# Chapter 9

# Photon and Matter Waves

## Quantization of Energy

In black body radiation, it was considered that the radiation was emitted continuously. In 1902, Planck had shown that, the energy from the body, was emitted in separate packets of energy. The energy of each packet is equal to hf, called a quantum energy i.e. $E = hf$, where $h = 6.63 \times 10^{-34}$ J.S is the called Planck's constant and f is the frequency of radiation. This theory is called Planck's quantum theory.

Again in 1905, Einstein explained photoelectric effect using quantum theory. He suggested that light of frequency 'f' consist of packets or quanta of energy hf.

In general for 'n' number of photons, the total energy is

$$E_n = nhf, \; n = 0, 1, 2, 3 \ldots\ldots\ldots$$

This means, energy is emitted in the form of discrete amount i.e. quanta (singular form "quantum"). Energy is multiple of fundamental energy hf, so energy is quantized.

## Electrons and Matter waves: De-Broglie Equation

The successful explanation of compton effect, photoelectric effect and black body radiation shows that electromagnetic radiation travels not in the form of a continuous stream of energy but in the form of tiny packets or bundles of energy. These packets of energy were called 'quanta'. For electromagnetic radiation these were called photon.

On the other hand, the successful explanation of phenomenon like, reflection, refraction, interference, diffraction and polarization cannot be explained unless wave nature of electromagnetic radiation is assumed.

Louis de-Broglie in 1924 Suggested his hypothesis that there is 'wave particle dualism'. The wave associated with material particles is called 'matter wave'.

To show the wave particle dualism he made the use of Planck's theory of quantum radiation and Einstein theory of relativity.

According to Planck's theory of quantum radiation, Energy of photon is given by,

$$E = hf = \frac{hc}{\lambda} \qquad \ldots\ldots\ldots(1)$$

Where, h is Planck's constant and f is frequency of radiation.

Again according to Einstein mass energy relationship, energy of photon is given by,

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

'c' is the velocity of light

Comparing (1) and (2)

$$\frac{hc}{\lambda} = mc^2$$

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

[Where p = mc = momentum of photon]

According to de-Broglie the wave length 'λ', of the wave associated with a moving particle having momentum p = mv is given by,

$$\lambda = \frac{h}{mv} \quad \text{.........(3)}$$

### The de - Broglie Electron Wave

According to de-Broglie if an electron is accelerated to various velocities at various potential, different waves having different wavelengths are produced.

For de-Broglie matter wave we have,

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad \text{.....(1)}$$

If an electron of mass 'm' is accelerated through the potential 'V' and velocity v then,

$$\frac{1}{2}mv^2 = eV \Rightarrow v = \sqrt{\frac{2eV}{m}} \quad \text{.....(2)}$$

$$\text{Therefore, } \lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}}$$

$$\text{Wave length of electron wave, } \lambda = \frac{h}{\sqrt{2meV}}.$$

### Characteristics of de- Broglie Matter wave

1. Two different velocities are associated with a matter wave - one is mechanical velocity or group velocity (v) and other is velocity of each component wave called wave or phase velocity (u).
2. The wave velocity of de- Broglie wave is greater than the velocity of electro magnetic wave.
3. The velocity of de-Broglie wave is different for different matter (i.e. not constant as velocity of electromagnetic wave).
4. The wave length of de-Broglie matter wave varies inversely with the mass of the particles.



## Wave and Group Velocity

The wave packet accompanies the particle and tell us where the particle may be found. To describe a localized particle we must use a wave packet. According to de-Broglie, each particle of matter in motion is associated with a group of wave differ slightly in wavelength and frequency called wave packet. The velocity of this group of wave or wave packet which is quantitatively equal to mechanical velocity of the particle is called group velocity.

Let us, mix two traveling waves that differ slightly in wavelength and frequency.

$$\psi_1 = A \sin(kx - \omega t)$$

$$\psi_2 = A \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

where, $\Delta k << k$ and $\Delta\omega << \omega$

The resulting wave is given by

$$\psi(x, t) = \psi_1 + \psi_2$$

$$\psi(x, t) = A \sin(kx - \omega t) + A \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

$$= 2A \sin\frac{(kx - \omega t + kx + \Delta k.x - \omega t - \Delta\omega.t)}{2} \cos\frac{(kx - \omega t - kx - \Delta k.x + \omega t + \Delta\omega.t)}{2}$$

$$= 2A \cos\frac{(\Delta\omega.t - \Delta k.x)}{2} \sin\frac{(2kx + \Delta k.x - 2\omega t - \Delta\omega.t)}{2}$$

since $\cos(-A) = \cos A$, and $\Delta k << k$ and $\Delta\omega << \omega$

$$\psi(x, t) = 2A \cos\frac{(\Delta k.x - \Delta\omega.t)}{2} \sin(kx - \omega t) \quad \text{.... (1)}$$

The resulting wave is thus the product of two traveling waves. The second term of equation (1) represents a wave having nearly the same frequency and wavelength as the original waves. The first term of equation (1) represents a wave having mach larger wave length (since $\lambda = \frac{2\pi}{\Delta k}$, $\Delta k$ is very small) and much smaller frequency. We can consider ψ as a wave similar to the original ones except that its amplitude, $2A\cos\frac{(\Delta k.x - \Delta\omega.t)}{2}$, is periodically varying forming the envelopes as shown in figure.

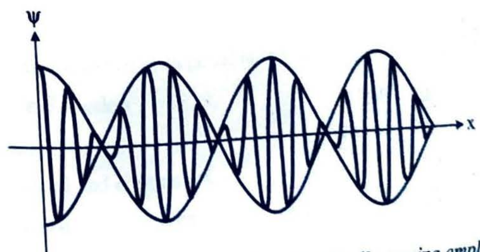



*Figure: A snapshot of a wave with a periodically varying amplitude.*

Each envelopes includes a group of wave, or a wave packet. Such a $\psi$ could be used to describe a beam of particles with one particle in each group.

This group of wave consist of different component waves. The velocity with which each component wave propagates is called phase or wave velocity. It is given by, $v = \frac{\omega}{k}$.

The envelopes (or the wave packets) travel with a velocity called the group velocity and is given by

$$v_{group} = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk} \qquad \text{.... (2)}$$

Since, $E = hf = \frac{h}{2\pi} \cdot 2\pi f = \hbar\,\omega$ and $p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k$

Equation (2) can be rewritten as

$$v_{group} = \frac{d\omega}{dk} = \frac{d(\hbar\omega)}{d(\hbar k)} = \frac{dE}{dP} \qquad \text{.... (3)}$$

We know that, for a particle of mass 'm' and velocity v,

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

Therefore, $v_{group} = \frac{dE}{dP} = \frac{d}{dP}\left(\frac{P^2}{2m}\right) = \frac{2P}{2m} = \frac{P}{m} = \frac{mv}{m}$

$$v_{group} = v$$

Therefore, the group velocity is equal to the particle velocity. From this result it can be concluded that the wave packet moves along with the particle.

**Relation Between group velocity and phase velocity**

We know

Wave vector $k = \frac{2\pi}{\lambda}$

$$\frac{dk}{d\lambda} = \frac{-2\pi}{\lambda^2}$$

and, $\omega = 2\pi f = \frac{2\pi u}{\lambda}$ [Since phase velocity, $u = f\lambda$]

$$\frac{d\omega}{d\lambda} = \frac{-2\pi u}{\lambda^2} + \frac{2\pi}{\lambda}\frac{du}{d\lambda}$$

Now, Group velocity, $v = \frac{d\omega}{dk} = \frac{d\omega/d\lambda}{dk/d\lambda}$

$$= \frac{-\lambda^2}{2\pi}\left(\frac{-2\pi u}{\lambda^2} + \frac{2\pi}{\lambda}\frac{du}{d\lambda}\right)$$

$$v = u - \lambda\frac{du}{d\lambda}$$



This is the relation between wave velocity (u) and group velocity v. This shows that wave velocity is always greater than group velocity.

## Wave Function and its Significance

A simple harmonic wave is represented by the equation, $y = a\sin(\omega t - kx)$. In such type of wave motion there is only the transfer of energy, but incase of matter wave, there is transfer of momentum (particle) in addition to the energy. The suitable function to represent wave function for matter wave is

$$\psi(x,t) = Ae^{-i(\omega t - kx)} \qquad \text{..... (1)}$$

Where A is called normalizing constant.

Since $E = \hbar\omega \Rightarrow \omega = \frac{E}{\hbar}$ and $P = \hbar k \Rightarrow k = \frac{P}{\hbar}$

Therefore, equation (1) can be rewritten as,

$$\psi(x,t) = Ae^{-i/\hbar(Et - Px)} \qquad \text{..... (2)}$$

The wave function $\psi$ has no physical meaning itself. When it is operated by Schrodinger wave equation, it describes the motion of the particle associated with it, as done by second law of motion in classical mechanics.

The only quantity having the physical meaning is the square of its magnitude. The quantity $P = |\psi|^2$ evaluated at a particular point at a particular time is proportional to the probability of finding the particle there at that time.

The probability of finding a particle in the volume element dx dy dz is $|\psi|^2$ dx dy dz or $|\psi|^2$ dv.

Since the total probability of finding the particle in the entire space is unity.

$$\int |\psi|^2 dv = \int \psi^* dv = 1.$$

Where, $\Psi^*$ is complex conjugage of $\psi$.

The wave function satisfying this condition is called normalized wave function. Every acceptable wave function can be normalized by multiplying it with an appropriate constant called normalizing constant.

If the product of a function $\psi_1(x)$ and the complex conjugate $\psi_2^*(x)$ of another function $\psi_2(x)$ vanishes when integrated with respect to x over a interval $a \le x \le b$, i.e. if,

$$\int_a^b \psi_1(x)\,\psi_2^*(x)\,dx = 0$$

Then $\psi_1(x)$ and $\psi_2(x)$ are said to be orthogonal in the interval (a, b).

**Characteristics of Wave Function**

1. It must be normalized.
2. It must be single valued and continuous.
3. If $\psi_1(x)$, $\psi_2(x)$ ........$\psi_n(x)$ are solution of Schrödinger wave equation (SWE) then the linear combination, $\psi(x) = a_1\psi_1(x) + a_2\psi_2(x) + ..... + a_n\psi_n(x)$ must be solution of SWE.
4. The wave function $\psi(x)$ must approach zero as $x \rightarrow \pm\infty$.

## Schrödinger Wave Equation

### Time Independent Schrödinger Equation

Schrödinger wave equation describes the motion of quantum mechanical particle as Newton's second law in classical mechanics.

The wave function for quantum mechanical particle is given by.

$$\psi(x,t) = A e^{-i(\omega t - kx)} = A e^{-\frac{i}{\hbar}(Et - Px)} \quad .....(1)$$

Differentiating this equation w.r.t. x

$$\frac{d\psi}{dx} = A\frac{iP}{\hbar} e^{-\frac{i}{\hbar}(Et - Px)} = \frac{iP}{\hbar}\psi$$

$$\text{or,} \quad P\psi = \frac{\hbar}{i}\frac{d\psi}{dx} = \frac{-i^2\hbar}{i}\frac{d\psi}{dx} = -i\hbar\frac{d\psi}{dx}$$

$$\text{Momentum operator } P = -i\hbar\frac{d}{dx} \quad ....(2)$$

Similarly, differentiating equation (1) two times with respect to x we get

$$\frac{d^2\psi}{dx^2} = \left(\frac{iP}{\hbar}\right)^2 \psi$$

$$P^2\psi^2 = -\hbar^2\frac{d^2\psi}{dx^2} \quad .....(3)$$

Consider a particle of mass m and potential energy 'V', moving with velocity v, then the total energy is given by.

$$E = \frac{1}{2}mv^2 + V = \frac{1}{2}\frac{(mv)^2}{m} + V = \frac{P^2}{2m} + V$$

Multiplying this equation with $\psi$,

$$\left(\frac{P^2}{2m} + V\right)\psi = E\psi$$

$$\Rightarrow -\frac{h^2}{2m}\frac{d^2\psi}{dx} + V\psi = E\psi$$

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

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

This is the time independent Schrödinger wave equation in one dimension.

### Time Dependent Wave Equation

The wave function describing the quantum mechanical particle is given by,

$$\psi(x,t) = A e^{-i/\hbar}(Et - Px) = \psi$$



Differentiating w.r.t. t

$$\frac{d\psi}{dt} = \frac{-iE}{\hbar} A e^{(-i/\hbar)(Et - Px)} = -\frac{iE}{\hbar}\psi$$

$$\Rightarrow E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt}$$

$$\text{or,} \quad E\psi = i\hbar\frac{d\psi}{dt} \quad ............(1)$$

Consider a particle of mass m and potential energy V, moving with a velocity, v then the total energy of the system is

$$E = K + U = \frac{1}{2}mv^2 + V = \frac{P^2}{2m} + V$$

Multiplying this equation both sides by $\psi$

$$E\psi = \frac{P^2\psi}{2m} + V\psi \quad ............(2)$$

From (1) and (2)

$$\left(\frac{P^2}{2m} + V\right)\psi = i\hbar\frac{d\psi}{dt}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = i\hbar\frac{d\psi}{dt} \quad ............(3)$$

The term $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]$ is recognized as Hamiltonian operator

$$\text{i.e. } H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V$$

Equation (3) can be rewritten as,

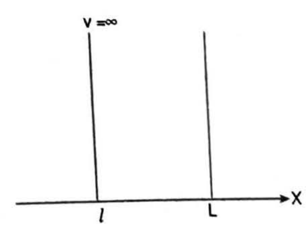
$$H\psi = i\hbar\frac{d\psi}{dt} \quad .............(4)$$

which is the time dependent Schrodinger wave equation

**Application of Schrodinger wave equation**

**1. A particle in an one dimensional infinitely deep potential well**

Consider a particle restricted to move along the x-axis between x = 0 and x = *l*. The potential energy V of the particle is zero inside the box, but rises to infinity on the outside.



i.e. $V = 0$ for $0 < x < l$

and $V = \infty$ for $x < 0$ and $x > l$

In such case the particle is said to be moving in an infinitely deep potential well.

The Schrödinger wave equation for the particle with in the box (V = 0) is.

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{.............(1)}$$

$$\text{let } k^2 = \frac{2mE}{\hbar^2} \quad \text{..............(2)}$$

$$\text{Therefore, } \frac{d^2\psi}{dx^2} + k^2\psi = 0$$

The solution of the equation is,

$$\psi(x) = A \sin kx + B \cos kx \text{ ....(3)}$$

where A and B are constants to be determined using boundary conditions.

Since the particle cannot have infinite energy, it cannot exist out side the box. Therefore, the wave function $\psi$ must be zero outside the box, or $\psi$ must be zero at the walls, i.e. at $x = 0$ and $x = l$

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

From equation (3)

$\Rightarrow 0 = 0 + B \Rightarrow B = 0$

Now equation (3) becomes, $\psi(x) = A\sin kx$.

Again, $\psi(x) = 0$ at $x = l$

$\Rightarrow 0 = A \sin kl$

$\Rightarrow \sin kl = 0$

$\Rightarrow \sin kl = \sin n\pi$, n = 0, 1, 2, 3...

$\Rightarrow kl = n\pi$

$$\Rightarrow k = \frac{n\pi}{l} \quad \text{...........(3)}$$

From equation (2) and equation (4), $\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{l^2}$

$$\Rightarrow E = \frac{n\pi^2\hbar^2}{2ml^2}, \; n = 1, 2, 3, 4, \ldots \quad \text{...........(4)}$$

This means the energy of particle in potential well is quantized. Each value of energy given by (4) is called eigen value and corresponding function is called eigen function.

Now substituting, $B = 0$ and $k = n\pi/l$ in equation (3), the allowed solutions of Schrödinger equation are.

$$\psi_n(x) = A \sin\frac{n\pi x}{l}$$



The coefficient A is called normalizing constant and can be determined using normalizing condition.

$$\int_0^l \psi\psi^* \, dx = 1$$

$$A^2 \int_0^l \sin^2\frac{(n\pi x)}{l} dx = 1$$

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

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

$$A^2 . \frac{l}{2} = 1$$

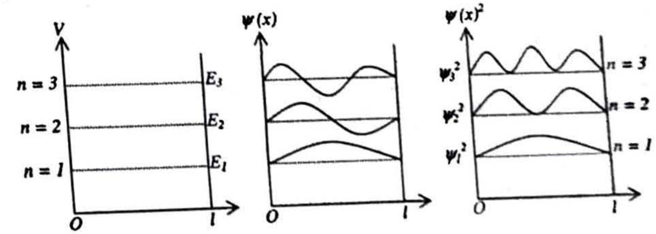
$$A = \sqrt{\frac{2}{l}}.$$

The normalized wave functions of the particles are therefore

$$\psi_n(x) = \sqrt{\frac{2}{l}} \sin\frac{n\pi x}{l}.$$

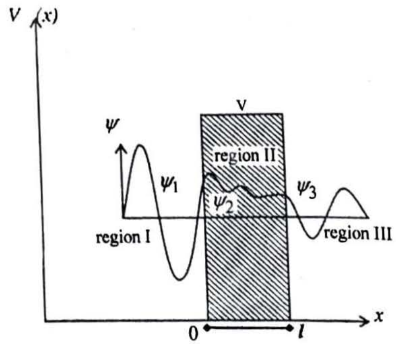
The first three eigen functions, $\psi_1$, $\psi_2$, $\psi_3$ together with the probability densities $|\psi_1|^2$, $|\psi_2|^2$, $|\psi_3|^2$ are shown in figure below.

It is obvious that the wave mechanical result is very different from the classical result. Classical mechanics predicts the same probability for the particle being any where in the box. But quantum mechanics predicts that the probability is different at different point.




2. **Barrier Tunneling**

Consider a barrier of potential V having width 'l'. When a moving particle of energy E < V be incident on the barrier from the left of region I, classically region II and III are forbidden to particle. But for quantum mechanics all regions are accessible to the particle. This is because, for relatively narrow barrier, in short time, the particle can allow to cross it. This effect of quantum mechanical particle is called barrier tunneling.




The potential function for the particle can be expressed as

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

The Schrödinger equation and their solutions for these region are as follows.

For region I

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

$$\text{or, } \frac{d^2\psi_1}{dx^2} + k_1^2\,\psi_1 = 0 \text{ where, } k_1^2 = \frac{2mE}{\hbar^2}$$

and the solution of this equation is

$$\psi_1 = Ae^{ik_1x} + B\,e^{-ik_1x} \qquad \text{.......(1)}$$

For region II, $\frac{d^2\psi_2}{dx^2} + \frac{2m\,(E-V)}{\hbar^2}\psi_2 = 0$

$$\text{or, } \frac{d^2\psi_2}{dx^2} - \frac{2m\,(V-E)}{\hbar^2}\psi_2 = 0$$

$$\text{or, } \frac{d^2\psi_2}{dx^2} - k_2^2\,\psi_2 = 0\text{, where } k_2^2 = \frac{2m\,(V-E)}{\hbar^2}$$

The solution of this equation is

$$\psi_2 = Ce^{k_2x} + De^{-k_2x} \qquad \text{.........(2)}$$

For region III, $\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$

$$\text{or, } \frac{d^2\psi_3}{dx^2} + k_1^2\,\psi_3 = 0 \text{ where } k_1^2 = \frac{2mE}{\hbar^2}$$

The solution of this equation is

$$\psi_3(x) = Fe^{ik_1x} + Ge^{-k_1x}$$



Since there is no reflected wave in region (III) so, the second term in the right side of expression for $\psi_3$ is zero.

$$\text{Therefore, } \psi_3(x) = Fe^{ik_1x} \qquad \text{.........(3)}$$

Using boundary conditions, at x = 0

$$\psi_1\big|_{x=0} = \psi_2\big|_{x=0}$$
$$A + B = C + D \qquad \text{.......(4)}$$

and $\psi'_1\big|_{x=0} = \psi'_2\big|_{x=0}$

$$ik_1 A - ik_1 B = k_2 C - k_2 D$$
$$A - B = \frac{k_2}{ik_1}(C - D) \qquad \text{.........(5)}$$

Adding equation (4) and (5)

$$2A = \left(1 + \frac{k_2}{ik_1}\right)C + \left(1 - \frac{k_2}{ik_1}\right)D \qquad \text{.........(6)}$$

Again using the boundary conditions at x = $l$

$$\psi_2\big|_{x=l} = \psi_3\big|_{x=l}$$
$$Ce^{k_2l} + De^{-k_2l} = Fe^{ik_1l} \qquad \text{....(7)}$$

and $\psi'_2\big|_{x=l} = \psi'_3\big|_{x=l}$

$$Ck_2\,e^{k_2l} - Dk_2e^{-k_2l} = F(ik_1)e^{ik_1l}$$
$$Ce^{k_2l} - De^{-k_2l} = \left(\frac{ik_1}{k_2}\right)Fe^{ik_1l} \qquad \text{.......(8)}$$

Adding equation (7) and (8)

$$2Ce^{k_2l} = \left(1 + \frac{ik_1}{k_2}\right)F\,e^{ik_1l}$$
$$\text{or, } 2C = \left(1 + \frac{ik_1}{k_2}\right)Fe^{ik_1l}\,e^{-k_2l} \qquad \text{........(9)}$$

and subtracting equation (8) from (7)

$$2De^{-k_2l} = \left(1 - \frac{ik_1}{k_2}\right)Fe^{ik_1l}$$
$$2D = \left(1 - \frac{ik_1}{k_2}\right)Fe^{ik_1l}\,.\,e^{k_2l} \qquad \text{.....(10)}$$

Multiplying equation (6) both sides by 2 and substituting the value of 2C and 2D from (9) and (10)

$$\frac{4A}{F} = \left(1 + \frac{k_2}{ik_1}\right)\left(1 + \frac{ik_1}{k_2}\right)e^{ik_1l}\,.\,e^{-k_2l} + \left(1 - \frac{k_2}{ik_1}\right)\left(1 - \frac{ik_1}{k_2}\right)e^{ik_1l}\,e^{k_2l}$$

$$\frac{4A}{F}e^{-ik_1l} = \left(1-\frac{ik_2}{k_1}\right)\left(1+\frac{ik_1}{k_2}\right)e^{-k_2l} + \left(1+\frac{ik_2}{k_1}\right)\left(1-\frac{ik_1}{k_2}\right)e^{k_2l}$$

$$\frac{4A}{F}e^{-ik_1l} = \frac{(k_1-ik_2)(k_2+ik_1)e^{-k_2l}}{k_1k_2} + \frac{(k_1+ik_2)(k_2-ik_1)}{k_1k_2}e^{k_2l}$$

or, $$\frac{4A}{F} = \frac{e^{ik_1l}}{k_1k_2}[(k_1k_2+ik_1^2-ik_2^2+k_1k_2)e^{-k_2l}+(k_1k_2-ik_1^2+ik_2^2+k_1k_2)e^{k_2l}]$$

$$= \frac{e^{ik_1l}}{k_1k_2}[\{2k_1k_2+i(k_1^2-k_2^2)\}e^{-k_2l}+\{2k_1k_2-i(k_1^2-k_2^2)\}e^{k_2l}]$$

$$\frac{4A}{F} = \frac{e^{ik_1l}}{k_1k_2}[2k_1k_2(e^{-k_2l}+e^{k_2l})+i(k_1^2-k_2^2)(e^{-k_2l}-e^{k_2l})]$$

$$\frac{2A}{F} = \frac{e^{ik_1l}}{k_1k_2}\left[2k_1k_2\left(\frac{e^{k_2l}+e^{-k_2l}}{2}\right)-i(k_1^2-k_2^2)\left(\frac{e^{k_2l}-e^{-k_2l}}{2}\right)\right]$$

$$= \frac{e^{ik_1l}}{k_1k_2}[2k_1k_2\cos h\, k_2l - i(k_1^2-k_2^2).\sin h\, k_2l]$$

$$\frac{A}{F} = e^{ik_1l}\left[\cos h\, k_2l - \frac{i(k_1^2-k_2^2)}{2k_1k_2}\sin hk_2l\right]$$

or, $$\frac{F}{A} = \frac{e^{-ik_1l}}{\cos h\, k_2l - i\dfrac{(k_1^2-k_2^2)}{2k_1k_2}\sin hk_2l} \qquad \text{.......... (11)}$$

The probability of tunneling is described by transmission coefficient. It represents the probability that the particle penetrates to the other side of the barrier and it is defined by

$$T = \left|\frac{F}{A}\right|^2 = \left(\frac{F}{A}\right)\left(\frac{F}{A}\right)^*$$

$$T = \frac{e^{-ik_1l}}{\cos hk_2l - i\dfrac{(k_1^2-k_2^2)}{2k_1k_2}\sin hk_2l} \times \frac{e^{ik_1l}}{\cos h\, k_2l + \dfrac{i(k_1^2-k_2^2)}{2k_1k_2}\sin h\, k_2l}$$

$$= \frac{1}{\cos h^2 k_2l + \dfrac{(k_1^2-k_2^2)^2}{4k_1^2k_2^2}\sin h^2 k_2l}$$

$$= \frac{4k_1^2k_2^2}{4k_1^2k_2^2\cos h^2 k_2 l + (k_1^2-k_2^2)^2\sin h^2 k_2l}$$

or, $$T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2\cos h^2 k_2l + (k_1^4+k_2^4-2k_1^2k_2^2)\sin h^2 k_2l}$$

$$= \frac{4k_1^2k_2^2}{4k_1^2k_2^2\cos h^2 k_2l + (k_1^4+k_2^4+2k_1^2k_2^2-4k_1^2k_2^2)\sin h^2 k_2l}$$

$$= \frac{4k_1^2k_2^2}{4k_1^2k_2^2(\cos h^2 k_2l - \sin h^2 k_2l) + (k_1^2+k_2^2)^2\sin h^2 k_2l}$$



$$= \frac{4k_1^2k_2^2}{4k_1^2k_2^2 + (k_1^2+k_2^2)^2\sin h^2 k_2l}$$

Using $k_1^2 = \frac{2mE}{\hbar^2}$ and $k_2^2 = \frac{2m(V-E)}{\hbar^2}$

$$T = \frac{\left(\dfrac{2m}{\hbar^2}\right)^2.4E(V-E)}{\left(\dfrac{2m}{\hbar^2}\right)^2[4E(V-E)+(E+V-E)^2.\sin h^2 k_2l]}$$

$$T = \frac{4E(V-E)}{4E(V-E)+V^2\sinh^2 k_2l} \qquad \text{...........(12)}$$

If the width of potential is very large, the term 4E (V - E) in the denominator of equation (12) can be neglected in comparison to $V^2 \sin h^2 k_2l$

And $\sin h\, k_2l = \frac{e^{k_2l}-e^{-k_2l}}{2} \approx \frac{e^{k_2l}}{2}$ for large '$l$'.

Equation (12) can be written as

$$T = \frac{4E(V-E)}{V^2\left(\dfrac{e^{k_2l}}{2}\right)^2} = \frac{16E(V-E)}{V^2}e^{-2k_2l}$$

$$T = \frac{16E(V-E)}{V^2}e^{-2k_2l} \qquad \text{...........(13)}$$

Equation (13) gives the probability of tunneling of the particle through potential barrier of width '$l$' and height V.

The reflection coefficient or the probability of refection of the particle at the barrier is given by.

$$R = \left|\frac{B}{A}\right|^2 = 1 - T$$

This is the superiority of quantum mechanics over the classical mechanics which shows that there is finite probability of emission of electron (β - emission) from the nucleus of an atom even the electron has lower energy than the energy by which it is bounded.

## Solved Examples

1. **A ball of mass 10 gm has velocity 100 cm/sec. Calculate the wave length associated with it. Why does not this wave nature show up our daily observations. Given, h = 6.62 ×10$^{-34}$ JS.**

***Solution:***

Here, m = 10 gm = 10 ×10$^{-3}$ kg, h = 6.62×10$^{-34}$ Js

We have,

$$\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}}{10\times10^{-3}\times1} = 6.62\times10^{-32}\text{ m}$$

This wavelength is much smaller than the dimensions of the balls therefore in such cases wave - like properties of matter can not be observed in our daily observations.

2. **Calculate the wave length associated with an electron subjected to a potential difference of 1.25 KV.**

***Solution:***

We have,

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

$$\text{Now, } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}} = \frac{6.62\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.6\times10^{-19}\times1.25\times10^{3}}}$$

$$\lambda = 0.347A^{\circ}$$

3. **Show that wave velocity is greater than velocity of light**

***Solution:***

We have, wave velocity, $u = f\lambda$

From Planck's law and Einstein's mass energy relation.

$$hf = mc^2$$

$$f = \frac{mc^2}{h}$$

Substituting f for u

$$u = \frac{mc^2}{h}.\lambda = \frac{mc^2}{h}\cdot\frac{h}{mv} = \frac{c^2}{v}$$

$$c^2 = uv$$

Since particle velocity (v) must be less than velocity of light (c), so wave velocity (u) is greater than velocity of light.

4. **Find the energy of the neutron in units of electron - volt whose de - Broglie wave length is 1A°. Given mass of neutron = $1.674\times10^{-27}$ kg, h = $6.62\times10^{-34}$ joule-sec.**

***Solution:***

Here, $\lambda = 1\ A^{\circ} = 1\times10^{-10}$ m, $m = 1.674\times10^{-27}$kg, $h = 6.62\times10^{-34}$ Joule / sec.

$$\text{We have, } E = \frac{1}{2}mv^2$$

$$\text{Also, } \lambda = \frac{h}{mv} \Rightarrow v = \frac{h}{m\lambda}$$

$$\text{Therefore, } E = \frac{1}{2}m\frac{h^2}{m^2\lambda^2} = \frac{h^2}{2m\lambda^2}$$

$$= \frac{(6.62\times10^{-34})^2}{2\times1.674\times10^{-27}\times(1\times10^{-10})^2}$$

$$= 1.3\times10^{-20}\text{ joule}$$

$$= \frac{1.3\times10^{-20}}{1.6\times10^{-19}} = 8.13\times10^{-2}\text{ eV}$$



5. **Show that group velocity is equal to particle velocity.**

The group velocity is given by

$$v_g = \frac{d\omega}{dk} = \frac{d(\hbar\omega)}{d(\hbar k)} = \frac{dE}{dP}\quad\left[\text{Since } E = hf = \frac{h}{2\pi}.2\pi f = \hbar\omega \text{ and } p = \frac{h}{\lambda} = \frac{h}{2\pi}.\frac{2\pi}{\lambda} = \hbar k\right]$$

$$\text{Since, } E = \frac{p^2}{2m}\text{ for free particle}$$

$$\text{Since, } v_g = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{2P}{m} = \frac{mv}{m} = v = \text{particle velocity.}$$

6. **An electron is confined to an infinite height box of size 0.1 nm. Calculate the ground state energy of the electron. How this electron can be put to the third energy level.**

***Solution:***

The energy of the particle in one dimensional rigid box of side $l$ is given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ml^2} = \frac{n^2h^2}{8ml^2} = \frac{(6.62\times10^{-34})^2\times n^2}{8\times9.1\times10^{-31}\times(10^{-10})^2}$$

$$= 6.03\times10^{-18}n^2\text{ joule}$$

$$= 37.7\ n^2\text{ eV}$$

In the ground state, $n = 1$, $E_1 = 37.7$ eV

For third energy level, $n = 3$, $E_3 = 37.7\times3^2 = 37.7\times9$ eV

$\therefore E_3 - E_1 = (9-1)\times37.7 = 301.5$ eV

Hence to put the electron to third energy level an extra energy of 301.5 ev is to be given.

7. **What voltage must be applied to an electron microscope to produce electrons of wave length 0.50 A°? Given, e = $1.6\times10^{-19}$ Coulomb, m = $9.0\times10^{-31}$ kg, h = $6.62\times10^{-34}$ Joule.sec.**

***Solution:***

$$\text{We have, } \frac{1}{2}mv^2 = eV$$

$$V = \frac{mv^2}{2e}$$

$$\text{The de-Broglie wavelength is given by, } \lambda = \frac{h}{mv} \Rightarrow v = \frac{h}{m\lambda}$$

$$\text{Therefore, } V = \frac{m}{2e}\cdot\frac{h^2}{m^2\lambda^2} = \frac{h^2}{2me\lambda^2}$$

$$= \frac{(6.62\times10^{-34})^2}{2\times9.1\times10^{-31}\times1.6\times10^{-19}\times(0.5\times10^{-10})^2}$$

$$= 602\text{ Volts.}$$

8. **The wave function of a particle confined in a box of length $l$ is $\psi(x) = \sqrt{\frac{2}{l}}\sin\frac{\pi x}{l}$.**

**Calculate the probability of finding the particle in the region $0 < x < \frac{l}{2}$.**

***Solution:***

The probability of finding the particle in the length 0 to $\frac{l}{2}$ is

$$P = \int_0^{l/2} (\psi)^2\,dx = \frac{2}{l}\int_0^{l/2} \sin^2\frac{\pi x}{l}\,dx$$

$$= \frac{1}{l}\int_0^{l/2} \left(1-\cos\frac{2\pi x}{l}\right) dx$$

$$= \frac{1}{l}\cdot\frac{l}{2} = \frac{1}{2} = 0.5$$

**9. Calculate the probability of transmission of $\alpha$ – particle through the rectangular barrier indicated below. Height of barrier V = 2 eV, energy of $\alpha$ particle, E = 1eV, barrier width, $l$ = 1A°, mass of $\alpha$ particle, m = $6.4\times10^{-27}$ kg.**

***Solution:***

We have,

Transmission probability, $T = \frac{16\,E\,(V-E)}{V^2}\,e^{-2k_2 l}$

Where, $k_2 = \sqrt{\frac{2m(V-E)}{\hbar^2}}$

Here, $\frac{16\,E(V-E)}{V^2} = \frac{16\times1\times1.6\times10^{-19}\times(2-1)\times1.6\times10^{-19}}{(2\times1.6\times10^{-19})^2}$

$= 4$

and $k_2 = \sqrt{\frac{2\times6.4\times10^{-27}\times(2-1)\times1.6\times10^{-19}}{(1.05\times10^{-34})^2}}$

$= 4.3\times10^{11}$

Now, $2k_2 l = 2\times4.3\times10^{11}\times1\times10^{-10} = 86.2$

Therefore $T = 4e^{-86.2}$

$= 1.465\times10^{-37}$

**10. Normalize the one dimensional wave function**

$$\Psi = A\sin\left(\frac{\pi x}{a}\right), 0 < x < a$$

$$= 0 \qquad \text{, outside}$$

**Solution.**

We have normalizing condition

$$\int_{-\infty}^{\infty} |\Psi|^2\,dx = 1$$



or $\int_0^a A^2\sin^2\frac{\pi x}{a}\,dx = 1$

or $\frac{A^2}{2}\int_0^a\left(1-\cos\frac{2\pi x}{a}\right)dx = 1$

or $\frac{A^2}{2}\cdot a = 1$

$\therefore\ A = \sqrt{\frac{2}{a}}$

Hence the normalized wave function is $\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}$.

**11. An electron moving is a wave has wave function $\Psi$ (x) = 2 sin2$\pi$x. Find the probability of finding the electron in the region x = 0.25 to 0.5 m.**

**Solution.**

The probability of finding the electron in given region is,

$$P = \int_{0.25}^{0.5} \Psi\,\Psi^*\,dx = \int_{0.25}^{0.5} 4\sin^2 2\pi x\,dx$$

$$P = 2\int_{0.25}^{0.5} 2\sin^2 2\pi x\,dx$$

$$= 2\int_{0.25}^{0.5} (1-\cos 4\pi x)$$

$$= 2\left[\int_{0.25}^{0.5} dx - \int_{0.25}^{0.5}\cos 4\pi x\,dx\right]$$

$$= 2\left[(x)\Big|_{0.25}^{0.5} - \frac{\sin 4\pi x}{4\pi}\Big|_{0.25}^{0.5}\right]$$

$= 2\,[(0.5-0.25)-0]$

$= [0.25-0]$

$= 0.5$

**12. A particle is moving in 1–D box of infinite potential. Evaluate the probability of finding the particle within range 1 Å at the centre of box when it is in lowest energy state.**

**Solution.**

$L = 1$ Å$= 1 \times 10^{-10}$ m

We have, wave function for the particle in infinite potential well

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

At the centre, $x = \frac{L}{2} = 0.5$ Å and for lowest energy state, $n = 1$.

Then,

$$\text{Probability} = \left(\sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\right)^2$$

$$= \left|\sqrt{\frac{2}{L}} \sin\frac{\pi}{2}\right|^2$$

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

The probability in the interval $\Delta x$ is, $P = |\Psi_1(x)|^2 \Delta x = \left(\frac{2}{L}\right) \Delta x = \frac{2 \times 0.5 \times 10^{-10}}{1 \times 10^{-10} \text{ m}} = 1$

## Exercise

1. What is wave function? Describe it's significance. Derive Schrodinger time dependent wave equation for a free particle like electron.
2. Determine the total energy of a particle using Schrodinger equation, when the potential energy has value $v = 0$ for $0 < x < a$ and $v = \infty$ for $x \leq 0$ and $x \geq a$.
3. Prove that energy levels are quantized, when the electron is confined in an infinite potential well of width 'a'.
4. What is barrier tunneling? Discuss and write the Schrodinger wave equation in each regions. Also write formula of transmission coefficient, T in this case.
5. Derive an expression for the energy of a particle in an one dimensional infinite deep potential well.
6. An electron is trapped in an one dimensional infinite potential well of width 'a' such that.

   $v = \infty$ for $x \leq 0$ and $x \geq a$

   $v = 0$ for $0 < x < a$



   Using boundary condition, prove that the total potential energy of system is $E = \frac{n^2 \pi^2 \hbar^2}{2ml^2}$.

   where symbols carry their usual meaning.

7. Discuss the significance of the wave function and deduce the time independent schrodinger equation.
8. A particle is confined in a box of width L. Find an expression for energy eigen value to show that the particle can have only discrete energy and momentum.
9. Define tunneling effect and derive the expression for reflection and transmission coefficient for a barrier of width 'a' and potential of height $V_0$.
10. 'Quantum mechanics is superior to the classical mechanics' support this statement explaining burrier tunneling.
11. Calculate the de-Broglie wavelength of neutron of energy 28.8eV, $h = 6.62 \times 10^{-34}$ Joule-sec, $m = 1.67 \times 10^{-27}$ kg.
12. Calculate the energy in electrn volt of an electron wave of $\lambda = 3 \times 10^{-2}$ m, Given $h = 6.62 \times 10^{-34}$ JS.
13. Calculate the de Broglie wave length of an $\alpha$ - particle accelerated through a potential difference of 2000 volts. Given mass of proton $= 1.67 \times 10^{-27}$ kg

    Plancks constant $= 6.62 \times 10^{-34}$ Joule-sec
14. Calculate the energy difference between the ground state ($n = 1$) and the first excited state for an electron in one dimensional rigid box of length 1 A°.
15. A beam of electron having energy of 3eV is incident on a potential barrier of height 4 eV. If the width of the barrier is 20 A°, Calculate the transmission probability.
16. An electron has a wave length 0.2 nm. What are the momentum and energy of electron.
17. An $\alpha$-particle is trapped in a nucleus whose radius is $1.4 \times 10^{-5}$m. What is the probability that an $\alpha$-particle will escape from the nucleus if its energy is 2 meV? The potential barrier at the surface of the nucleus is 4 meV.
18. Find the minimum energy of an electron in a box of width 2A°.
19. An electron with kinetic energy 5 eV is incident on a barrier height 10 eV. Calculate the probability that an electron (a) will tunnel through the barrier and (b) will be reflected?
20. Normalize the wave-function $\psi(x)$ given by $\psi(x) = A \sin\frac{\sin 2n\pi x}{l}$ in the region $0 \leq x, \leq l$.
21. The energy of an electron constrained to move in one dimensional box of length 4.0 A° is $9.664 \times 10^{-17}$J. Find out the order of excited state and the momentum of electron in that state.

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