

Module-II

Quantum Physics

PART-B Long Answer Questions

1. Compare a particle with a wave and discuss about dual nature of radiation.

Ans. Wave:-

- A wave is not located at a definite point, instead it is spread out over a relatively large region of space.
- A wave is nothing but spreading of disturbance in a medium. The characteristics/properties of waves are 1) Amplitude (A) 2) Time period 3) Frequency (ν) 4) Wavelength (λ) 5) Phase velocity (v) 6) Intensity (I).
- Generally, the displacement regarding wave is

$$y = A \sin \omega t.$$

Particle:-

- It has mass and is located at a definite point, and can move from one place to another. It gives energy when slowed down or stopped.
- The particle is specified by 1) Mass (m) 2) velocity (v) 3) Momentum (P) 4) Energy (E) etc.
- The motion of particle can be explained by Newton's second law of motion

$$F = dP/dt = m dv/dt = ma.$$

Radiation: Wave-Particle Duality

- The photo electric effect and the Compton Effect established that light behaves as a flux of photons.
- On the other hand, the phenomena of interference, diffraction and polarization can be explained only when light is treated as a continuous wave.
- Neither of the modes can separately explain all the experimental facts.
- The particle nature and wave nature appear mutually exclusive.
- So, Light exhibits both wave nature and particle nature i.e., called as wave-particle duality.

2. Enlist physical significance of wave function according to Schrodinger and Max –Born Interpretation

Ans. Physical Significance of wave function:

Wave function is a mathematical tool used in quantum mechanics to describe any physical system and it is denoted by ' Ψ '.

- ❖ The wave nature of matter introduced an uncertainty in the location of the position of the particle because a wave cannot be set exactly at this position (or) at that position.
- ❖ The amplitude of the wave tells us about the probability of finding particle in space at a particular instant. A large wave amplitude means a large probability of finding the particle at that position.
- ❖ Mathematically, to explain it, scientists introduced a new physical quantity called wave function.
- ❖ It is a variable quantity i.e., associated with a moving particle at any position (x,y,z) and time t and it relates probability of a finding the particle at that point and time.
- ❖ It must be well behaved it is single valued and continuous everywhere.
- ❖ It is a complex quantity and individually has no meaning.
- ❖ To explain it, Max Born suggested a new idea about the physical significance of Ψ which is generally accepted now a days.
- ❖ According to Max Born $\Psi \Psi^* = |\psi|^2$ is real and positive, it has physical meaning. It represents the probability of finding the particle in the state Ψ .
- ❖ Since the wave function is a complex quantity, it may be expressed in terms of
- ❖
$$\Psi(x,y,z) = (a+ib)$$
- ❖ Where a,b are real function of the variables (x,y,z,t) and $i = \sqrt{-1}$
- ❖ The complex conjugate of Ψ is given by
- ❖
$$\Psi^*(x,y,z) = (a-ib)$$

Multiplying the two equations, we have

$$\Psi \Psi^* = (a+ib)(a-ib) = a^2 + b^2$$

According to Max Born

$$P = \Psi \Psi^* = |\psi_{(x,y,z)}|^2 = a^2 + b^2$$

Thus the product of Ψ and Ψ^* is real and positive if $\Psi \neq 0$

And is known as the probability density of the particle associated with the de-Broglie wave.

The probability of the finding the particle in a volume $dv = dx.dy.dz$ is given by

$$\text{Probability (p)} = |\psi|^2 dx dy dz$$

For the total probability of finding the particle somewhere is

$$p = \int \int \int |\psi|^2 dx dy dz = 1$$

A wave function ψ satisfying the above relation is called a normalized wave function.

3. Matter waves are new kind of waves. Justify this concept by discussing different properties of matter waves.

Ans.

Matter Waves or de-broglie-waves: The waves associated with a material particle are called as matter waves.

Properties of Matter Waves:

- ❖ Lighter is the particle, smaller the value of mass m , greater is the wavelength associated with it. Therefore wave behavior is significant for micro particles whereas wave associated with macro bodies can never be detected.
- ❖ If $v = 0$, then $\lambda = \infty$, i.e. wave becomes indeterminate.
- ❖ This shows that matter waves are generated only when material particles are in motion.
- ❖ Smaller is the velocity of the particle, greater is the wavelength associated with it.
- ❖ Matter waves are produced by the motion of particles and are independent of charge. ($\lambda = h/mv$). i.e., matter waves are neither electromagnetic waves nor acoustic waves but they are a new kind of waves.
- ❖ It can be shown that the matter waves can travel faster than light i.e. the velocity of matter waves can be greater than the velocity of light.
- ❖ No single phenomenon exhibits both particle nature and wave nature simultaneously.

4. Using Planck's and Einstein's theory of radiation, Show that the wavelength associated with an electron of mass 'm' and kinetic energy 'E' is given by $\frac{h}{\sqrt{2mE}}$

Ans.

- ❖ The waves associated with the material particles are called as de-Broglie waves or matter waves & the wave length associated with matter waves are called as de-Broglie wave-length or matter wave-length (λ).

$$\text{de-broglie wave-length is given by } \lambda = \frac{h}{p} = \frac{h}{mv}$$

According to the planck's theory of radiation, the energy of photon is given by

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

h - planck's constant, ν -frequency of photon

According to Einstein mass energy relation

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

m-mass of a photon

c-velocity of light

$$\lambda = \frac{h}{mc} = \frac{h}{p} \text{(3)}$$

From equation of (1) & (2)

Where p-momentum of photon = mc

m-mass of photon, c-speed of light

But according to de-broglie theory

Momentum of electron particle(p) = mv

m-mass of e's , v-velocity of electron particle

$$\text{de-broglie wave-length}(\lambda) = \lambda = \frac{h}{p} = \frac{h}{mv} \text{ -----(4)}$$

Eq.(4) gives the expression for de-broglie wave-length.

we know that the kinetic energy of particle i.e. $E = \frac{1}{2}mv^2$ (5)

Multiply Eq-(5) by 'm' on both sides, we get

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

$$2Em = m^2v^2$$

$$mv = \sqrt{2mE}$$

$$\lambda = \frac{h}{\sqrt{2mE}} \text{ (6)}$$

5. Determine an expression for the wavelength associated with an electron, accelerated by a potential V.

Ans.

If a charged particle is accelerated through a potential difference(V), then the kinetic energy of the particle is given as

$$E = eV$$

But we have kinetic energy (E) of particle i.e. $E = \frac{1}{2}mv^2$

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

$$2eV = mv^2$$

Multiply by 'm' on both sides we get

$$2meV = m^2v^2$$

$$mv = \sqrt{2meV}$$

⁻³⁴

$$h = 6.6 \times 10 \text{ J-S}$$

We have de-broglie wavelength $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}}$

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$$

⁻³⁴

$$h = 6.625 \times 10 \text{ Js}$$

⁻³¹

$$m = 9.1 \times 10 \text{ kg}$$

⁻¹⁹

$$e = 1.6 \times 10 \text{ c}$$

6. Explain the difference between a matter wave and an electromagnetic wave.

Ans.

MATTER WAVE	EM WAVE
Matter wave is associated with a particle.	Oscillating charged particle gives rise to electromagnetic wave.
Wavelength depends on the mass of the particle and its velocity $\lambda = h/mv$	Wavelength depends on the energy of the photon $\lambda = hc/E$
Can travel with a velocity greater than the velocity of light.	Travels with velocity of light.
Matter wave is not electromagnetic wave.	Electric field and magnetic field oscillate perpendicular to each other.
Matter wave require medium for propagation	Electromagnetic waves do not require medium i.e., they travel in vacuum also.

7. Describe Davisson Germer experiment with a neat diagram and explain how it established the proof for wave nature of electrons.

Davisson and Germer's experiment:-

First practical evidence for the wave nature of matter waves was given by C.J. Davisson and L.H. Germer in 1927. This was the first experimental support to de Broglie's hypothesis.

Principle: The electrons which are coming from the source are incident on the target and the electrons get diffracted. These diffracted electrons produce a diffraction pattern. It shows(explains) the wave nature of matter waves.

Experimental Arrangement:-

Electron gun G

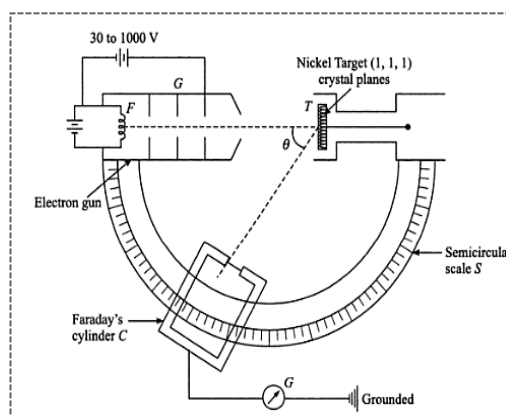
Filament F.

Target T (large single crystal of Ni)

Faraday cylinder C

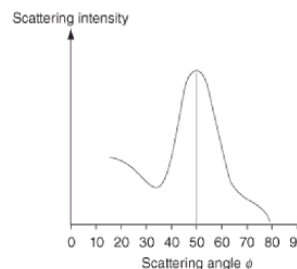
Semi circular Scale S

Galvanometer G

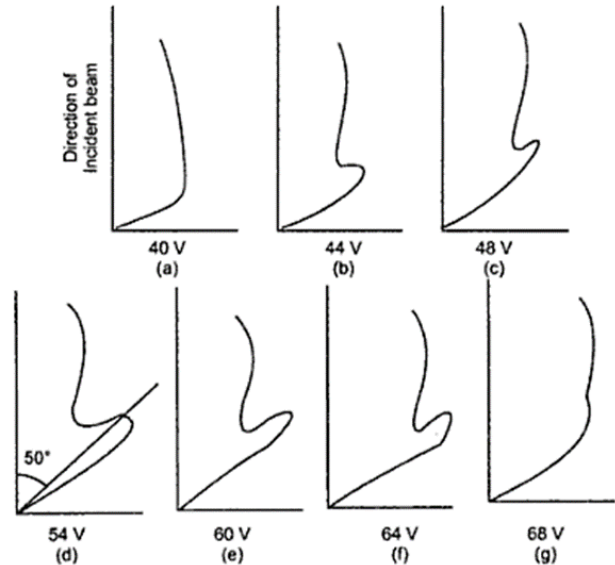


Working:

- ❖ When tungsten filament 'F' is heated by a LTB then e's are produced. These e's are accelerated by High voltage(HTB).
- ❖ The accelerated e's are collimated into a fine beam of pencil by passing them through a system of pin-holes.
- ❖ This beam of electrons is allowed to incident on nickel crystal which acts as target. Then e's are scattered in all the directions.
- ❖ The intensity of scattered e's is measured by the circular scale arrangement. In this arrangement, an electron or movable collector (Double walled faraday cylinder) is fixed to circular scale which can collect the electrons and can move along the circular scale.
- The electron collector (Double walled faraday cylinder) is connected to a sensitive galvanometer to measure the intensity of electron beam entering the collector at different scattering angles(θ).



- A graph is plotted between the scattering angle (θ) and the number of scattered electron's as shown in above figure.
- The intensity of scattered electrons is maximum at $\theta = 50^\circ$ & accelerating voltage = 54V.
- ❖ A bump is started at 44 volts and it is gradually increases become maximum at 54 volts beyond that bump decreases at 60V and disappear on further increasing the voltage.



If θ is the correspondence angle of

diffraction at the Bragg's plane then θ and Φ are related as $\theta = \frac{180 - \Phi}{2}$

So if θ is diffraction angle, n is order of maxima, then from Bragg's law $2d\sin\theta = n\lambda$.

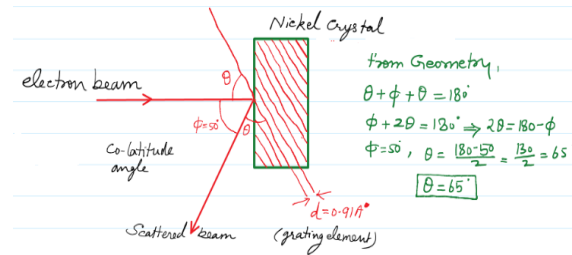
Davisson & Germer observed that maximum diffraction occurs at

$\Phi = 50^\circ$ & $d = 0.91 \text{ \AA}$.

Now, $\Phi = 50^\circ \Rightarrow \theta = \frac{180 - 50}{2} = 65^\circ$.

Therefore, $\lambda = 2d\sin\theta$ {for $n=1$ }

$$\begin{aligned} &= 2 \times 0.91 \times \sin 65^\circ \\ &= 1.65 \text{ \AA} \end{aligned}$$



From de-broglie wave length(λ):

$$\lambda = \frac{12.27}{\sqrt{V}}$$

But $V = 54\text{v}$

$$\lambda = \frac{12.27}{\sqrt{54}} = 1.67 \text{ \AA}$$

$$\lambda = 1.67 \text{ \AA}$$

It has been proved both the practical & theoretical wavelengths are almost equal. Hence the wave nature of particle is proved experimentally.

8. Considering dual nature of electron, derive Schrodinger's time independent wave equation for the motion of an electron.

Ans.

SCHRODINGER TIME INDEPENDENT WAVE EQUATION

If a particle of mass 'm' moving with velocity 'v' is associated with a group of waves, let ψ be the wave function of the particle. Also let us consider a simple form of progressing wave represented by the eqn,

$$\text{wave function } \psi = \psi_0 \sin(\omega t - kx) \text{-----} > (1)$$

$$\text{Where } \Psi = \Psi(x)$$

$$\Psi_0 \text{ is amplitude,}$$

$$k = 2\pi/\lambda,$$

$$\omega = 2\pi\nu = \frac{2\pi}{T},$$

The **Schrödinger wave equation** is a linear partial differential equation that governs the wave function of a quantum-mechanical system.

Now, differentiating (1) with respect to 'x' we get

$$\begin{aligned} \frac{\partial \psi}{\partial x} &= -K \psi_0 \cos(\omega t - kx) \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} &= -K^2 \psi_0 \sin(\omega t - Kx) \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} &= -K^2 \Psi \text{ [from (1)} \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} + K^2 \Psi &= 0 \text{-----} (2) \end{aligned}$$

OR

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \Psi = 0 \text{-----} (3)$$

we know that Debroglie wavelength $\lambda = h/mv$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \text{-----} (4)$$

Now, we know that the total energy E of the particle is sum of its kinetic energy K and potential energy V

Therefore,

$$E = K + V \text{ and } K = \frac{1}{2} m v^2 \Rightarrow$$

$$m v^2 = 2m (E - V) \text{-----} (5)$$

From (4) & (5)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m(E-V)}{h^2} \psi = 0$$

The value of $h/2\pi$ is considered as \hbar

Therefore, $\hbar = h/2\pi$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2} \psi = 0 \text{ ----- (6)}$$

This is Schrodinger time independent wave equation in 1-D

In three dimensional it can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m(E-V)}{\hbar^2} \psi = 0 \text{ ----- (7)}$$

9. Assuming that a particle of mass m is confined in a field free region between impenetrable walls in infinite height at $x = 0$ and $x = a$, show that the permitted energy levels of a particle are given by $n^2 h^2 / 8ma^2$

Ans.

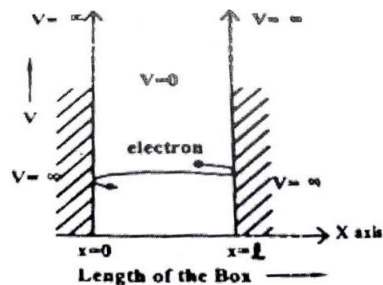
- Let us consider a particle of mass ' m ' moving with velocity ' v ' along x-direction and is confined between to infinite potential rigid walls, so that the particle has no chance of escaping from them. Therefore, the particle bounces back and forth between two walls as shown in fig.
- Let the potential energy of electron inside the box is constant and can be taken as zero for simplicity.

Inside the box

The particle exist inside the box; therefore the probability of finding the electron inside the box is not equal to zero and the potential energy is zero.

$$\text{i.e., } \Psi(x) \neq 0 \quad \text{when } x > 0 \text{ and } x < L$$

$$V(x) = 0$$



To calculate the probability of finding particle within the box, let us consider one dimensional time independent Schrodinger wave equation

$$\text{i.e.,} \quad \frac{d^2\Psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V(x))\Psi = 0 \quad \dots\dots\dots(1)$$

Inside the box, the potential energy $V(x) = 0$

Therefore, equation (1) becomes

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2mE}{h^2}\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 \quad \dots\dots\dots(2)$$

$$\text{Where,} \quad K^2 = \frac{8\pi^2mE}{h^2} \quad \dots\dots\dots(3)$$

Eq. (2) is a second order differential equation; therefore it should have solution with two arbitrary constants.

∴ The solution for equation (2) is given by

$$\Psi(x) = A\sin Kx + B\cos Kx \quad \dots\dots\dots(4)$$

Where A and B are called as arbitrary constants, which can be found by applying the boundary conditions.

Boundary condition at $x=0$

At $x = 0$, the probability of the finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(0) + B \cos K(0)$$

$$0 = 0 + B$$

$$\therefore B = 0 \quad \dots\dots\dots(5)$$

Boundary condition at $x=L$

At $x = L$, the probability of finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(L) + B \cos K(L)$$

$$0 = A \sin K(L) + (0) \cos K(L)$$

$$A \sin K(L) = 0$$

Since $A \neq 0$; $\sin K(L) = 0$ (6)

We know that, $\sin n\pi = 0$ (7)

Comparing these two equations, we can write

$$K(L) = n\pi$$

$$K = \frac{n\pi}{L} \text{(8)}$$

$$K^2 = \frac{n^2\pi^2}{L^2} \text{(9)}$$

Substituting the values of 'B' and 'K' in equation (4),

Equation (4) becomes

$$\Psi_n(x) = A \sin \frac{n\pi x}{L} \text{(10)}$$

This equation represents the wave function associated with moving free electron inside the box.

Energy of the Particle

From the equations (3) & 9

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

$$K^2 = \frac{n^2\pi^2}{L^2}$$

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

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

This is an expression for the energy of the particle

Each value of E_n is known as Eigen value

The various Eigen values of an electron enclosed in a 1D box is shown in Fig.

If $L = a$

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

10. Discuss the results from the eigen values, eigen functions and probability density for a particle in a one dimensional potential box of infinite height. Also sketch the figures.

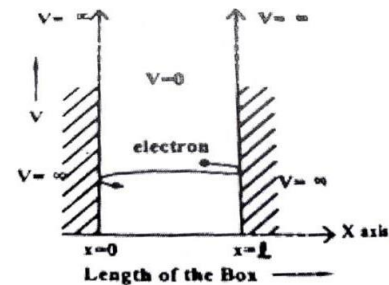
- Let us consider a particle of mass 'm' moving with velocity 'v' along x-direction and is confined between two infinite potential rigid walls, so that the particle has no chance of escaping from them. Therefore, the particle bounces back and forth between two walls as shown in fig.
- Let the potential energy of electron inside the box is constant and can be taken as zero for simplicity.

Inside the box

The particle exists inside the box; therefore the probability of finding the electron inside the box is not equal to zero and the potential energy is zero.

$$\text{i.e., } \Psi(x) \neq 0 \quad \text{when } x > 0 \text{ and } x < L$$

$$V(x) = 0$$



To calculate the probability of finding a particle within the box,

let us consider one-dimensional time-independent Schrödinger wave equation

$$\text{i.e., } \frac{d^2\Psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V(x))\Psi = 0 \quad \dots\dots\dots(1)$$

Inside the box, the potential energy $V(x) = 0$

Therefore, equation (1) becomes

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2mE}{h^2}\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 \quad \dots\dots\dots(2)$$

$$\text{Where, } K^2 = \frac{8\pi^2mE}{h^2} \quad \dots\dots\dots(3)$$

Eq. (2) is a second-order differential equation; therefore it should have a solution with two arbitrary constants.

∴ The solution for equation (2) is given by

$$\Psi(x) = A\sin Kx + B\cos Kx \quad \dots\dots\dots(4)$$

Where A and B are called as arbitrary constants, which can be found by applying the boundary conditions.

Boundary condition at x =0

At x = 0, the probability of the finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(0) + B \cos K(0)$$

$$0 = 0 + B$$

$$\therefore B = 0 \quad \dots\dots\dots(5)$$

Boundary condition at x =L

At x = L, the probability of finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(L) + B \cos K(L)$$

$$0 = A \sin K(L) + (0) \cos K(L)$$

$$A \sin K(L) = 0$$

$$\text{Since } A \neq 0; \sin K(L) = 0 \quad \dots\dots\dots(6)$$

$$\text{We know that, } \sin n\pi = 0 \quad \dots\dots\dots(7)$$

Comparing these two equations, we can write

$$K(L) = n\pi$$

$$K = \frac{n\pi}{L} \quad \dots\dots\dots(8)$$

$$K^2 = \frac{n^2\pi^2}{L^2} \quad \dots\dots\dots(9)$$

Substituting the values of 'B' and 'K' in equation (4),

Equation (4) becomes

$$\Psi_n(x) = A \sin \frac{n\pi x}{L} \quad \dots\dots\dots(10)$$

This equation represents the wave function associated with moving free electron inside the box.

Normalization of the Wave function:

It is the process by which the probability (P) of finding the particle or electron inside the box can be done.

The total probability that the particle is somewhere in the box must be unity

$$\text{i.e., } P = \int_0^L |\Psi_n(x)|^2 dx = 1 \quad \dots\dots\dots(11)$$

[Since the particle present inside the box between the length 0 to L, then the limits are chosen between 0 to L]

Substituting equation (10) in equation (11), we get

$$\begin{aligned} P &= \int_0^L A^2 \sin^2 \frac{n\pi x}{L} dx = 1 \\ A^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx &= 1 \\ A^2 \int_0^L \frac{1}{2} \left[1 - \cos \frac{2n\pi x}{L} \right] dx &= 1 \quad (\text{as } \cos 2\theta = 1 - 2\sin^2 \theta) \end{aligned}$$

$$\left(\frac{A^2}{2} \right) \left[x - \frac{L}{2\pi n} \sin \frac{2\pi n x}{L} \right]_0^L = 1$$

Since, $\sin n\pi = 0$, $\sin 2n\pi$ is also $= 0$

Equation (12) can be written as

$$\begin{aligned} \frac{A^2}{2} [L] &= 1 \\ A^2 &= \frac{2}{L} \end{aligned}$$

$$A = \sqrt{\frac{2}{L}} \quad \dots\dots\dots(13)$$

Substituting the values of 'A' in equation (10)

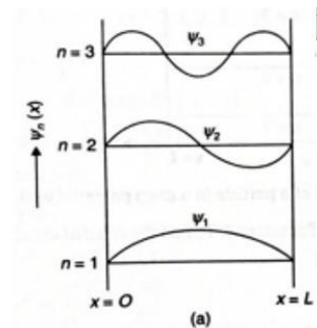
$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \dots\dots\dots(14)$$

Each value of wave function is known as Eigen function. The various Eigen functions of an electron enclosed in a 1D box is shown in Fig.

Case 1: If $n=1$, then $\Psi_1(x)$ has two nodes at $x=0$, and $x=L$

Case 2: If $n=2$, then $\Psi_2(x)$ has three nodes at $x=0$ and $x=\frac{L}{2}$ and $x=L$.

Case 3: If $n=3$, then $\Psi_3(x)$ has four nodes at $x=0$ and $x=\frac{L}{3}$ and $x=\frac{2L}{3}$ and $x=L$. Therefore $\Psi_n(x)$ has $(n+1)$ nodes.



Energy of the Particle

From the equations (3) & 9

$$K^2 = \frac{8\pi^2 m E}{h^2}$$

$$K^2 = \frac{n^2 \pi^2}{L^2}$$

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

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

This is an expression for the energy of the particle

Each value of E_n is known as Eigen value

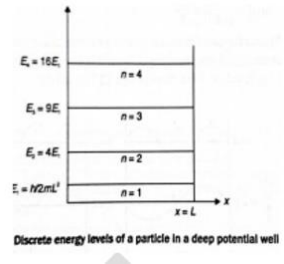
The various Eigen values of an electron enclosed in a 1D box is shown in Fig.

Case 1: If $n=1$, then $E_1 = \frac{h^2}{8mL^2}$

Case 1: If $n=2$, then $E_2 = \frac{4h^2}{8mL^2} = 4E_1$

Case 1: If $n=3$, then $E_3 = \frac{9h^2}{8mL^2} = 9E_1$ and so on

Therefore, energy levels of electron are discrete.



11. Show that the energies of a particle confined between two rigid walls of infinite potential are quantized.

Ans. Write 10th Question Answer.

12. What is de-Broglie wave? Derive expression for de Broglie wavelength associated with a particle having mass m and velocity v .

Ans.

Matter Waves or de-broglie-waves: The waves associated with a material particle are called as matter waves.

de-broglie concept of dual nature of matter waves:-

In 1924, Louis de-broglie suggested that matter waves also exhibit dual nature like radiation(light).

They are

I. Wave nature

II. Particle nature

Wave nature of matter waves is verified by Davisson & Germer experiment, G.P.Thomson experiment etc.

Particle nature of matter waves is verified by photo-electric effect, Compton effect etc.

de-broglie hypothesis:-

- 1) The universe consists of matter and radiation(light) only
- 2) Matter waves also exhibit dual nature like radiation.

3) The waves associated with the material particles are called as de-Broglie waves or matter waves & the wave length associated with matter waves are called as de-Broglie wave-length or matter wave-length (λ).

4) de-broglie wave-length is given by $\lambda = \frac{h}{p} = \frac{h}{mv}$

Expression for de-broglie wave-length(λ) in various form:-

According to the planck's theory of radiation, the energy of photon is given by

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

h- planck's constant, ν -frequency of photon

According to Einstein mass energy relation

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

m-mass of a photon

c-velocity of light

From equation of (1) & (2)

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

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

Where p-momentum of photon = mc

m-mass of photon, c-speed of light

But according to de-broglie theory

Momentum of electron particle(p) = mv

m-mass of e's , ν -velocity of electron particle

$$\text{de-broglie wave-length}(\lambda) = \lambda = \frac{h}{p} = \frac{h}{mv} \quad \text{-----(4)}$$

Eq.(4) gives the expression for de-broglie wave-length.

13. Discuss different phenomenon's that show the behavior of light radiation interacting with matter.

Ans. Blackbody Radiation:

- An object might absorb some and reflect

some of the radiation.

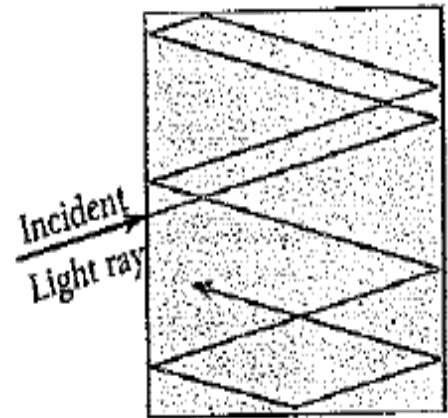
- An idealized **blackbody** is a material object that **absorbs all of the radiation** falling on it, and hence **appears as black** under reflection when illuminated from outside.

- **Blackbody** is a **perfect absorber** as well as a **perfect emitter** of radiation

- **Practical blackbody:** A hollow cavity with internal walls that perfectly reflect EM radiation and has a small hole on its surface.

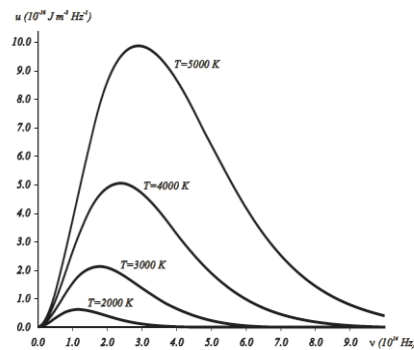
- The radiation entered through this hole gets completely absorbed due to successive reflections.

- The hole behaves as a perfect emitter when this cavity is heated to a temperature T , and the hole will eventually begin to glow as T increases.



- A blackbody emits thermal radiation on heating.

- This radiation consists of a **continuous distribution of frequencies** ranging from infrared to ultraviolet.



- **Classical Physics failed** to explain continuous distribution of frequencies.

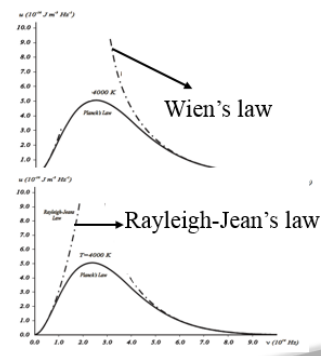
- Stefan-Boltzmann law,

$$P = a\sigma T^4$$

- Wien's energy distribution, $u(\nu, T) = A\nu^3 e^{-\beta\nu/T}$

- Rayleigh-Jean's energy distribution

$$u(\nu, T) = \frac{8\pi\nu^2}{c^3} kT.$$



Planck's Quantum Theory

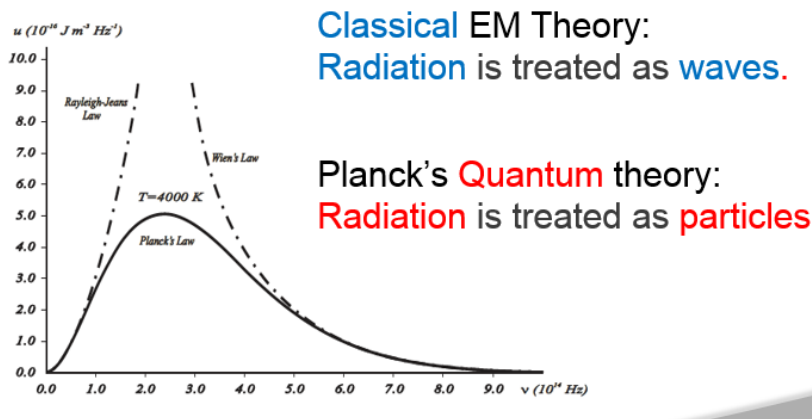
- Planck postulated that energy of radiation emitted by oscillating charges must be integer multiples of $h\nu$:

$$E = nh\nu, \quad n = 0, 1, 2, 3, \dots$$

where h is a universal constant and $h\nu$ is the energy of a “quantum” of radiation.

- Planck’s energy distribution,

$$u(\nu, T) = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{h\nu/kT} - 1}.$$



Photoelectric Effect

- Hertz observed that when a metal is irradiated with light, electrons were ejected from it.

Experimental Observations:

- If frequency of the incident radiation ν is smaller than metal's threshold frequency ν_0 , no electron can be emitted irrespective of the intensity I .
- At $\nu > \nu_0$, number of electrons ejected increases with I of light but does not depend on ν .
- In experiments, increasing intensity alone does not help in ejecting the electron from a metal.
- These experimental facts indicate that concept of gradual accumulation, continuous absorption, of energy by the electron, as predicted by classical physics is indeed erroneous.
- Einstein assumed that light is made of particles each carrying an energy $h\nu$, called a photon.
- When beam of light of ν is incident on a metal, each photon transmits all its energy $h\nu$ to an electron near the surface.

- So, photon is entirely absorbed by the electron. The electron thus absorb energy only in quanta of $h\nu$, irrespective of I of incident radiation.

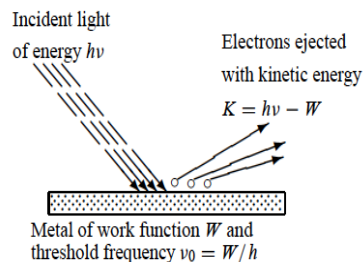
- If $h\nu > W$, metal's work function (energy required to dislodge electron from metal) electron will then be knocked out.

- If, $h\nu < W$, No electron emits.

$$h\nu = W + K ;$$

K is K.E of ejected electron.

This gives proper explanation that **K.E of the ejected electron increases linearly with ν .**



Atomic Stability:

- Classical Physics to electrons

- * Atom consists of (+ve) nucleus and (–ve) electrons.

- * The attraction b/n +ve & –ve \rightarrow collapse of atom.

- * Electron experiences a centripetal force.

An accelerated charged particle radiates energy as

EM waves \rightarrow collapse of atom.

Atom is not stable???

Classical Physics fails.

- Following Planck's QUANTA concept and Einstein's PHOTON concept, Bohr's model for Hydrogen atom.

- He argued that atoms can be found only in **discrete states of energy**.

- The emission or absorption of radiation takes place only in discrete amounts $h\nu$ that results from the transitions b/n various discrete states of energy.

So, **Atoms are stable.**

- Blackbody radiation, Photoelectric effect, Atomic model predicts **the particle behavior of radiation.**

14. Write major differences between classical mechanics and quantum mechanics.

Classical Mechanics	Quantum Mechanics
It describes physics of macroscopic objects.	It describes physics of microscopic objects.
Newton's laws are used for <u>macroparticle</u> dynamics.	Schrodinger's equations are used for <u>microparticle</u> dynamics.
The dynamics are completely deterministic and future is predictable.	The dynamics are <u>indeterministic</u> and future prediction is impossible.
Matter is treated as particles and radiation is treated as waves.	Both matter and radiation exhibit wave-particle duality.
The energies of a <u>macroparticle</u> are arbitrary including zero.	The energies of a <u>microparticle</u> are discrete and zero is excluded.

15. Differentiate between ψ and $|\psi|^2$.

Ans. Wave function:

- The quantity whose variations make up matter waves is called the wave function and denoted by ψ .
- It connects the particle nature and its associated wave nature.
- Wave functions are usually complex with both real and imaginary parts.

$$\psi = A + iB$$

Physical Significance of Wave function

- ψ itself doesn't have any physical meaning, the square of its absolute magnitude $|\psi|^2$, is proportional to the probability of finding the particle.
- It is usually convenient to have $|\psi|^2$ be equal to the probability density P of finding the particle rather than merely proportional to P as *particle exists somewhere over t* .

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 1. \quad (1)$$

This is a normalized wave function.

16. Highlight the conditions for an acceptable wave function.

Ans. Properties of Wave function: Write 2nd Question Answer

17. Extend the one dimensional problem to 3 dimensions and hence give the equations for eigen values and eigen functions.

Ans. Write 10th Question Answer

18. Why matter waves are observed for particles of atomic or nuclear size.

Ans. Write 3rd Question Answer.

19. Explain the concept of phase velocity and group velocity deduce a relation between them

Ans. Group Velocity, V_{gr} :

The group of waves, as a whole must travel with the particle velocity v . Hence the group velocity of the matter waves,

$$\overline{v_{gr}} = \bar{v}$$

Phase Velocity, V_{ph} :

Each wave of the group of matter waves travel with a velocity is known as the phase velocity of the wave. It is given by

$$V_{ph} = \frac{\omega}{k}$$

$$= \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

Relation between Group velocity and Phase velocity

$$= \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

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

$$E = h\nu = mc^2$$

$$v_{ph} = \frac{c^2}{v}$$

$$v_{gr} \times v_{ph} = c^2$$

20. Derive the equation for energy of a particle confined in a 1-D infinite square well and explain energy quantization, zero-point energy and spatial nodes.

Ans. Write 9th Question Answer and

The quantum behavior in the box include

Energy quantization: It is not possible for the particle to have any arbitrary definite energy. Instead only discrete definite energy levels are allowed.

Zero-point Energy: The lowest possible energy level of the particle, called the zero-point energy, is non-zero.

Spatial-nodes: In contrast to classical mechanics the Schrodinger equation predicts that for some energy levels there are nodes, implying positions at which the particle can never be found.

PART-C Short Answer Questions

1. Relate the dependency of wavelength of matter waves on velocity and mass of material particle.

Ans.

Properties of Matter Waves:

- ❖ Lighter is the particle, smaller the value of mass m , greater is the wavelength associated with it. Therefore wave behavior is significant for micro particles whereas wave associated with macro bodies can never be detected.
- ❖ If $v = 0$, then $\lambda = \infty$, i.e. wave becomes indeterminate.
- ❖ This shows that matter waves are generated only when material particles are in motion.
- ❖ Smaller is the velocity of the particle, greater is the wavelength associated with it.
- ❖ It can be shown that the matter waves can travel faster than light i.e. the velocity of matter waves can be greater than the velocity of light.

2. Write an expression for de-Broglie wavelength in terms of momentum and kinetic energy.

$$\text{de-broglie wave-length is given by } \lambda = \frac{h}{p} = \frac{h}{mv}$$

According to the planck's theory of radiation, the energy of photon is given by

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

h - planck's constant, ν -frequency of photon

According to Einstein mass energy relation

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

m -mass of a photon

c -velocity of light

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

From equation of (1) & (2)

Where p -momentum of photon = mc

m -mass of photon, c -speed of light

But according to de-broglie theory

Momentum of electron particle(p) = mv

m-mass of e's , v-velocity of electron particle

$$\text{de-broglie wave-length}(\lambda) = \lambda = \frac{h}{p} = \frac{h}{mv} \quad \text{-----(4)}$$

Eq.(4) gives the expression for de-broglie wave-length.

we know that the kinetic energy of particle i.e. $E = \frac{1}{2}mv^2$ (5)

Multiply Eq-(5) by 'm' on both sides, we get

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

$$2Em = m^2v^2$$

$$mv = \sqrt{2mE}$$

$$\lambda = \frac{h}{\sqrt{2mE}} \quad \text{... .. (6)}$$

3. Explain the conception of light behaving both as a particle and wave.

Ans. Radiation: Wave-Particle Duality

- The photo electric effect and the Compton Effect established that light behaves as a flux of photons.
- On the other hand, the phenomena of interference, diffraction and polarization can be explained only when light is treated as a continuous wave.
- Neither of the modes can separately explain all the experimental facts.
- The particle nature and wave nature appear mutually exclusive.
- So, Light exhibits both wave nature and particle nature i.e., called as wave-particle duality.

4. Explain the concept of Heisenberg uncertainty principle

- ✓ If ' Δx ' & ' Δp ' are uncertainties in the measurement of position & momentum of the particle then mathematically this uncertainties of this physical variables is written as

$$\Delta x. \Delta p \geq \frac{h}{4\pi} \quad \text{... .. (1)}$$

Explanation:-

(i) If $\Delta x = 0$. i.e., the position of a particle is measured accurately, then from eq-(1).

$$\Delta p = \frac{h}{\Delta x. 4\pi}$$
$$\Delta p = \frac{h}{0} = \infty$$

It means that, the momentum of the particle can't be measured.

(ii) If $\Delta p = 0$. i.e., the momentum of a particle is measured accurately, then from eq-(1).

$$\Delta x = \frac{h}{\Delta p \cdot 4\pi}$$

$$\Delta p = \frac{h}{0} = \infty$$

- ✓ From the above said observations made by Heisenberg, he clearly states that it is impossible to design an experiment to prove the wave & particle nature of matter at any given instant of time.
- ✓ If one measures position or momentum accurately, then there will be an uncertainty in the other.

5. Prove that matter waves travel with a velocity greater than velocity of light. Also justify it.

Ans. Group Velocity, V_{gr} :

The group of waves, as a whole must travel with the particle velocity v . Hence the group velocity of the matter waves,

$$\overline{v_{gr}} = \bar{v}$$

Phase Velocity, V_{ph} :

Each wave of the group of matter waves travel with a velocity is known as the phase velocity of the wave. It is given by

$$V_{ph} = \frac{\omega}{k}$$

$$= \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

Relation between Group velocity and Phase velocity

$$= \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

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

$$E = h\nu = mc^2$$

$$v_{ph} = \frac{c^2}{v}$$

$$v_{gr} \times v_{ph} = c^2$$

6. Write one dimensional time independent Schrodinger equation associated with matter wave.

Ans. If a particle of mass 'm' moving with velocity 'v' is associated with a group of waves, let ψ be the wave function of the particle. Also let us consider a simple form of progressing wave represented by the eqn,

$$\text{wave function } \psi = \psi_0 \sin(\omega t - kx) \text{-----} > (1)$$

$$\text{Where } \Psi = \Psi(x)$$

Now, differentiating (1) with respect to 'x' we get

$$\begin{aligned} \frac{\partial \psi}{\partial x} &= -K \psi_0 \cos(\omega t - kx) \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} &= -K^2 \psi_0 \sin(\omega t - Kx) \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} &= -K^2 \Psi \text{ [from (1)} \\ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} + K^2 \Psi &= 0 \text{-----} (2) \end{aligned}$$

OR

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \Psi = 0 \text{-----} (3)$$

we know that Debroglie wavelength $\lambda = h/mv$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \text{-----} (4)$$

Now, we know that the total energy E of the particle is sum of its kinetic energy K and potential energy V

Therefore,

$$\begin{aligned} E &= K + V \text{ and } K = \frac{1}{2} m v^2 \Rightarrow \\ m v^2 &= 2m (E - V) \text{-----} (5) \end{aligned}$$

From (4) & (5)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m (E - V)}{h^2} \Psi = 0$$

The value of $h/2\pi$ is considered as \hbar

Therefore, $\hbar = h/2\pi$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E - V)}{\hbar^2} \Psi = 0 \text{-----} (6)$$

This is Schrodinger time independent wave equation in 1-D

7. Explain the feature of wave function which connects the particle nature and wave nature of matter wave.

- ❖ The wave nature of matter introduced an uncertainty in the location of the position of the particle because a wave cannot be set exactly at this position (or) at that position.
- ❖ The amplitude of the wave tells us about the probability of finding particle in space at a particular instant. A large wave amplitude means a large probability of finding the particle at that position.
- ❖ Mathematically, to explain it, scientists introduced a new physical quantity called wave function.
- ❖ It is a variable quantity i.e., associated with a moving particle at any position (x,y,z) and time t and it relates probability of a finding the particle at that point and time.
- ❖ It must be well behaved it is single valued and continuous everywhere.
- ❖ It is a complex quantity and individually has no meaning.
- ❖ To explain it, Max Born suggested a new idea about the physical significance of Ψ which is generally accepted now a days.
- ❖ According to Max Born $\Psi \Psi^* = |\psi|^2$ is real and positive, it has physical meaning. It represents the probability of finding the particle in the state Ψ .

8. Describe behavior of matter waves by giving any two of its properties.

Matter Waves or de-broglie-waves: The waves associated with a material particle are called as matter waves.

Properties of Matter Waves:

- ❖ Lighter is the particle, smaller the value of mass m, greater is the wavelength associated with it. Therefore wave behavior is significant for micro particles whereas wave associated with macro bodies can never be detected.
- ❖ If $v = 0$, then $\lambda = \infty$, i.e. wave becomes indeterminate.
- ❖ This shows that matter waves are generated only when material particles are in motion.
- ❖ Smaller is the velocity of the particle, greater is the wavelength associated with it.

9. Define Phase Velocity associated with a matter wave.

Ans.

Each wave of the group of matter waves travel with a velocity is known as the phase velocity of the wave. It is given by

$$v_{ph} = \frac{\omega}{k}$$

$$= \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

10. Define Group velocity associated with a matter wave.

Ans. The group of waves, as a whole must travel with the particle velocity v . Hence the group velocity of the matter waves,

$$\overline{v_{gr}} = \bar{v}$$

11. Write expressions for eigen function and eigen values for a particle in one dimensional square well box of infinite potential.

Ans.

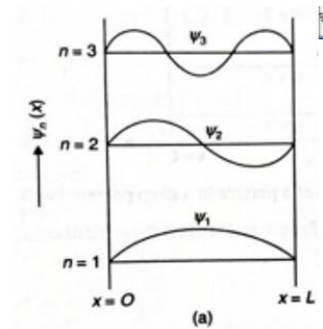
$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \dots \dots \dots (14)$$

Each value of wave function is known as Eigen function. The various Eigen functions of an electron enclosed in a 1D box is shown in Fig.

Case 1: If $n=1$, then $\Psi_1(x)$ has two nodes at $x=0$, and $x=L$

Case 2: If $n=2$, then $\Psi_2(x)$ has three nodes at $x=0$ and $x=\frac{L}{2}$ and $x=L$.

Case 3: If $n=3$, then $\Psi_3(x)$ has four nodes at $x=0$ and $x=\frac{L}{3}$ and $x=\frac{2L}{3}$ and $x=L$. Therefore $\Psi_n(x)$ has $(n+1)$ nodes.



Energy of the Particle

From the equations (3) & 9

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

$$K^2 = \frac{n^2\pi^2}{L^2}$$

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

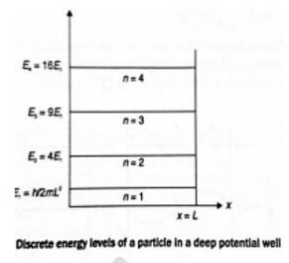
$$E_n = \frac{n^2h^2}{8mL^2}$$

This is an expression for the energy of the particle
Each value of E_n is known as Eigen value
The various Eigen values of an electron enclosed in a 1D box is shown in Fig.

Case 1: If $n=1$, then $E_1 = \frac{h^2}{8mL^2}$

Case 1: If $n=2$, then $E_2 = \frac{4h^2}{8mL^2} = 4E_1$

Case 1: If $n=3$, then $E_3 = \frac{9h^2}{8mL^2} = 9E_1$ and so on
Therefore, energy levels of electron are discrete.



12. Discuss about Normalization condition as postulated by Max Born.

- ❖ According to Max Born $\Psi \Psi^* = |\psi|^2$ is real and positive, it has physical meaning. It represents the probability of finding the particle in the state Ψ .
- ❖ Since the wave function is a complex quantity, it may be expressed in terms of
- ❖ $\Psi(x,y,z) = (a+ib)$
- ❖ Where a,b are real function of the variables (x,y,z,t) and $i = \sqrt{-1}$
- ❖ The complex conjugate of Ψ is given by
- ❖ $\Psi^*(x,y,z) = (a-ib)$

Multiplying the two equations, we have

$$\Psi \Psi^* = (a+ib)(a-ib) = a^2 + b^2$$

According to Max Born

$$P = \Psi \Psi^* = |\psi_{(x,y,z)}|^2 = a^2 + b^2$$

Thus the product of Ψ and Ψ^* is real and positive if $\Psi \neq 0$

And is known as the probability density of the particle associated with the de-Broglie wave.

The probability of the finding the particle in a volume $dv = dx.dy.dz$ is given by

$$\text{Probability (p)} = |\psi|^2 dx dy dz$$

For the total probability of finding the particle somewhere is

$$p = \int \int \int |\psi|^2 dx dy dz = 1$$

A wave function ψ satisfying the above relation is called a normalized wave function.

13. What is the Schrödinger's interpretation of complex and not observable wave function?

Ans. Physical Significance of wave function:

Wave function is a mathematical tool used in quantum mechanics to describe any physical system and it is denoted by ' Ψ '.

- ❖ The wave nature of matter introduced an uncertainty in the location of the position of the particle because a wave cannot be set exactly at this position (or) at that position.
- ❖ The amplitude of the wave tells us about the probability of finding particle in space at a particular instant. A large wave amplitude means a large probability of finding the particle at that position.

- ❖ Mathematically, to explain it, scientists introduced a new physical quantity called wave function.
- ❖ It is a variable quantity i.e., associated with a moving particle at any position (x,y,z) and time t and it relates probability of finding the particle at that point and time.
- ❖ It must be well behaved it is single valued and continuous everywhere.
- ❖ It is a complex quantity and individually has no meaning.
- ❖ To explain it, Max Born suggested a new idea about the physical significance of Ψ which is generally accepted now a days.
- ❖ According to Max Born $\Psi \Psi^* = |\psi|^2$ is real and positive, it has physical meaning. It represents the probability of finding the particle in the state Ψ .
- ❖ Since the wave function is a complex quantity, it may be expressed in terms of
- ❖ $\Psi(x,y,z) = (a+ib)$
- ❖ Where a,b are real function of the variables (x,y,z,t) and $i = \sqrt{-1}$

14. How energy of a particle confined in a potential box is related to the width of the box.

Ans.

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

This is an expression for the energy of the particle

Each value of E_n is known as Eigen value

The various Eigen values of an electron enclosed in a 1D box is shown

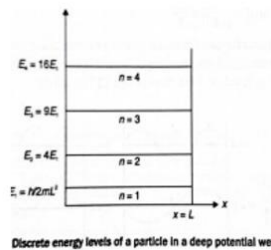
Fig.

Case 1: If $n=1$, then $E_1 = \frac{h^2}{8mL^2}$

Case 1: If $n=2$, then $E_2 = \frac{4h^2}{8mL^2} = 4E_1$

Case 1: If $n=3$, then $E_3 = \frac{9h^2}{8mL^2} = 9E_1$ and so on

Therefore, energy levels of electron are discrete.



15. Write about probability density of moving material particle as explained by Born and Schrodinger.

According to Max Born

$$P = \Psi \Psi^* = |\psi_{(x,y,z)}|^2 = a^2 + b^2$$

Thus the product of Ψ and Ψ^* is real and positive if $\Psi \neq 0$

And is known as the probability density of the particle associated with the de-Broglie wave.

The probability of finding the particle in a volume $dv = dx.dy.dz$ is given by

$$\text{Probability (p)} = |\psi|^2 dx dy dz$$

For the total probability of finding the particle somewhere is

$$p = \int \int \int |\psi|^2 dx dy dz = 1$$

A wave function ψ satisfying the above relation is called a normalized wave function.

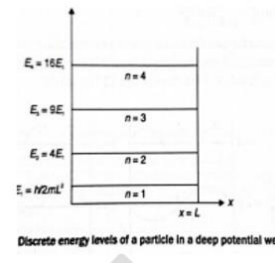
16. What is the minimum energy possessed by the particle in an infinitely deep potential well?

$$\text{Case 1: If } n=1, \text{ then } E_1 = \frac{h^2}{8mL^2}$$

$$\text{Case 1: If } n=2, \text{ then } E_2 = \frac{4h^2}{8mL^2} = 4E_1$$

$$\text{Case 1: If } n=3, \text{ then } E_3 = \frac{9h^2}{8mL^2} = 9E_1 \text{ and so on}$$

Therefore, energy levels of electron are discrete.



Zero-point Energy: The lowest possible energy level of the particle, called the zero-point energy, is non-zero.

17. Discuss about the nature of the walls of the box in which a particle is bound.

The quantum behavior in the box include

Energy quantization: It is not possible for the particle to have any arbitrary definite energy. Instead only discrete definite energy levels are allowed.

Zero-point Energy: The lowest possible energy level of the particle, called the zero-point energy, is non-zero.

Spatial-nodes: In contrast to classical mechanics the Schrodinger equation predicts that for some energy levels there are nodes, implying positions at which the particle can never be found.

18. What happens to the wavefunction associated with a particle in an infinitely deep potential well

Probability of the location of the particle

The probability of finding a particle over a small distance dx at x is given by

$$P(x)dx = |\Psi_n(x)|^2 dx$$

$$P(x)dx = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

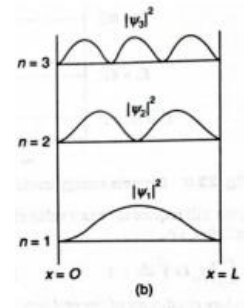
Thus the probability density for one dimensional motion is

$$P(x)dx = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$$

The probability density is maximum when

$$\frac{n\pi x}{L} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}$$

$$x = \frac{L}{2n}, \frac{3L}{2n}, \frac{5L}{2n}$$



Case 1: If $n=1$, then the probability of position of the particle is at $x = \frac{L}{2}$

Case 2 : If $n=2$, then the probability of position of the particle is at $x = \frac{L}{4}$ and $\frac{3L}{4}$

Case 3: If $n=3$, then the probability of position of the particle is at

$x = \frac{L}{6}$ and $\frac{3L}{6}$ and $\frac{5L}{6}$

19. What is the boundary condition for normalized wave function?

According to Max Born

$$P = \Psi \Psi^* = |\psi_{(x,y,z)}|^2 = a^2 + b^2$$

Thus the product of Ψ and Ψ^* is real and positive if $\Psi \neq 0$

And is known as the probability density of the particle associated with the de-Broglie wave.

The probability of the finding the particle in a volume $dv = dx.dy.dz$ is given by

$$\text{Probability (p)} = |\psi|^2 dx dy dz$$

For the total probability of finding the particle somewhere is

$$p = \int \int \int |\psi|^2 dx dy dz = 1$$

A wave function ψ satisfying the above relation is called a normalized wave function.

20. Define square well potential associated with a bound electron moving along one dimension.

- Let us consider a particle of mass 'm' moving with velocity 'v' along x-direction and is confined between to infinite potential rigid walls, so that the particle has no chance of escaping from them. Therefore, the particle bounces back and forth between two walls as shown in fig.

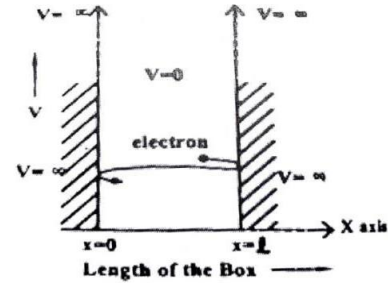
- Let the potential energy of electron inside the box is constant and can be taken as zero for simplicity.

Inside the box

The particle exist inside the box; therefore the probability of finding the electron inside the box is not equal to zero and the potential energy is zero.

$$\text{i.e., } \Psi(x) \neq 0 \quad \text{when } x > 0 \text{ and } x < L$$

$$V(x) = 0$$



To calculate the probability of finding particle within the box,

let us consider one dimensional time independent Schrodinger wave equation

$$\text{i.e., } \frac{d^2\Psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V(x))\Psi = 0 \quad \dots\dots\dots(1)$$

Inside the box, the potential energy $V(x) = 0$

Therefore, equation (1) becomes

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2mE}{h^2}\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 \quad \dots\dots\dots(2)$$

$$\text{Where, } K^2 = \frac{8\pi^2mE}{h^2} \quad \dots\dots\dots(3)$$

Eq. (2) is a second order differential equation; therefore it should have solution with two arbitrary constants.

∴ The solution for equation (2) is given by

$$\Psi(x) = A\sin Kx + B\cos Kx \quad \dots\dots\dots(4)$$

Where A and B are called as arbitrary constants, which can be found by applying the boundary conditions.

Boundary condition at $x = 0$

At $x = 0$, the probability of the finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(0) + B \cos K(0)$$

$$0 = 0 + B$$

$$\therefore B = 0 \quad \dots\dots\dots(5)$$

Boundary condition at $x = L$

At $x = L$, the probability of finding the electron is zero, i.e., $\Psi(x) = 0$

Equation (4) becomes

$$0 = A \sin K(L) + B \cos K(L)$$

$$0 = A \sin K(L) + (0) \cos K(L)$$

$$A \sin K(L) = 0$$

$$\text{Since } A \neq 0; \sin K(L) = 0 \quad \dots\dots\dots(6)$$

$$\text{We know that, } \sin n\pi = 0 \quad \dots\dots\dots(7)$$

Comparing these two equations, we can write

$$K(L) = n\pi$$

$$K = \frac{n\pi}{L} \quad \dots\dots\dots(8)$$

$$K^2 = \frac{n^2\pi^2}{L^2} \quad \dots\dots\dots(9)$$

Substituting the values of 'B' and 'K' in equation (4),

Equation (4) becomes

$$\Psi_n(x) = A \sin \frac{n\pi x}{L} \quad \dots\dots\dots(10)$$

This equation represents the wave function associated with moving free electron inside the box.

Energy of the Particle

From the equations (3) & 9

$$K^2 = \frac{8\pi^2 m E}{h^2 \pi^2}$$
$$K^2 = \frac{n^2 \pi^2}{L^2}$$

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

This is an expression for the energy of the particle

Each value of E_n is known as Eigen value

The various Eigen values of an electron enclosed in a 1D box is shown in Fig.

If $L = a$

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