves are called De Broglie waves or matter waves and are described by the relation.

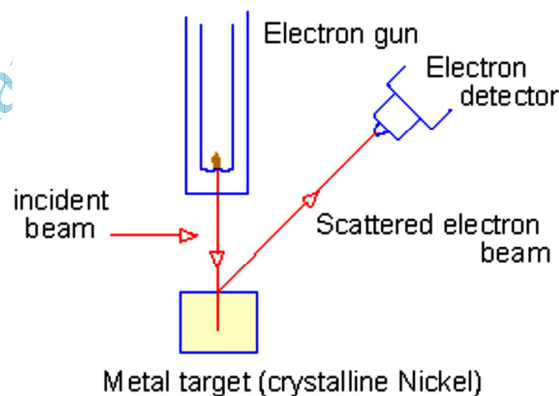
$$\lambda = \frac{h}{p}$$

#### 50.4 De Broglie Hypothesis

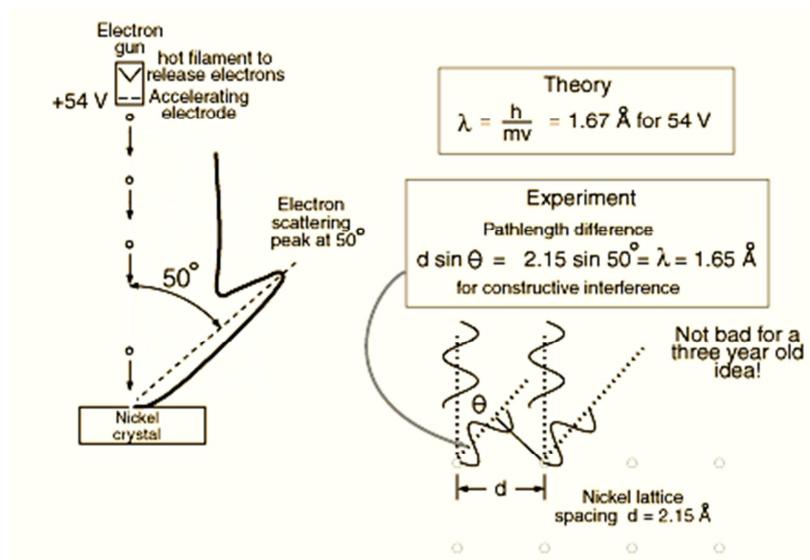
The De Broglie equation  $\lambda = \frac{h}{p} = \frac{h}{mv}$  describes the wave behavior of particles. As the value of Planck's constant  $h$  is very small and is of the order of  $\approx 10^{-34}$ , the wavelength associated with ordinary object (e.g., A moving tennis ball) is so small and is difficult to observe. But for the small objects like electrons and neutron etc., the wave behavior of particles is dominant. It is because of the reason that mass of electron and neutron are very small as compared to an ordinary tennis ball.

#### 50.5 The Davison-Germer Experiment

The De Broglie hypothesis was confirmed by Davison and Germer. The schematic diagram of Davison and Germer experimental setup is shown in the figure.



The electrons from a heated filament F are accelerated by an adjustable potential difference  $V$ . The beam of electrons is allowed to fall on a nickel crystal. The diffracted beam of electrons is detected by a movable detector at different values of angles.



It is observed that there is a strong diffracted beam obtained for  $\phi = 50^\circ$  and  $V = 54 \text{ volts}$ . This situation is similar to the diffraction of light produced by the diffraction grating.

In nickel crystal, the atoms are arranged in definite order; hence the crystal surface acts like a diffraction grating. The first order maxima is obtained at an angle  $\phi = 50^\circ$ . The wavelength associated with electrons can be determined by using the equation:

$$m\lambda = D \sin \theta$$

Here  $m = 1$  for the first order diffraction peak  
 Inter-planer spacing for nickel  $D = 215 \text{ pm}$   
 Angle of diffraction  $\phi = 50^\circ$

$$\Rightarrow 1 \times \lambda = 215 \times 10^{-12} \times \sin 50$$

$$\Rightarrow \lambda = 165 \text{ pm}$$

The wavelength of the matter wave, can be find out by using de Broglie hypothesis:

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

The kinetic energy of the electron is:

$$\frac{1}{2}mv^2 = Ve \Rightarrow v = \sqrt{\frac{2Ve}{m}}$$

$$\Rightarrow \lambda = \frac{h}{m\sqrt{\frac{2Ve}{m}}}$$

By putting the value of constants  $h, m, e$  and  $V = 54 \text{ volts}$ , we have:

$$\lambda = 166.4 \text{ pm}$$

Hence the value of de Broglie wavelength is in good agreement with the experimentally observed wavelength associated with electrons.

### 50.6 G. P. Thomson Experiment

In 1927, G. P. Thomson (son of J. J. Thomson) performed an experiment and confirmed the de Broglie equation of matter waves.

He obtained a fine beam of electrons accelerated through a potential difference of 15 kV and made it to fall on a target which was not a single crystal, but it was made up of a large number of tiny, randomly oriented crystallites (powdered aluminum).

A photographic plate was placed parallel to the target on which the diffraction pattern was obtained. It was observed that the diffraction pattern of electrons was very similar to the diffraction of X-rays. As the diffraction is a wave property, so the wave nature of electrons was confirmed experimentally.

The wavelength of the matter waves associated with the electrons can be determined by using the Bragg's equation:

$$2d \sin \theta = m\lambda \quad \text{----- (1)}$$

Where  $d$  is the inter-planer spacing,  $\theta$  is the glancing angle and  $m$  is the order of diffraction.

If  $V$  is the potential difference through which the electrons are accelerated, then the kinetic energy of electrons is:

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

$$v = \sqrt{\frac{2Ve}{m}}$$

According to de Broglie hypothesis

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

$$\Rightarrow \lambda = \frac{h}{m\sqrt{\frac{2Ve}{m}}} = \frac{h}{\sqrt{2me}} \quad \text{----- (2)}$$

G. P. Thomson observed that the de Broglie wavelength associated with moving electrons was good in agreement with experimentally observed value, that was find out by using Bragg's law.

The atomic structure of solids are studied the diffraction beam of electrons. The electrons are less penetrating than X-rays, so the electrons are used to study the surface morphology of solids.

### 50.7 Waves and Particles

The evidence of the matter is wave like is very strong. On the other hand, the evidence that a matter is particle like is equally as strong. In these situations, the description of wave as well as the particle nature of matter has remained a challenge for the scientists. One property that we like for the particles (even particles with the wave like nature) to have the ability to be localized. For example, an electron in an atom of 0.1 m diameter is localized in certain region of space. On the other hand, a wave cannot be localized in space and time like a particle.

The amplitude of a matter wave carries information about the location of the particle. The wave has the large amplitude where the particle is likely to be found, and it has the small amplitude where the particle is unlikely to be found. If the wave has the constant amplitude throughout a given region of space, the particle is equally likely to be found anywhere in that region. If the amplitude of the matter wave is zero in a specific region, then the particle never found there.

### 50.8 Localizing Wave in Space

Consider a wave moving along x-axis extends from  $x = -\infty$  to  $x = \infty$ . This wave has a sharply defined wavelength  $\lambda_0$ . There is nothing about this wave that will suggest the localization in space that we associate with the particle. Such a wave has no beginning, no end, and no such distinct mark. If this wave were describing a particle, we would say that the particle could be found anywhere between  $x = -\infty$  to  $x = \infty$ , and it is completely un-localized.

Often it is convenient to work, not with the wavelength, but with the wave number  $k = \frac{2\pi}{\lambda}$ . For the present case, the wave has a sharply defined wave number  $k_0 = \frac{2\pi}{\lambda_0}$ .

On the other hand, a wave packet is associated with a moving particle. Many waves adds up to make a wave packet of length  $\Delta x$  and adds to zero everywhere else. Thus for the present case, the particle is localized in space. The particle is likely to be found in the region of size  $\Delta x$  and unlikely to found outside that region.

This wave packet no longer contains a single wave number  $k_0$  but rather a spread of wave numbers centered about  $k_0$ . Let  $\Delta k$  is the rough measure of the spread of wave numbers. The product of  $\Delta x$  and  $\Delta k$  is proves to be of the order of unity:

$$\Delta x \Delta k \approx 1$$

This expression tells that the smaller the value of  $\Delta x$ , the larger must be the range of wave numbers  $\Delta k$ . Conversely, the narrower the spread in  $\Delta k$ , the less localized the particle will be.

### 50.9 Localizing Wave in Time

A particle is localized in space as well as in time. So, the space variable  $x$  must be replaced by time variable  $t$  (as the wavelength  $\lambda_0$  by the time period  $T_0$ ). And the wave number  $k_0$  must be replaced by the angular frequency  $\omega_0$ .

Similarly, the spread of wave number  $\Delta k$  must be replaced by  $\Delta\omega$  and the displacement  $\Delta x$  by the interval of time  $\Delta t$ . So we have

$$\Delta\omega \Delta t \approx 1$$

It means that the product  $\Delta\omega \Delta t$  is of the order of unity.

### 50.10 Heisenberg's Uncertainty Relationship

Let the motion of the particle is along x-axis, then according to the de Broglie Hypothesis:

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

The angular wave number is

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{\left(\frac{h}{p_x}\right)} = \frac{2\pi}{h} p_x$$

Also

$$\Delta k = \Delta \left( \frac{2\pi}{h} p_x \right)$$

$$\Delta k = \frac{2\pi}{h} \Delta p_x$$

For a particle, we have

$$\Delta x \left( \frac{2\pi}{h} \Delta p_x \right) \approx 1$$

$$\Delta x \Delta p_x \approx \frac{h}{2\pi}$$

If the motion of the particle depends upon the three coordinates  $x$ ,  $y$ ,  $z$ , the generalizing above relation, we have:

$$\Delta x \Delta p_x \approx \frac{h}{2\pi}$$

$$\Delta y \Delta p_y \approx \frac{h}{2\pi}$$

$$\Delta z \Delta p_z \approx \frac{h}{2\pi}$$

These are known as Heisenberg's Uncertainty Relationships. According to these relationships:

*It is not possible to determine both the position and the momentum of a particle with ultimate precision.*

The width  $\Delta x$  of the wave packet indicates the probable location of the particle, and  $\Delta p_x$  is the range in momentum. So, the Uncertainty principle may also be stated as:

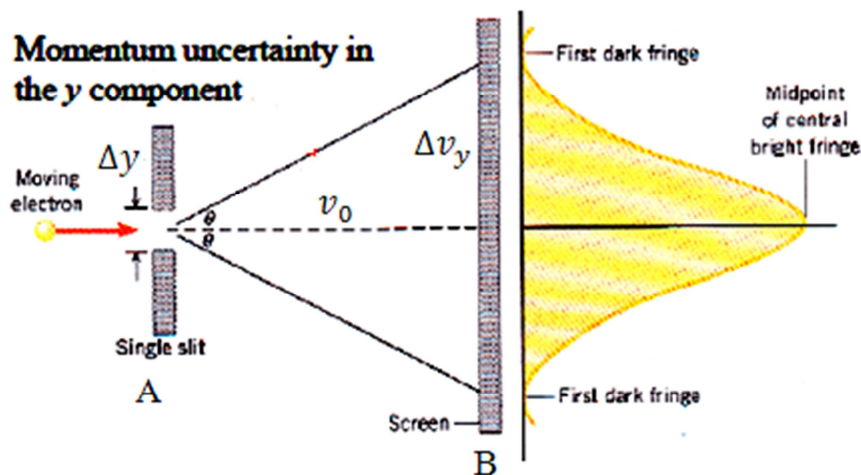
*A particle cannot be described by a wave packet in which the position and momentum have arbitrary small ranges.*

It means that due to the wave nature, the exact position  $x$  of a particle cannot be determine, but it will be in the range  $\Delta x$ .

Similarly, the true or exact momentum of the particle  $p_x$  cannot be determined, but it will be in the range of  $\Delta p_x$ .

**50.11 Uncertainty Principle and Single-Slit Diffraction**

Consider the experiment of diffraction of electrons by single slit. Let a beam of electrons moving with speed  $v_0$  passes through a single slit of width  $\Delta y$ . The diffraction pattern is obtained on the screen B as shown in the figure.



Due to the wave nature, the electron beam bends on the either side of the central point producing the diffraction pattern. Let  $\Delta v_y$  is the uncertainty in the component of velocity along  $y$ - axis for the first minimum, then we have

$$\tan \theta = \frac{\Delta v_y}{v_0}$$

Consider the angle  $\theta$  is very small, then  $\tan \theta \approx \theta$ :

$$\theta = \frac{\Delta v_y}{v_0} \quad \text{----- (1)}$$

In case of location of the first minimum of diffraction, we have:

$$D \sin \theta = m\lambda$$

Here  $m=1$  and if  $\theta$  is very small, then  $\sin \theta \approx \theta$

$$D\theta \approx \lambda$$

$$\because D = \Delta y$$

$$\Delta y \theta \approx \lambda$$

$$\theta \approx \frac{\lambda}{\Delta y} \quad \text{-----} \quad (2)$$

Comparing equation (1) and (2),

$$\frac{\Delta v_y}{v_0} \approx \frac{\lambda}{\Delta y}$$

$$\Delta v_y \Delta y \approx \lambda v_0$$

According to the de Broglie hypothesis:  $\lambda = \frac{h}{p} = \frac{h}{mv_0}$

$$\Rightarrow \Delta v_y \Delta y \approx \left( \frac{h}{mv_0} \right) v_0$$

$$\Rightarrow m \Delta v_y \Delta y \approx h$$

$$\Rightarrow \Delta p_y \Delta y \approx h$$

This is the form of uncertainty principle, which may be stated as:

*The product of uncertainty in momentum and uncertainty in position of a particle is of the order of plank's constant h.*

It means that, if the position of the particle is made more and more precise, the uncertainty in the momentum of the particle increases and vice versa. On other words,

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

### 50.12 The Energy-Time Uncertainty Relationship

The wave nature of a particle can be represented by the wave packet having angular frequency  $\omega$ . So the spread of angular frequency  $\Delta\omega$  and the time interval are related as:

$$\Delta\omega \Delta t \approx 1 \quad \text{-----} \quad (1)$$

Einstein's photon equation is

$$E = h\nu$$

$$\nu = \frac{E}{h}$$

The uncertainty in the frequency of the matter waves:

$$\Delta\nu = \frac{\Delta E}{h}$$

As  $\Delta\omega = 2\pi\Delta\nu = 2\pi \frac{\Delta E}{h}$ , put in equation (1):

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

This is another form of Uncertainty principle. It may be stated as:

*It is not possible to determine both the energy and time co-ordinates with ultimate precision.*



### 50.13 The Wave Function

The wave nature of a particle can be represented by wave function  $\psi$ , which is the function of space and time co-ordinates. The behavior of the particle in terms of wave can be determined by knowing the wave function for every point in the space and for every instant of time:

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

Consider a matter wave associated with a particle of mass  $m$  travelling in the direction of increasing  $x$  and on which no force acts, so called free particle. To describe the displacement associated with such a wave, the American physicist Erwin Schrodinger introduced a quantity  $\psi(x, t)$  for such a free particle, called wave function. The wave function for a free particle moving in the direction of increasing  $x$  is given by:

$$\psi(x, t) = \psi_0 e^{i(kx - \omega t)}$$

Here  $\psi_0$  is the amplitude of the wave,  $k \left( = \frac{2\pi}{\lambda} \right)$  is the wave number and  $\omega (= 2\pi f)$  is the angular frequency. As this wave function contains the imaginary number  $i (= \sqrt{-1})$ , so it a complex quantity.

The physical interpretation of the wave function was given by the German Physicist Max Born. He asserted that physical meaning should not be given to  $\psi$  itself, but to the product of  $\psi$  and its complex conjugate  $\psi^*$ . Specifically, Born postulated:

*The product  $\psi\psi^* dx$  gives the probability that the particle in question will be found between position  $x$  and  $x + dx$ .*

In quantum mechanics, we cannot say where a particle is' we can only say where it is likely to be. We call the product  $\psi\psi^*$  the probability density, symbol  $P(x)$ , so that

$$P(x) = \psi\psi^*$$

Even though the wave function  $\psi(x, t)$  is a complex quantity, but the probability density is always a real number.

For the free particle, the probability density is described as:

$$P(x) = [\psi_0 e^{i(kx - \omega t)}][\psi_0 e^{i(kx - \omega t)}] = |\psi_0|^2$$

Thus the probability density  $P(x)$  of a free particle is constant and is independent of  $x$  or  $t$ . Thus we conclude that the particle can be find with equal probability, at any point along the  $x$  directin from  $x = -\infty$  to  $x = +\infty$ .

This inability to pin down the location of a free particle is in complete accord with Heisenberg Uncertainty principle.

### 50.14 Schrodinger's Equation

The Schrodinger equation is used to find out the expression of wave function of moving particle in a specific direction. As it is described earlier, that a wave function is the function of both space and time variables. So we can write the wave function for the particle moving along  $x -$  axis as:

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

That is, the wave function of a particle can be described as the product of space dependent wave function  $\psi(x)$  and time dependent wave function  $\psi(t)$ . In the rest of the chapter we will focus our attention to the space dependent portion of wave function.

Now the Schrodinger's equation for a particle travelling in the  $x -$ direction is:

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

where  $E$  is the total energy of the particle and  $U(x)$  is its potential energy.

### 50.15 Schrodinger's Equation for a Free Particle

If the particle is a free particle, its potential energy  $U(x)$  is a constant which we can take to be zero for all values of  $x$ . The total energy  $E$  of the moving particle must be taken entirely kinetic. That is, in which we must have  $E = K = \frac{p^2}{2m}$ , in which  $p$  is the momentum of the particle. With this assumption, the Schrodinger's equation becomes:

$$\begin{aligned} -\frac{h^2}{8\pi^2m} \frac{d^2\psi(x)}{dx^2} &= E\psi(x) \\ \Rightarrow -\frac{d^2\psi(x)}{dx^2} &= \frac{8\pi^2mE}{h^2}\psi(x) \end{aligned}$$

$$\text{Put } \frac{8\pi^2mE}{h^2} = k^2 \quad \text{-----} \quad (1)$$

where  $k$  is the wave number.

$$\begin{aligned} \Rightarrow -\frac{d^2\psi(x)}{dx^2} &= k^2\psi(x) \\ \Rightarrow \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) &= 0 \end{aligned}$$

Putting  $\frac{d^2}{dx^2} = D^2$ , we have

$$\Rightarrow D^2\psi(x) + k^2\psi(x) = 0$$

$$\Rightarrow (D^2 + k^2)\psi(x) = 0$$

For characteristic solution, we have:

$$D^2 + k^2 = 0$$

$$D^2 = -k^2$$

$$D = \pm k$$

The characteristic solution of this equation will be:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{-----} \quad (2)$$

As the particle is moving along positive x-direction, so the equation (2) will become:

$$\psi(x) = Ae^{ikx} \quad \text{-----} \quad (3)$$

where A is the amplitude of the wave. The expression in equation (3) is wave function for the free particle moving along x – direction.

### Probability Density

For the free particle, the probability density P(x) is described as:

$$P(x) = [A e^{ikx}][A e^{-ikx}] = A^2$$

Thus the probability density of a free particle is  $A^2$  constant and is independent of  $x$  or  $t$ .

Thus we conclude that the particle can be find with equal probability, at any point along the x-direction from  $x = -\infty$  to  $x = +\infty$ .

### Wave Number

From equation (1), we have

$$k^2 = \frac{8\pi^2 mE}{h^2}$$

For the free particle, the total energy  $E = K = \frac{p^2}{2m}$ , in which  $p$  is the momentum of the particle.

$$\Rightarrow k^2 = \frac{8\pi^2 mE}{h^2} = \frac{8\pi^2 mp^2}{2m h^2} = \frac{4\pi^2 p^2}{h^2}$$

$$\Rightarrow k = \frac{2\pi p}{h} = \frac{2\pi}{(h/p)}$$

Using de Broglie hypothesis, we have

$$\Rightarrow k = \frac{2\pi}{\lambda}$$

### 50.16 Particle in a Well or One Dimensional Box

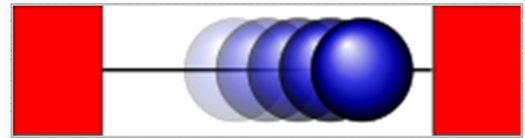
Let a particle of mass  $m$  is moving in a one-dimensional box of length  $L$ . Consider that the particle moves back and forth along  $x$ -axis between the perfectly hard and infinite high walls of the box, from  $x = 0$  to  $x = L$ , and no force acts on it during its motion. The particle suffers elastic collisions and its total energy  $E$  remains constant.

As there is no force acting on the particle, therefore

$$F = \frac{dV}{dx} = 0$$

$$\Rightarrow V = \text{constant}$$

For convenience, we take the potential energy of the particle as zero, i.e.,  $V = 0$ , inside the box. Since the walls of the box are infinitely high, therefore the potential energy of the particle outside the box is infinite.



Since the particle cannot have an infinite amount of energy, so it cannot exist outside the box. Hence the wave function of the particle  $\psi(x)$  is zero for  $x \leq 0$  and  $x \geq L$ .

$$-\frac{\hbar^2}{8\pi^2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$\frac{\hbar^2}{8\pi^2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) = 0$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2m}{\hbar^2} E\psi(x) = 0$$

$$\text{Put } \frac{8\pi^2mE}{\hbar^2} = k^2 \quad \text{----- (1)}$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

Putting  $\frac{d^2}{dx^2} = D^2$ , we have

$$\Rightarrow D^2\psi(x) + k^2\psi(x) = 0$$

$$\Rightarrow (D^2 + k^2)\psi(x) = 0$$

For characteristic solution, we have:

$$D^2 + k^2 = 0$$

$$D^2 = -k^2$$

$$D = \pm k$$

The characteristic solution of this equation will be:

$$\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}$$

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

$$\psi(x) = (A_1 + A_2) \cos kx + (iA_1 - iA_2) \sin kx \quad \text{--}$$

$$\text{----- (2)}$$

Let  $iA_1 - iA_2 = A$

$$A_1 + A_2 = B$$

Thus equation (2) will become:

$$\psi(x) = A \sin kx + B \cos kx \quad \text{--}$$

$$\text{----- (3)}$$

Where the constants A and B can be evaluated from the boundary conditions, which are:

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

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

Applying the 1<sup>st</sup> boundary condition, the equation (3):

$$B = 0$$

Applying the 2<sup>nd</sup> boundary condition:

$$\sin kL = 0$$

$$kL = n\pi, \text{ where } n \text{ is an integer}$$

$$k = \frac{n\pi}{L} \quad \text{----- (4)}$$

Thus equation (3) will become:

$$\psi(x) = A \sin \frac{n\pi}{L} x \quad \text{----- (5)}$$

The solution of the wave function for the particle in a box, since we have not yet determined the constant A. for this purpose, we make use of the normalization condition:

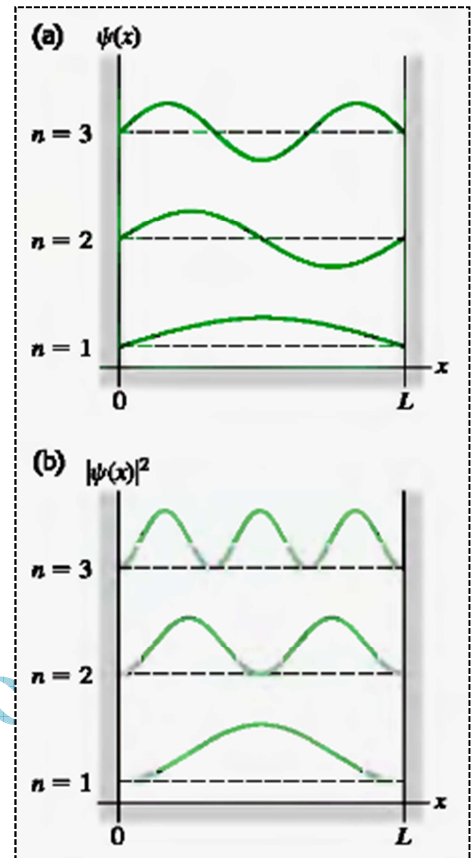
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

For the present case:

$$\int_0^L |\psi(x)|^2 dx = 1$$

$$\Rightarrow \int_0^L A^2 \sin^2 \left( \frac{n\pi}{L} x \right) dx = 1$$

$$\Rightarrow A^2 \int_0^L \left[ 1 - \cos \left( \frac{2n\pi}{L} x \right) \right] dx = 1$$



$$\Rightarrow A^2 \frac{L}{2} = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

Thus the equation (4) will become:

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$$

**Energy of the particle in the Box**

From equation (1) and (4), we have:

$$\frac{8\pi^2 mE}{h^2} = \frac{n^2 \pi^2}{L^2}$$

$$E_n = \frac{n^2 h^2}{8mL^2} \text{ ----- (6)}$$

For  $n = 1$ ,  $E_1 = \frac{h^2}{8mL^2}$ . Thus the equation (6) will become:

$$E_n = n^2 E_1$$

This shows that the particle in the box have discrete values. Hence, the energy of the particle in the box is quantum box is quantized.

**50.17 The Potential Step and Barrier Tunneling**

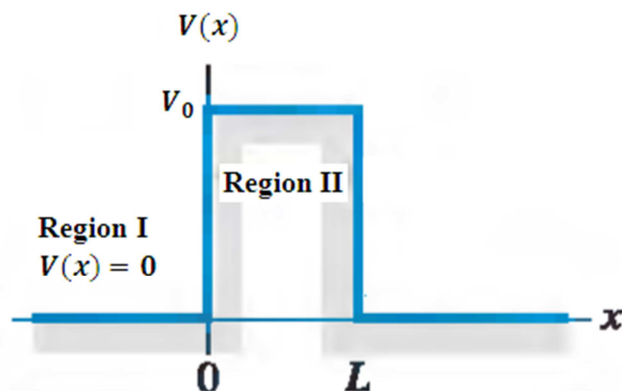
When a particle is moving in a region of a constant potential suddenly comes across another region of different constant potential, the common boundary of the two regions is called potential step. In the figure, the height of the potential step is  $V_0$ , say at  $x = 0$ . According to the classical physics, the particle coming from region I, approach the potential barrier of potential step with energy,  $E > V_0$  and are slow down by the force  $F = -\frac{\partial V}{\partial x}$ , so that the kinetic energy is converted into potential energy. If the particles have sufficient energy to overcome the barrier, then there will be total transmission. And if  $E \leq V_0$ , then the particles are stopped by the barrier and their motion will be reversed. In this case, there is the total reflection of the beam.

Quantum mechanically, for this potential step, we have the potential function as:

$$V(x) = 0 \text{ for } x < 0$$

$$V(x) = 0 \text{ for } x \geq 0$$

For the present case, the Schrodinger



wave equation will be:

$$\begin{aligned}
 &-\frac{h^2}{8\pi^2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \\
 \Rightarrow &\frac{h^2}{8\pi^2m} \frac{d^2\psi(x)}{dx^2} + [E + V(x)]\psi(x) = 0 \\
 \Rightarrow &\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2m}{h^2} [E + V(x)]\psi(x) = 0 \quad \text{----- (1)}
 \end{aligned}$$

**Case-1.  $E > V_0$**

**i) Region-1**

Let the particles with total energy E moves from region-I to region-II along x-axis. In region-I,  $V(x) = 0$ . Therefore, the equation (1) will become:

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{8\pi^2mE}{h^2}\psi_1(x) = 0$$

Put  $\frac{8\pi^2mE}{h^2} = k_1^2$  ----- (2)

where  $k$  is the wave number.

$$\Rightarrow \frac{d^2\psi_1(x)}{dx^2} + k_1^2\psi_1(x) = 0$$

The characteristic solution of this equation will be:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad \text{----- (3)}$$

The first and the second term of equation (3) represent the incident and reflected particles respectively.

**ii) Region-II**

For region-II,  $V(x) = V_0$ . Therefore, the equation (1) for the case of region-II will be:

$$\frac{d^2\psi_2(x)}{dx^2} + \frac{8\pi^2m}{h^2}[E - V_0]\psi_2(x) = 0$$

Put  $\frac{8\pi^2m(E+V_0)}{h^2} = k_2^2$  ----- (4)

where  $k_2$  is the wave number.

$$\Rightarrow \frac{d^2\psi_2(x)}{dx^2} + k_2^2\psi_2(x) = 0$$

The characteristic solution of this equation will be:

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \quad \text{----- (5)}$$

In equation (5), the first term represents the transmitted wave. And the second term represents a wave coming from  $+\infty$  in the negative direction. Clearly, for  $x > 0$ , no particle can flow to region-I and D must be zero.

Therefore, the equation (5) becomes:

$$\psi_2(x) = Ce^{ik_2x} \quad \text{-----} \quad (6)$$

**iii) Continuity Statements at  $x = 0$**

The continuity of  $\psi$  implies that  $\psi_1 = \psi_2$  at  $x = 0$

$$\Rightarrow A + B = C \quad \text{-----} \quad (7)$$

Also the continuity  $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$  at  $x = 0$

$$\Rightarrow k_1(A - B) = k_2C \quad \text{-----} \quad (8)$$

Putting value of  $C$  in equation (8) from equation (7):

$$\begin{aligned} k_1(A - B) &= k_2(A + B) \\ \Rightarrow k_1A - k_1B &= k_2A + k_2B \\ \Rightarrow A(k_1 - k_2) &= B(k_1 + k_2) \\ \Rightarrow B &= \frac{(k_1 - k_2)}{(k_1 + k_2)}A \quad \text{-----} \quad (9) \end{aligned}$$

Putting value of  $B$  in equation (7), from equation (9):

$$\begin{aligned} C &= A + \frac{(k_1 - k_2)}{(k_1 + k_2)}A \\ C &= \left(\frac{2k_2}{k_1 + k_2}\right)A \quad \text{-----} \quad (10) \end{aligned}$$

It should be noted that  $A$  is the amplitude of incident beam, while  $B$  and  $C$  represent the amplitude of the reflected and transmitted beams, respectively.

Since the probability density associated with a wave function is proportional to the square of the amplitude of that function, we can represent the barrier transmission coefficient as:

$$T = \frac{|C|^2}{|A|^2}$$

And a reflection coefficient for the barrier surface at  $x = 0$  as:

$$R = \frac{|B|^2}{|A|^2}$$

**Case-2.  $E < V_0$**

**Region-I.**

When  $E$  is less than  $V_0$ , then solution of Schrodinger wave equation for region-I is:

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{8\pi^2mE}{h^2}\psi_1(x) = 0$$

$$\text{Put } \frac{8\pi^2mE}{h^2} = k_1'^2 \quad \text{-----} \quad (11)$$

where  $k$  is the wave number.

$$\Rightarrow \frac{d^2\psi_1(x)}{dx^2} + k_1'^2\psi_1(x) = 0$$



The characteristic solution of this equation will be:

$$\psi_1(x) = A'e^{ik_1x} + B'e^{-ik_1x} \quad \text{----- (12)}$$

The first and the second terms corresponds to the incident and reflected beams respectively.

**Region-II.**

When  $E$  is less than  $V_0$ , then solution of Schrodinger wave equation for region-II is:

$$\frac{d^2\psi_2(x)}{dx^2} + \frac{8\pi^2m}{h^2} [E - V_0]\psi_2(x) = 0$$

As  $V_0 > E$ , therefore the Schrodinger wave equation will become:

$$\frac{d^2\psi_2(x)}{dx^2} - \frac{8\pi^2m}{h^2} [V_0 - E ]\psi_2(x) = 0$$

Put  $\frac{8\pi^2m(V_0-E)}{h^2} = k'^2_2$  ----- (13)

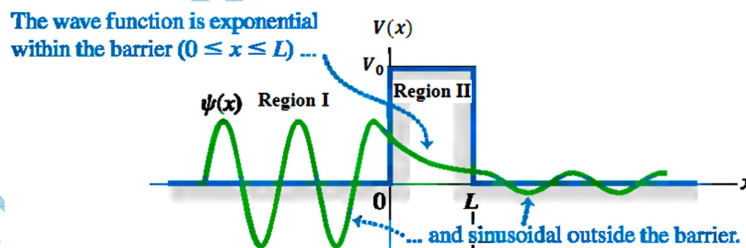
where  $k$  is the wave number.

$$\Rightarrow \frac{d^2\psi_2(x)}{dx^2} + k'^2_2\psi_2(x) = 0$$

The characteristic solution of this equation will be:

$$\psi'_2(x) = C'e^{k'_2x} + D'e^{-k'_2x} \quad \text{----- (14)}$$

The first and the second terms corresponds to the incident and reflected beams respectively. The equation 13 describes that there is always be a probability for a particle to move through a barrier.



**District Khushab**

