

**MODULE 1: Quantum Mechanics:**

de Broglie Hypothesis, Heisenberg's Uncertainty Principle and its application (Broadening of Spectral Lines), Principle of Complementarity, Wave Function, Time independent Schrödinger wave equation (Derivation), Physical significance of a wave function and Born Interpretation, Expectation value and its physical significance, Eigen functions and Eigen values, Particle inside one dimensional infinite potential well, Role of higher dimensions (Qualitative), Waveforms and Probabilities, Particle inside a finite potential well and quantum tunnelling, Numerical Problems.

**Module - 1 Blow-up**

Subtopics	Topics to be covered	Duration
De-Broglie Hypothesis & Matter Waves	Wave-particle duality, de-Broglie wavelength formula ( $\lambda = h/p$ ) Derivation by analogy)	½ Hour
Heisenberg's Uncertainty Principle (HUP)	Mathematical relations $\Delta x \cdot \Delta p \geq h/2$ , $\Delta E \cdot \Delta t \geq h/2$ , applications to spectral line broadening, Atomic stability.	1 Hour
Complementarity Principle & Wave Function	Bohr's complementarity principle, Probabilistic nature of quantum mechanics and Born interpretation of wave function $\psi$	½ Hour
Schrödinger Wave Equation	Derivation of the time-independent Schrödinger equation from the classical wave equation in 1D, Extension to 3D(mention).	1 Hour
Eigen values and Eigen functions, Infinite 1D Potential Well	Eigen values and Eigen functions (qualitative), Schrodinger Wave Equation for 1D infinite potential well, Solutions of Schrödinger equation in an infinite well, Quantization of energy levels, normalization of wave function, Waveforms and Probabilities	1 ½ Hour
Higher Dimensions, Expectation Values,	Extension to 2D & 3D(Qualitative), expectation values of position, momentum, energy and physical significance,	½ Hour
Finite Potential Well & Tunneling	Finite square well solutions (only equations and solutions), concept of barrier penetration, quantum tunneling, applications in devices	1 Hour
Numerical Problems	Calculations on de-Broglie wavelength from Energy, uncertainty principle(Energy and time), Energy eigenvalues (Particle in 1D Box)	2 Hour

**De-Broglie Hypothesis- Dual nature of matter**

Light exhibits the phenomenon of interference, diffraction, photoelectric effect and Compton Effect. The phenomenon of interference, diffraction can only be explained with the concept that light travels in the form of waves. The phenomenon of photoelectric effect and Compton Effect can only be explained with the concept of Quantum theory of light. It means to say that light possess particle nature. Hence it is concluded that light exhibits dual nature namely wave nature as well as particle nature.

- 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 wavelength associated with matter waves are called as De-Broglie wavelength or matter wavelength ( $\lambda$ ).

4) De-Broglie wavelength is given by  $\lambda = \frac{h}{p} = \frac{h}{mv}$

### De-Broglie's Wavelength: Expression by analogy:

A particle of mass 'm' moving with velocity 'v' possess energy given by

$$E = mc^2 \rightarrow (1) \quad (\text{Einstein's Equation})$$

According to Planck's quantum theory the energy of quantum of frequency 'v' is  $E = h\nu \rightarrow (2)$

From (1) & (2)  $mc^2 = h\nu$  since  $\nu = c/\lambda$

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

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

$$\frac{mc}{h} = \frac{1}{\lambda}$$

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

But w.k.t momentum  $p = mc$  or  $= mv$  since  $v \approx c$

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

This is known as De-Broglie wavelength.

### De-Broglie's Wavelength in terms of Kinetic Energy:

For a free particle the total energy is same as its kinetic energy which is given by 'E'

$$E = \frac{1}{2}mv^2 \rightarrow (1)$$

Multiply and divide equation (1) by 'm'  $E = \frac{m^2v^2}{2m}$

But w.k.t  $p = mv$ , then

$$E = \frac{p^2}{2m} \quad \text{or } p = \sqrt{2mE} \rightarrow (2)$$

By De-Broglie wave-length is given by  $\lambda = \frac{h}{p} \rightarrow (3)$

Substitute equation (2) in (3) we get,  $\lambda = \frac{h}{\sqrt{2mE}} \rightarrow (4)$

Equation (4) represents De-Broglie's Wavelength in terms of Kinetic Energy.

**De-Broglie's Wavelength in terms of Voltage:**

Let us consider an electron of mass 'm' and having a charge 'e' accelerated by a potential 'V' volt from rest to a velocity 'v' or 'c'

$$\text{Work done on electron} = eV \rightarrow (1)$$

$$\text{Kinetic Energy of an electron} = \frac{1}{2}mv^2 \rightarrow (2)$$

Equating eqn (1) and (2),  $\text{Work done} = \text{Kinetic Energy}$

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

$$2eV = mv^2$$

Multiply 'm' on both sides,  $2meV = m^2v^2$

$$mv = \sqrt{2meV} \rightarrow (3)$$

By De-Broglie wavelength is given by  $\lambda = \frac{h}{p} \rightarrow (4)$

Substitute equation (3) in (4) we get,  $\lambda = \frac{h}{\sqrt{2meV}} \rightarrow (4)$

Equation (4) represents De-Broglie's Wavelength in terms of voltage.

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

**Heisenberg's Uncertainty Principle:**

The discovery of dual nature of material particle imposes a serious hurdle in locating the exact position and momentum of a particle simultaneously. This wax was removed by "Werner Heisenberg" in 1927 by proposing a significant principle. Later it was called Heisenberg's uncertainty principle or Heisenberg's principle of indeterminacy.

**"It is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy."**

If ' $\Delta x$ ' & ' $\Delta p$ ' are uncertainties in the measurement of position & momentum of the particle then mathematically this uncertainties of this physical variables is written as

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

Similarly, the uncertainties in measuring energy and time interval we can write

$$\Delta E. \Delta t \geq \frac{h}{4\pi}$$

And the uncertainties in measuring angular momentum & angular displacement as

$$\Delta L. \Delta \theta \geq \frac{h}{4\pi}$$

**Applications:-**

- (i) It explains the non-existence of e's in the nucleus.
- (ii) It gives the binding energy of an e's in atom.
- (iii) It calculates the radius of Bohr's first orbit.

**Application of Heisenberg's Uncertainty Principle - (Non-existence of electron inside the nucleus - Non Relativistic):**

The radius of the nucleus atom is of the order of  $10^{-14}m$ . If the electron is confined within the nucleus, the uncertainty in its position must not be greater than  $10^{-14}m$ .

W.K.T Heisenberg's Uncertainty Principle  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$  ----- (1)

Where,  $\Delta x$  is the uncertainty in position (which is radius of the nucleus atom) and  $\Delta p$  is uncertainty in momentum.

If  $\Delta x$  is the maximum uncertainty in position (i.e., radius of the nucleus atom  $10^{-14}m$ ) then,  $\Delta p$  is given by  $\Delta p \geq \frac{h}{4\pi \cdot \Delta x}$

$$\Delta p \geq \frac{6.63 \times 10^{-34}}{4\pi \cdot 10^{-14}} = 5.27 \times 10^{-21} Kg \, m/s \text{ ----- (2)}$$

Equation (2) tells the minimum value of momentum of a particle.

Using Non-Relativistic equation of energy of an electron is given by  $E = \frac{p^2}{2m_e}$

Where,  $m_e$  – rest mass of an electron =  $9.11 \times 10^{-31} \, kg$

$$E = \frac{5.27 \times 10^{-21}}{2 \times 9.11 \times 10^{-31}} = 1.527 \times 10^{-11} \, J$$

In terms of electron volts (eV),  $E = \frac{1.527 \times 10^{-11}}{1.602 \times 10^{-19}} = 95318352.06 \, eV$  or  $E_{min} = 95MeV$

Thus if an electron exists inside the nucleus it should possess the minimum energy 95MeV. But through beta-decay the energy emitted from the nucleus is of the order of 3-4MeV only.

***∴ Electrons cannot exist within the nucleus.***

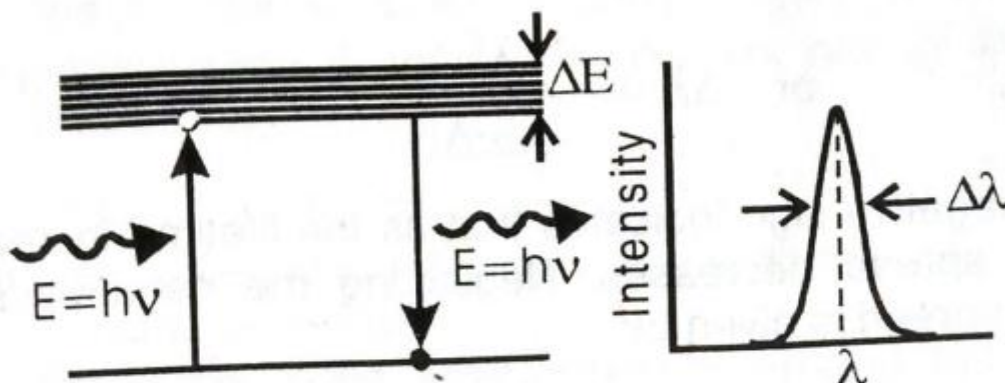
**Broadening of Spectral Lines:**

A shorter lifetime of an excited state corresponds to a larger  $\Delta t$ . According to the energy-time uncertainty relation, a larger  $\Delta t$  leads to a greater uncertainty in the energy ( $\Delta E$ ) of the state.

**Broadening of spectral line (Line width):**

When an atom absorbs a photon it rises to the excited state and it can stay for a definite time in the excited state, called the lifetime. Lifetimes of excited levels are typically of the order of  $10^{-8}$  sec. As the atom completes its lifetime in the excited state, on its own

accord without the influence of external agency, it comes to the ground state by emitting a photon of energy exactly equal to the energy.



Difference between the two levels as shown in Fig.1.9. The energy of the emitted photon is given by

$$E = h\nu = \frac{hc}{\lambda} \dots\dots\dots(1)$$

Where 'h' is Planck's constant,

'ν' is frequency,

'c' is velocity of light in vacuum and

'λ' is wavelength.

Differentiating Eq. (1) with respect to λ we get

$$\Delta E = -\frac{hc \Delta \lambda}{\lambda^2} \dots\dots\dots(2)$$

The momentum of the emitted photon is  $p = \frac{h}{\lambda}$

According to Heisenberg's uncertainty principle, the finite lifetime Δt of the excited state means there will be an uncertainty in the energy of the emitted photon given by

$$\Delta E \geq \frac{\hbar}{2\Delta t} \dots\dots\dots(3)$$

Substituting for ΔE from equation(2) and applying the condition for minimum uncertainty is we get

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

$$-\frac{hc \Delta \lambda}{\lambda^2} = \frac{\hbar}{2\Delta t}$$

$$\text{or } -\frac{hc \Delta \lambda}{\lambda^2} = \frac{h}{4\pi\Delta t}$$

$$\text{or } \Delta \lambda = \frac{\lambda^2}{4\pi c\Delta t}$$

Where the negative sign indicates that as the lifetime increases the wavelength spreads decreases. Neglecting the negative sign, the wavelength spread is given by

$$\Delta\lambda = \frac{\lambda^2}{4\pi c\Delta t}$$

This shows that for a finite lifetime of the excited state, the measured value of the emitted photon wavelength will have spread of wavelengths around the mean value  $\lambda$ . This uncertainty in the measured value of wavelength demands for very narrow spread, the lifetime of the excited state must be very high of the order of  $10^{-3}$ sec. Such excited levels are called metastable states. This concept has been adopted in the production of laser light.

### Principle of Complementarity:

#### **Statement:**

Principle of complementarity as stated by Bohr “In a situation where the wave aspect of the system is revealed, its particle aspect is concealed (hidden) and in a situation where the particle aspect is revealed its wave aspect is concealed (hidden). Revealing both simultaneously is impossible; the wave and aspects are complementary.”

#### **Alter:**

The consequences of uncertainty is that both particle and wave aspects of matter cannot be measured in the same experiment. Now suppose that an experiment is designed to measure particle properties of matter, then it implies that in these errors in the measurement of position coordinates  $\Delta x$  and time coordinates  $\Delta t$  should be zero. This in turn means that momentum and energy, and hence the wave aspects  $\left(\lambda, \frac{h}{p}, \gamma = \frac{E}{h}\right)$  are completely unknown. Similarly, if an experiment measures the wave aspects ( $\Delta p$  and  $\Delta E$ ) are zero, the position and time ( $\Delta x$  and  $\Delta t$ ) are zero.

**Explanation:** If an experiment is designed to measure the particle nature of matter, during this experiment errors of measurement of both position and time is zero and hence and hence momentum, energy and the wave nature of the matter are completely unknown and vice versa.

### Wave function:

A physical situation in quantum mechanics is represented by a function called wave function.

Or The probability of finding a particle in space, at any given instant of time is characterized by a function  $\Psi(x, y, z)$ , called as wave function

It is denoted by ‘ $\psi$ ’. It accounts for the wave like properties of particles.

Wave function is obtained by solving Schrodinger equation.

Mathematically it is given by

$$\psi = Ae^{i(kx - \omega t)}$$

### **Properties of Wave Functions:**

Physically acceptable wave function  $\Psi$  must satisfy the following conditions,

#### **1. $\Psi$ is single valued everywhere**

If  $\Psi$  has more than one value at any point, it would mean more than one value of probability of finding the particle at that point, which is obviously ridiculous. Therefore  $\Psi$  must be single valued everywhere.

#### **2. $\Psi$ is finite everywhere**

If  $\Psi$  is infinite at a point there will be large probability of finding the particle at that point this violates the uncertainty principle therefore  $\Psi$  must be finite or zero value at any point and hence  $|\Psi|^2$  represents probability.

#### **3. $\Psi$ and its first derivatives $d\Psi/dx$ with respect to its variables are continuous everywhere**

This is necessary from Schrödinger's equation itself which shows that  $d\Psi/dx$  must be finite everywhere. Further, the existence of is continuous function, which implies that the function of  $\Psi$  is also continuous everywhere.

### **Physical significance of a wave function:**

- 1) The probability of finding a particle in space, at any given instant of time is characterized by a function  $\Psi(x, y, z)$ , called as wave function.
- 2) It relates the particle and the wave statistically.
- 3) It gives the information about the particle behavior.
- 4) It is a complex quantity.
- 5)  $|\Psi|^2$  represents the probability density of the particle, which is real and positive.

### **Born interpretation:**

The wave function  $\Psi$  just as itself has no direct physical meaning. It is more difficult to give a physical interpretation to the amplitude of the wave. The amplitude of the wave function  $\Psi$  is certainly not like displacement in water wave or the pressure wave nor the waves in stretched string. It is a very different kind of wave. The quantity-squared absolute value of the amplitude gives the probability of finding the particle per unit volume at the given location in space and is referred to as probability density. This is also referred to as Born interpretation. It is given by

$$P(x) = |\Psi|^2$$

Thus, in one dimension the probability of finding a particle in the width  $dx$  of length  $x$

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

Similarly, in three dimension, the probability of finding a particle in a given small volume  $dv$  of volume  $V$  is given by



$$P dv = |\Psi|^2 dv$$

Here  $dv = dx dy dz$  and  $P$  is the probability of finding the particle at given location per unit volume and is called Probability density. Since  $\Psi$  is a complex quantity,  $|\Psi|^2 = \Psi \Psi^*$  and the product is real number.  $\Psi^*$  is the complex conjugate of  $\Psi$ .

### Time independent Schrödinger wave equation (Derivation):

According to de-Broglie's idea of matter which consists of particles of mass 'm' moving with a velocity 'v' has a wave system and its wavelength is given by,  $\lambda = \frac{h}{mv}$

But we know that waves are produced when something oscillates, the quantity that vibrates to produce matter waves can be indicated by  $\Psi$ . The period changes in  $\Psi$  produces a wave system similar to period changes in the displacement of 'x'. Hence  $\Psi$  is the displacement of

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right)$$

$$\text{or } \frac{\partial^2 \Psi}{\partial t^2} = v^2 \nabla^2 \Psi \quad \text{----- (1)}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \frac{\partial^2 \Psi}{\partial x^2} \quad \text{----- (1) for One dimension}$$

Where,  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  is a laplacian operator.

The solution for equation (1) gives  $\Psi$  as periodic variations in terms of time t,

$$\Psi_{(x,y,z,t)} = \Psi_0(x,y,z) e^{-i\omega t} \text{ or } \Psi = \Psi_0 e^{-i\omega t} \quad \text{----- (2)}$$

Where,  $\Psi_0$  = amplitude of the wave and  $\omega$  = angular velocity of the wave

The position vectors of a particle, whose Cartesian coordinates are x,y,z is given by

$$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$$

$$\text{So equation (2)} \quad \Psi_{(r,t)} = \Psi_0(r) e^{-i\omega t} \quad \text{----- (3)}$$

Differentiate equation (3) with respect to 't' twice,

$$\frac{\partial \Psi}{\partial t} = (-i\omega) \Psi_0(r) e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = (-i\omega)(-i\omega) \Psi_0(r) e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = (-\omega^2) \Psi_0(r) e^{-i\omega t}$$

$$\text{Or } \frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi \quad \text{----- (4)}$$

Comparing equation (1) and (4) we get,

$$-\omega^2 \Psi = v^2 \nabla^2 \Psi$$



$$\text{Or } \frac{\partial^2 \Psi}{\partial x^2} + \frac{\omega^2}{v^2} \Psi = 0 \text{ ----- (5)}$$

We know that  $\omega = 2\pi\gamma$  and  $v = \gamma\lambda$

$$\text{Now equation (5) becomes } \frac{\partial^2 \Psi}{\partial x^2} + \frac{4\pi^2 \gamma^2}{\gamma^2 \lambda^2} \Psi = 0$$

$$\text{Or } \frac{\partial^2 \Psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \Psi = 0 \text{ -----(6)}$$

We know that De-Broglie wavelength,  $\lambda = \frac{h}{p}$

$$\text{Then equation (6) becomes, } \frac{\partial^2 \Psi}{\partial x^2} + \frac{4\pi^2 p^2}{h^2} \Psi = 0 \text{ -----(7)}$$

Total energy E of the particle is sum of kinetic energy  $\frac{1}{2}mv^2$  and potential energy V.

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

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

$$E = \frac{p^2}{2m} + V \quad (\text{since } m^2 v^2 = p^2)$$

$$E - V = \frac{p^2}{2m}$$

$$\text{or } p^2 = 2m(E - V) \text{ -----(8)}$$

$$\text{Substitute equation (8) in (7), } \frac{\partial^2 \Psi}{\partial x^2} + \frac{4\pi^2 \cdot 2m(E-V)}{h^2} \Psi = 0$$

$$\text{Or } \frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0 \text{ ----- (9)}$$

Taking  $\hbar = \frac{h}{2\pi}$ , hence equation (9) becomes

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2} \Psi = 0 \text{ -----(10)}$$

**Equation (9) and (10) are called as Schroedinger time independent wave equation.**

Note : For a Free Particle  $V=0$ , then equation (9) becomes  $\frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 mE}{h^2} \Psi = 0 \text{ -----(11)}$

### Role of higher dimensions:

#### **Particle in 2D potential well:**

The solution for one-dimensional potential well can be extended to for a two dimensional potential well. In a two dimensional potential box, the particle (electron) can move in 'x' and 'y' directions. Therefore instead of one quantum number 'n', we have use two quantum numbers  $n_x$  and  $n_y$  corresponding the two co-ordinate axis (i.e.,) x and y respectively.

Let us consider a particle enclosed in a two-dimensional potential well of length 'a' and 'b' along x and y-axis respectively as shown in figure.

Since the particle inside 2-D well has an elastic collisions with the walls, the potential energy of the electron inside the well is constant and can be taken as zero for simplicity.

Therefore, we say that outside the well and on the wall of the well, the potential energy is infinity ( $\infty$ ).

As per the boundary conditions

$$\text{At, } V(x, y) = 0 \text{ when } 0 < x < a,$$

$$V(x, y) = 0 \text{ when } 0 < y < b \quad (\text{condition - 1})$$

Within these boundary conditions, the particle exists and we need to find the energy values and the wave functions.

$$\text{At, } V(x, y) = \infty \text{ when } 0 \geq x \geq a,$$

$$V(x, y) = \infty \text{ when } 0 \geq y \geq b \quad (\text{condition - 2})$$

In this area the particle does not exist and therefore the wave function is zero.

Let us consider the two dimensional time independent Schrodinger wave equation,

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

Note: For a Free Particle  $V=0$ , then equation becomes  $\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{8\pi^2 m E}{h^2} \Psi = 0 \dots \dots \dots (12)$

Equation (12) is a partial differential equation, in which  $\Psi$  is a wave function of two variables 'x' and 'y'.

### Particle in 3D potential well:

Let us consider a particle in a 3-dimensional potential well of length a, b and c along x, y and z axis respectively as shown in figure.

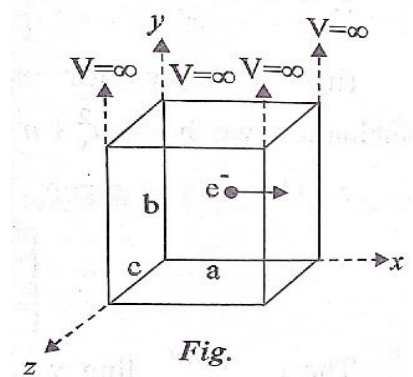
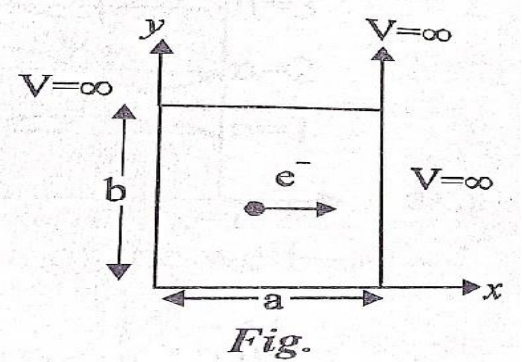
Since the particle inside 3-D well has an elastic collisions with the walls, the potential energy of the electron inside the well is constant and can be taken as zero for simplicity.

Therefore, we say that outside the well and on the wall of the well, the potential energy is infinity ( $\infty$ ).

As per the boundary conditions

$$\text{At, } V(x, y, z) = 0 \text{ when } 0 < x < a,$$

$$V(x, y, z) = 0 \text{ when } 0 < y < b$$



$$V(x, y, z) = 0 \text{ when } 0 < x < c$$

(condition – 1)

Within these boundary conditions, the particle exists and we need to find the energy values and the wave functions.

$$\text{At, } V(x, y, z) = \infty \text{ when } 0 \geq x \geq a,$$

$$V(x, y, z) = \infty \text{ when } 0 \geq x \geq b,$$

$$V(x, y, z) = \infty \text{ when } 0 \geq x \geq c \quad (\text{condition} - 2)$$

In this area the particle does not exist and therefore the wave function is zero.

Let us consider the two dimensional time independent Schrodinger wave equation,

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

Note: For a Free Particle  $V=0$ , then equation becomes

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m E}{h^2} \Psi = 0 \dots\dots\dots (13)$$

Equation(13) is a partial differential equation, in which  $\Psi$  is a wave function of two variables 'x', 'y' and 'z'.

### Expectation Value:

In quantum mechanics, measurements are probabilistic. The expectation value (average value) of an observable A is the statistical mean outcome obtained from repeated measurements on identically prepared quantum systems.

Mathematical Definition For a normalized wave function  $\psi(x,t)$ , the expectation value of an operator  $\hat{A}$  is

$$\langle A \rangle = \int_{-\infty}^{+\infty} \psi^*(x, t) \hat{A} \psi(x, t) dx$$

Where,  $\psi^*(x, t)$  is the complex conjugate of  $\psi(x, t)$

### Examples:

#### 1. Position:

$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\psi(x, t)|^2 dx$$

Represents the average position of the particle.

#### 2. Momentum:

$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x, t) \left( -i\hbar \frac{\partial}{\partial x} \right) \psi(x, t) dx$$

Represents the average momentum.

## 3. Energy:

$$\langle E \rangle = \int_{-\infty}^{+\infty} \psi^*(x, t) \hat{H} \psi(x, t) dx$$

where  $\hat{H}$  is the Hamiltonian operator.

Physical Significance:

- $\langle A \rangle$  gives the average value of observable A from many measurements.
- It is not necessarily a value seen in a single measurement.
- Provides a macroscopic meaning to microscopic quantum states.
- Links quantum mechanics with classical averages.

**Properties of Expectation Values**

1. Linearity:  $\langle aA + bB \rangle = a\langle A \rangle + b\langle B \rangle$
2. Reality: For Hermitian operators (observables), expectation values are always real.
3. Time Evolution (Ehrenfest's theorem):

$$\frac{d}{dt} \langle x \rangle = \frac{\langle p \rangle}{m}, \quad \frac{d}{dt} \langle p \rangle = - \left\langle \frac{\partial V}{\partial x} \right\rangle$$

Showing that quantum averages approximately follow classical mechanics.

Summary

- Expectation value = quantum average of a physical quantity.
- Connects quantum probabilities with experimental outcomes.
- Provides the bridge between quantum mechanics and classical physics.

**Eigen functions and Eigen Values:**

Any physical system is defined by its momentum, position, energy etc., Two important physical quantities of a system in quantum mechanics are wave function and energy. The solution of wave function are called Eigen function. The solution has to satisfy the following criteria in quantum mechanics.

- 1) The wave function must not be single value everywhere.
- 2) It must be finite everywhere.
- 3) The wave function and its first derivatives with variable must be continuous everywhere.

All such acceptable wave functions are called **Eigen functions**.

Once Eigen functions are known, it can be used in Schroedinger equation to determine the energy of the system. We can get restricted set of energy values. These set of values are called Eigen values.

**Particle inside one dimensional potential well of infinite depth:**

We know that Schrodinger time independent wave equation for a free particle is

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 m E}{h^2} \Psi = 0 \text{ --- (1)}$$

By assuming that  $k^2 = \frac{8\pi^2 m E}{h^2}$  --- (2)

Now equation (1) becomes,  $\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0$

equation (2) can be re written as,  $E = \frac{k^2 h^2}{8\pi^2 m}$  --- (4)

Equation (3) is similar to equation of simple harmonic motion and so that the solution can be written as

$$\Psi(x) = A \sin kx + B \cos kx \text{ --- (5)}$$

Where, A and B are called as arbitrary constants.

To evaluate the constants A and B in equation (5) we can use the Boundary conditions.

Boundary conditions:

(i)  $\Psi = 0$ , When  $x = 0$

Substitute in equation (5)  $0 = 0 + B \cos 0$

$$B = 0 \text{ --- (6)}$$

(ii)  $\Psi = 0$ , When  $x = L$

Substitute in equation (5)  $0 = A \sin kL + B \cos kL$

From equation (6)  $B = 0$ , then

$$0 = A \sin kL + 0 \text{ --- (7)}$$

$$\therefore A \neq 0, \text{ then } \sin kL = 0$$

$\sin kL$  is "0" when  $kL$  takes the value of  $n\pi$ , i.e.  $kL = n\pi$

Where n is positive integer,  $n = 1, 2, 3, \dots$

$$\therefore k = \frac{n\pi}{L} \text{ --- (8)}$$

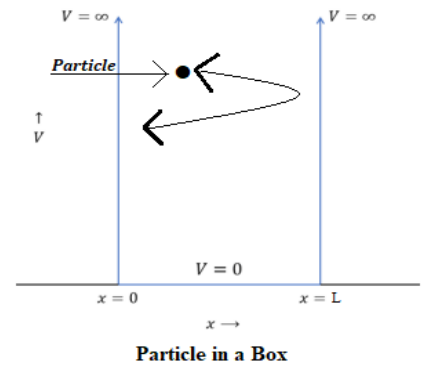
Substitute equation (8) in (4) we get

$$E = \frac{\left(\frac{n\pi}{L}\right)^2 h^2}{8\pi^2 m}$$

Or  $E_n = \frac{n^2 h^2}{8mL^2} \text{ --- (9)}$

Substitute equation (8) in (5) we get  $\Psi_n(x) = A \sin \frac{n\pi x}{L} \text{ --- (10)}$

Equation (9) is known as Eigen values and Equation (10) is known as Eigen function.



**To evaluate the constant “A”:**

The constant “A” is determined by normalization of wave function as follows.

Probability density is given by  $\int_0^L \Psi \cdot \Psi^* dx = 1$  ——— (11)

We know that  $\Psi_n(x) = A \sin \frac{n\pi x}{L}$

Then,  $\Psi \cdot \Psi^* = A \sin \frac{n\pi x}{L} \times A \sin \frac{n\pi x}{L}$

$$\Psi \cdot \Psi^* = A^2 \sin^2 \left( \frac{n\pi x}{L} \right) \text{ ——— (11a)}$$

Now equation (11) becomes,  $\int_0^L A^2 \sin^2 \left( \frac{n\pi x}{L} \right) dx = 1$   $\left( \sin^2 \theta = \frac{1 - \cos 2\theta}{2} \right)$

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

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

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

The second term in the integral becomes zero at both the limits.

$$\therefore \text{equation becomes, } \frac{A^2}{2} [x]_0^L = 1$$

$$\text{Thus, } \frac{A^2}{2} [L] = 1$$

$$A = \sqrt{\frac{2}{L}} \text{ ——— (12)}$$

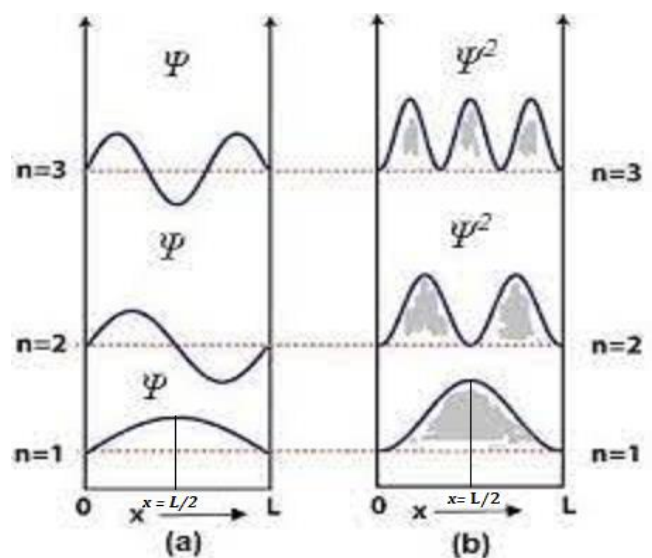
On substituting  $A = \sqrt{\frac{2}{L}}$  in equation (10), we get the normalized wave function of a particle in a

$$\text{box, } \Psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \text{ ——— (13)}$$

Equation (13) is known as **Normalized wave function**.

The first three Eigen functions  $\Psi_1, \Psi_2, \Psi_3$  together with the probability densities

$|\Psi_1|^2, |\Psi_2|^2, |\Psi_3|^2$  and Eigen values  $E_1, E_2, E_3$  are as shown in figure (a) & (b) respectively for  $n = 1, 2$  & 3.



- 1) In every case  $\Psi_1$  and  $|\Psi_1|^2$  equal to zero at  $x = 0$  and  $x = L$  at the boundaries of the box.
- 2) The probability of a particle present in a box is i.e.,  
 For  $n=1$ , the probability is maximum at  $x = \frac{L}{2}$   
 For  $n=2$ , the probability at  $x = \frac{L}{2}$   
*is zero but maxima at  $x = \frac{L}{4}$   
 and  $x = \frac{3L}{4}$ .*

### Expectation value:

In quantum mechanics, the expectation value is the probabilistic expected value of the result (measurement) of an experiment. It can be thought of as an average of all the possible outcomes of a measurement as weighted by their likelihood. Expectation value as such it is not the most probable value of a measurement. In the real sense the expectation value may have zero probability of occurring. Let us consider a particle moving along the x-axis. The result of a measurement of the position  $x$  is a continuous random variable.

Consider a wave function  $\Psi(x,t)$ . The  $|\Psi_{(x,t)}|^2$  value is a probability density for the position observable and  $|\Psi_{(x,t)}|^2 dx$  is the probability of finding the particle between  $x$  and  $x+dx$  at time  $t$ . Thus, if a measurement of position is repeated many times in an identical way on an identical particle in identical circumstances, many possible outcomes are possible and the expectation value of these outcomes is, according to the following equation.

$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\Psi_{(x,t)}|^2 dx$$

### Probability density:

If  $\psi$  is a complex no. then its complex conjugate is obtained by replacing  $i$  by  $-i$ ,  $\psi$  alone do not have any meaning but only  $\psi\psi^*$  gives the probability of finding the particle. In quantum mechanics we cannot assert where exactly a particle is. We cannot say where it is likely to be  $P(x) = \psi\psi^*$  or Probability density is given by  $\int_0^L \Psi \cdot \Psi^* dx = 1$



**Normalization of wave function:**

Normalization: If the particle exists somewhere at all the time. Let be the wave function associated with the particle, then the probability density of particle in a volume element is  $|\Psi|^2$ . If we further extend the case, where the particle is definitely present in some region or space, as per the statistical rule the normalization is given by  $\int_0^V |\Psi|^2 dV = 1$

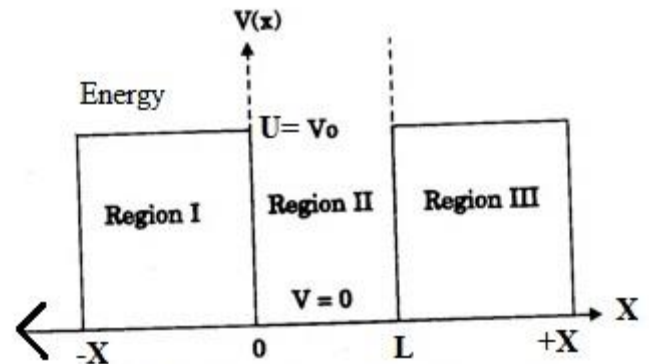
This is because, a value 1 for probability means, it is clearly a certainty. However, in the above case if we are not at all certain about locating the particle in a finite volume anywhere in the space, then the expectation will become limited to the extent that it exists somewhere in space. Then the limits in equation extend  $-\infty$  to  $+\infty$  to and the probability becomes.

$$\int_{-\infty}^{+\infty} |\Psi|^2 dV = 1$$

**Particle in a Finite Potential Well:**

Fig shows a square potential well of width L. consider a particle with energy E moving along the X-axis. The energy E of the trapped particle less than the height U of the barriers.

Schrodinger steady state equation for regions I and III is



**Fig- Finite potential well**

$$\frac{d^2\Psi}{dx^2} + \frac{2m(E - U)}{\hbar^2} \Psi = 0 \dots \dots \dots (1)$$

$$\text{Put, } \frac{\sqrt{2m(U-E)}}{\hbar} = -a^2 \dots \dots \dots (1a)$$

$$\text{Equation (1) becomes, } \frac{d^2\Psi}{dx^2} - a^2 \Psi = 0 \dots \dots \dots (2)$$

The solution to equation(2) are

$$\Psi_I = Ae^{ax} + B^{-ax} \dots \dots \dots (3)$$

$$\Psi_{III} = Ce^{ax} + De^{-ax} \dots \dots \dots (4)$$

For  $\Psi$  to remain finite as  $x \rightarrow \pm\infty$ , we must have  $B = 0$  and  $C = 0$ ,

$$\text{then equation (3) and (4) becomes, } \Psi_I = Ae^{ax} \dots \dots \dots (5)$$

$$\Psi_{III} = De^{-ax} \dots \dots \dots (6)$$

These wave functions decrease exponentially inside the barriers at the sides of the well.

Schrodinger equation for region II is  $\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2} \Psi = 0 \dots \dots \dots (7)$

Solution for equation (7) is  $\Psi_{II} = F \sin \frac{\sqrt{2mE}}{\hbar}x + G \cos \frac{\sqrt{2mE}}{\hbar}x = 0 \dots \dots \dots (8)$

At the boundaries  $x = 0$  and  $x = L$ , the wave function inside and outside must have the same value and the same slope.

$$\Psi_I = \Psi_{II} \text{ and } \frac{d\Psi_{II}}{dx} = \frac{d\Psi_I}{dx} \text{ at } x = 0 \dots \dots \dots (A)$$

$$\Psi_{II} = \Psi_{III} \text{ and } \frac{d\Psi_{II}}{dx} = \frac{d\Psi_{III}}{dx} \text{ at } x = L \dots \dots \dots (B)$$

These conditions when applied to diff w.r.t x at (x=0), equation (5) and (8) yield the following relation

$$\text{eqn(5), } \Psi_I = Ae^{ax} \text{ (when } x = 0) \text{ becomes } \Psi_I = A \dots \dots \dots (8a)$$

Similarly eqn(8)  $\Psi_{II} = F \sin \frac{\sqrt{2mE}}{\hbar}x + G \cos \frac{\sqrt{2mE}}{\hbar}x = 0$  (when  $x = 0$ ) becomes

$$\Psi_{II} = G \dots \dots \dots (8b)$$

We can write by equating (8a) and (8b) from boundary condition yields to

$$G = A \dots \dots \dots (9)$$

$$\text{And also we can, } F \frac{\sqrt{2mE}}{\hbar} = aA \dots \dots \dots (10)$$

As substitute eqn(6) and eqn(8) in eqn(B) at  $x=L$

$$\left( \frac{d\Psi_{II}}{dx} = \frac{d\Psi_{III}}{dx} \right) \text{ (at } x = L)$$

$$F \sin \frac{\sqrt{2mE}}{\hbar}L + G \cos \frac{\sqrt{2mE}}{\hbar}L = De^{-aL} \dots \dots \dots (11)$$

$$\text{diff now eqn becomes, } F \frac{\sqrt{2mE}}{\hbar} \cos \frac{\sqrt{2mE}}{\hbar}L - G \frac{\sqrt{2mE}}{\hbar} \sin \frac{\sqrt{2mE}}{\hbar}L = -aDe^{-aL} \dots \dots \dots (12)$$

$$\text{Now eqn (9) and (10) gives } \frac{F}{a} \frac{\sqrt{2mE}}{\hbar} = A$$

We can write it as ,  $F = Ga \frac{\hbar}{\sqrt{2mE}} \dots\dots\dots(13)$

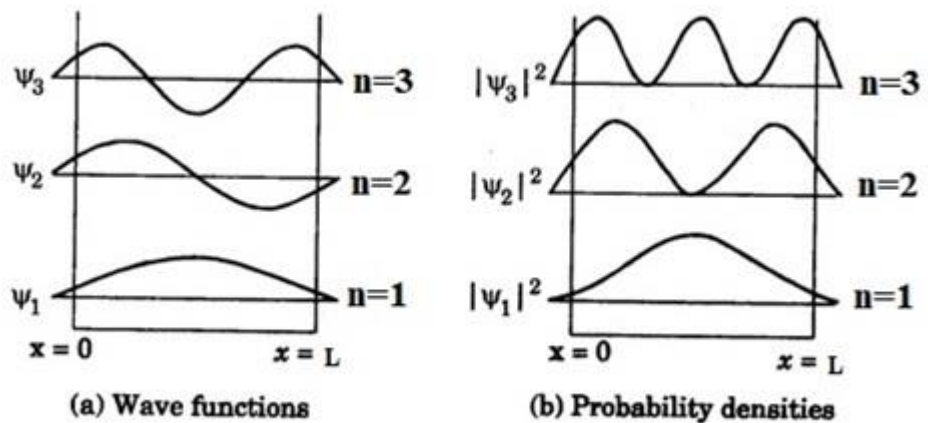
Equation (13) together with eqn (11) and (12) yields,

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}L\right) = \frac{2a\frac{\sqrt{2mE}}{\hbar}}{\frac{2mE}{\hbar^2} - a^2}$$

or we can write  $\tan\left(\frac{\sqrt{2mE}}{\hbar}L\right) = \frac{2\sqrt{E(U-E)}}{2E-U} \dots\dots\dots(14)$

Also we can say  $U=V_0$ , then equ(14) becomes,  $\tan\left(\frac{\sqrt{2mE}}{\hbar}L\right) = \frac{2\sqrt{E(V_0-E)}}{2E-V_0} \dots\dots\dots(14)$

Only those energy levels of  $E$  satisfy this relation are the allowed energy states. Thus the energy is quantised. The allowed energy levels are found by numerical or graphical methods.



The wave functions for the first three allowed energy values and the corresponding probability densities for finding the particle at different locations are shown in figure.(a) and (b) respectively.

### Quantum Tunnelling:

Concept: Classically, a particle with  $E < V_0$  cannot cross a barrier. Quantum mechanically, the wave function extends into and even through the barrier, giving a finite probability of transmission — this is tunnelling.

Barrier Penetration Probability For a barrier of height  $V_0$  and width  $L$ :

$$T \approx e^{-2\kappa L}, \quad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

### Physical Examples

1. Alpha decay in nuclei.
2. Scanning tunnelling microscope (STM).
3. Tunnel diodes in electronics.
4. Proton tunnelling in stellar fusion

**MODULE 1 - NUMERICALS – DE-BROGLIE WAVELENGTH**

1. Calculate the de-Broglie wavelength associated with neutron of mass  $1.674 \times 10^{-27}$  kg moving with one tenth part of the velocity of light.

*Data:* Mass of the neutron:  $1.674 \times 10^{-27}$  kg,

Velocity of light,  $c = 3 \times 10^8$  m/s

Velocity of neutron  $v = \frac{1}{10} \times c = 3 \times 10^7$  m/s

To Find: De Broglie wavelength,  $\lambda = ?$

Solution: De Broglie wavelength,  $\lambda = \frac{h}{mv}$

$$\lambda = \frac{6.6 \times 10^{-34}}{(1.074 \times 10^{-27})(3 \times 10^7)} = 1.314 \times 10^{-14} \text{ m}$$

**$\therefore$  De – Broglie wavelength associated of the neutron is  $1.314 \times 10^{-14}$  m**

2. A particle of mass  $0.5 \text{ MeV}/c^2$  has kinetic energy 100eV. Find its de-Broglie wavelength.

*Data:* Mass of the particle  $m = 0.5 \text{ MeV}/c^2$ ,

(Dec. 2014 | Jan 2020, Dec 2019 | Mar 2022–18S)

Kinetic energy  $E = 100 \times 1.609 \times 10^{-19}$  J

Velocity of light,  $c = 3 \times 10^8$  m/s

Velocity of neutron  $v = \frac{1}{10} \times c = 3 \times 10^7$  m/s

To find: De Broglie wavelength,  $\lambda = ?$

Solution: De Broglie wavelength,  $\lambda = \frac{h}{mv}$

We have, mass of the particle,  $m = 0.5 \frac{\text{MeV}}{c^2} = \frac{0.5 \times 10^6 \times 1.602 \times 10^{-19}}{3 \times 10^8} = 8.9 \times 10^{-31} \text{ kg}$

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 8.9 \times 10^{-31} \times 100 \times 1.602 \times 10^{-19}}} = 1.24 \times 10^{-10} \text{ m}$$

**$\therefore$  The De Broglie wavelength of the particle is  $1.24 \times 10^{-10}$  m**

3. Evaluate De Broglie Wavelength of helium nucleus that is accelerated through 500V.

(Mar 2022–21S)

*Data:* Mass of proton = mass of neutron =  $1.67 \times 10^{-27}$  kg.

Potential difference = 500V

To Find: De Broglie wavelength,  $\lambda = ?$

Solution: A Helium nucleus has 2 protons and 2 neutrons.

$\therefore$  Mass of nuclues =  $4m \times 1.67 \times 10^{-27}$  kg

since there are 2 protons, the charge on the nuclues,  $q = 2 \times 1.602 \times 10^{-19}$

we have the equation for de broglie wavelength,  $\lambda = \frac{h}{\sqrt{2mE}}$

But, for a charge of  $q$  accelerated through a potential  $V$ , the energy is given by  $E = qV$  (assuming its initial velocity as zero).

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{6.63 \times 10^{-34}}{\sqrt{2(4 \times 1.67 \times 10^{-27})(2 \times 1.602 \times 10^{-19}) \times 500}} = 4.53 \times 10^{-13} \text{ m}$$

**$\therefore$  The de broglie wavelength is  $4.53 \times 10^{-13}$  m**

4. Calculate the energy of the neutron in eV, if its De-Broglie wavelength is

$3 \text{ \AA}$  and  $m_n = 1.67 \times 10^{-27} \text{ kg}$ . (Aug 2022–21S)

*Data:* Wavelength,  $\lambda = 3 \text{ \AA} = 3 \times 10^{-10} \text{ m}$

mass of neutron,  $m_n = 1.67 \times 10^{-27} \text{ kg}$

To find: Energy of the neutron in terms of eV,  $E = ?$

Solution: De – Broglie wavelength,  $\lambda = \frac{h}{\sqrt{2mE}}$

$$\text{or rearranging, } E = \frac{h^2}{2 \times m \times \lambda^2} = \frac{(6.63 \times 10^{-34})^2}{2 \times 1.67 \times 10^{-27} \times (3 \times 10^{-10})^2} = 1.462 \times 10^{-21} \text{ J}$$

$$\text{in terms of eV, } = \frac{1.462 \times 10^{-21}}{1.602 \times 10^{-19}} = 0.9 \times 10^{-2} \text{ eV.}$$

$\therefore$  **Energy of the neutron in terms of eV,  $E = 0.9 \times 10^{-2} \text{ eV}$**

5. Compute the De-Broglie wavelength for an electron moving with one tenth part of the velocity of light. (Dec 2018 –17S)

Data: Mass of the electron =  $9.11 \times 10^{-31} \text{ kg}$ ,

Velocity of light,  $c = 3 \times 10^8 \text{ m/s}$

Velocity of neutron  $v = \frac{1}{10} \times c = 3 \times 10^7 \text{ m/s}$

To Find: De Broglie wavelength,  $\lambda = ?$

Solution: De Broglie wavelength,  $\lambda = \frac{h}{mv}$

$$\lambda = \frac{6.6 \times 10^{-34}}{(9.11 \times 10^{-31})(3 \times 10^7)} = 24.25 \times 10^{-12} \text{ m}$$

$\therefore$  **De – Broglie wavelength associated of the neutron is  $1.314 \times 10^{-14} \text{ m}$**

6. The kinetic energy of an electron is equal to energy of photon with a wavelength of 560nm. Calculate the de Broglie wavelength of the electron. (Jan-2025-22S-CSE STREAM)

The kinetic energy of an electron = energy of photon with  $\lambda = 560 \times 10^{-9} \text{ m}$

$$E = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{560 \times 10^{-9}} = 3.549 \times 10^{-19} \text{ J}$$

7. The inherent uncertainty in the measurement of time spent by Iridium 199 nuclei in the excited state is found to be  $1.4 \times 10^{-10}$  sec. estimate the uncertainty that result in its energy in the excited state.

Data: Uncertainty in time  $\Delta t = 1.4 \times 10^{-10}$  sec

(Sep 2020 | Feb 2021-18S)

To find: Uncertainty in energy  $\Delta E = ?$

By Heisenberg's uncertainty principle,  $\Delta E = \frac{h}{4\pi\Delta t}$

$$\Delta E = \frac{6.63 \times 10^{-34}}{4\pi \times 1.4 \times 10^{-10}} = 3.77 \times 10^{-25} J$$

$$\Delta E = 2.35 \times 10^{-6} eV$$

$$\therefore \text{Uncertainty in energy } \Delta E = 2.35 \times 10^{-6} eV$$

8. A spectral line of Wavelength  $5461 \text{ \AA}$  has a width of  $10^{-4} \text{ \AA}$ . Evaluate the minimum time spent by the electron in the upper energy state.

(Aug 2022-18S)

Data: wavelength of the spectral line  $\lambda = 5461 \times 10^{-10} m$

Width of the spectral lines (also means uncertainty in the wavelength value),

$$\Delta\lambda = 10^{-4} \times 10^{-10} m = 10^{-14} m$$

To find:

The minimum time sent by the electrons in the upper state (also means the uncertainty in the measurement of time for the system),  $\Delta t = ?$

Solution : We have the equation  $E = hv = \frac{hc}{\lambda}$

$$\Delta E = hc \Delta \left[ \frac{1}{\lambda} \right] \text{ or}$$

$$\Delta E = hc \frac{\Delta\lambda}{\lambda^2} \dots \dots \dots (1)$$

As per the uncertainty principle.  $\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$

$$\text{Or } \Delta t \geq \frac{h}{4\pi \cdot \Delta E} \dots \dots \dots (2)$$

Sing eqn(1), the right side of the above inequality can be written as,

$$\begin{aligned} \Delta t &= \frac{h}{4\pi \cdot \Delta E} = \frac{h\lambda^2}{4\pi(hc \cdot \Delta\lambda)} = \frac{\lambda^2}{4\pi(c \cdot \Delta\lambda)} \\ &= \frac{(5461 \times 10^{-10})^2}{4\pi \times 3 \times 10^8 \times 10^{-14}} \\ \Delta t &= 0.8 \times 10^{-8} \text{ second.} \end{aligned}$$

Thus, Using the above in the inequality (2), we have,

$$\Delta t = 0.8 \times 10^{-8} \text{ second}$$

$\therefore$  The minimum time spent by the electrons is,  $\Delta t = 0.8 \times 10^{-8} \text{ second}$

9. The position and momentum of an electron with energy  $0.5 \text{ KeV}$  are determined. What is the minimum percentage of uncertainty in its momentum, if the uncertainty in the measurement of its position is  $0.5 \text{ \AA}$ . (Mar 2022- 21S)

Data: Energy of electron,  $E = 0.5 \times 10^3 eV = 0.5 \times 10^3 \times 1.602 \times 10^{-19} J$

Maximum uncertainty in position,  $\Delta x = 0.5 \text{ \AA} = 0.5 \times 10^{-10} m$

To find:

Minimum percentage uncertainty in momentum =?

Solution: We have the uncertainty principle given by,  $\Delta x \cdot \Delta P_x \geq \frac{h}{4\pi}$

$$\Delta P_x \geq \frac{h}{4\pi \times \Delta x} = \frac{6.63 \times 10^{-34}}{4\pi \times 0.5 \times 10^{-10}} = 1.06 \times 10^{-24}$$

$$\therefore \text{Uncertainty in momentum} = 1.06 \times 10^{-24}$$

We have the equation for momentum,  $P = \sqrt{2mE} = \sqrt{2 \times 9.11 \times 10^{-31} \times 1.6 \times 10^{-19}}$   
 $\therefore \text{Momentum } P = 1.207 \times 10^{-23}$

$$\therefore \text{Percentage uncertainty in momentum} = \frac{\text{Uncertainty in momentum}}{\text{momentum}} \times 100$$

$$= \frac{1.06 \times 10^{-24}}{1.207 \times 10^{-23}} \times 100 = 8.8$$

$$\therefore \text{Percentage of uncertainty} = 8.8$$

10. An electron has a speed of 100m/s. The inherent uncertainty in its measurement is 0.005%. Calculate the corresponding uncertainty in the measurement of the position.  
 (CSE Stream, JAN/FEB – 2023 | 22S)

$$\text{Solution: } \Delta v = 100 \times \frac{0.005}{100} = 0.005 \text{ m/s}$$

$$\Delta x \geq \frac{h}{4\pi m \Delta v} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.005} = 0.0115 \text{ m}$$

Uncertainty in the measurement of the position,  $\Delta x = 0.0115 \text{ m}$

11. In the measurement of position and momentum that involved an uncertainty of 0.003%, the speed of an electron was found to be 800m/s. Calculate the corresponding uncertainty that arises in determining its position. (EEE Stream, JAN/FEB – 2023)

$$\text{Solution: } \Delta v = 800 \times \frac{0.003}{100} = 0.024 \text{ m/s}$$

$$\Delta x \geq \frac{h}{4\pi m \Delta v} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.024} = 2.41 \times 10^{-3} \text{ m}$$

12. In a measurement of position and velocity of an electron moving with a speed of  $6 \times 10^5 \text{ m/s}$ , Calculate the highest accuracy with its position could be determined, if the inherent error in the measurement of its velocity is 0.01% for the speed. (CSE Stream, JUNE/JULY – 2023 | 22S)

$$\text{Solution: } \Delta v = 6 \times 10^5 \times \frac{0.01}{100} = 60 \text{ m/s}$$

$$\Delta x \geq \frac{h}{4\pi m \Delta v} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 60} = 9.65 \times 10^{-7} \text{ m}$$



## MODULE 1 - NUMERICALS – ENERGY EIGENVALUES (PARTICLE IN 1D BOX)

13. An electron bound in a one-dimensional potential well of width  $1\text{\AA}$ , but infinite well height. Find its energy values in the ground state and in the first two excited states.

(Dec 2018–17S, Jan 2019 | July 2019 | Aug 2021–18S)

Data: Width of the potential well,  $L = 1\text{\AA} = 10^{-10}\text{m}$

To find: Values of energy of the electron in the ground and the first two excited states  
i.e.  $E_1 = ?$ ,  $E_2 = ?$ ,  $E_3 = ?$

Solution: The energy of the electron in a one-dimensional infinite potential well is given by,

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

Where, the values of E that we get for  $n=1, 2$  and  $3$  correspond respectively to  $E_1, E_2$  and  $E_3$ .

$$\therefore E_1 = \frac{n^2 h^2}{8mL^2} = \frac{1^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2}$$

$$\therefore E_0 = E_1 = 6.0314 \times 10^{-18}\text{J} = 37.64\text{ eV}$$

$$E_2 = \frac{n^2 h^2}{8mL^2} = \frac{2^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2} = 4 \times 6.0314 \times 10^{-18}\text{J}$$

$$\therefore E_2 = 2.4125 \times 10^{-17}\text{J} = 150.54\text{ eV}$$

$$E_3 = \frac{n^2 h^2}{8mL^2} = \frac{3^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2} = 9 \times 6.0314 \times 10^{-18}\text{J}$$

$$\therefore E_3 = 5.4282 \times 10^{-17}\text{J} = 338.7\text{ eV}$$

$\therefore$  The values of Energy of the electron in the ground and the first two excited states are respectively to

$$E_1 = 6.0314 \times 10^{-18}\text{J or } 37.64\text{ eV},$$

$$E_2 = 2.4125 \times 10^{-17}\text{ or } 150.54\text{ eV and}$$

$$E_3 = 5.4282 \times 10^{-17}\text{J or } 338.7\text{ eV}$$

14. An electron bound in a one dimensional potential well of height and width of  $0.2\text{nm}$ . Calculate energy required for the ground state and its first two excited states.

(Sep 2020 – 18S, Aug 2022–21S)

**NOTE: SOLVE AS PER PROBLEM-15**

15. Calculate the energy of the first three states for an energy of an electron in one dimensional potential well of width  $1\text{\AA}$ . (CSE Stream, JAN/FEB – 2024 | 22S)

Data: Width of the potential well,  $L = 1\text{\AA} = 10^{-10}\text{m}$

To find: Values of energy of the electron in the ground and the first two excited states  
i.e.  $E_1 = ?$ ,  $E_2 = ?$ ,  $E_3 = ?$

Solution: The energy of the electron in a one-dimensional infinite potential well is given by,

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

Where, the values of E that we get for  $n=1, 2$  and  $3$  correspond respectively to  $E_1, E_2$  and  $E_3$ .

$$\therefore E_1 = \frac{n^2 h^2}{8mL^2} = \frac{1^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2}$$

$$\therefore E_0 = E_1 = 6.0314 \times 10^{-18} J = 37.64 \text{ eV}$$

$$E_2 = \frac{n^2 h^2}{8mL^2} = \frac{2^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2} = 4 \times 6.0314 \times 10^{-18} J$$

$$\therefore E_2 = 2.4125 \times 10^{-17} J = 150.54 \text{ eV}$$

$$E_3 = \frac{n^2 h^2}{8mL^2} = \frac{3^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(10^{-10})^2} = 9 \times 6.0314 \times 10^{-18} J$$

$$\therefore E_3 = 5.4282 \times 10^{-17} J = 338.7 \text{ eV}$$

∴ The values of Energy of the electron in the ground and the first two excited states are respectively to

$$E_1 = 6.0314 \times 10^{-18} J \text{ or } 37.64 \text{ eV} ,$$

$$E_2 = 2.4125 \times 10^{-17} \text{ or } 150.54 \text{ eV and}$$

$$E_3 = 5.4282 \times 10^{-17} J \text{ or } 338.7 \text{ eV}$$

16. Calculate the first three energy states for an electron in one dimensional potential well of width of 0.1nm.

(Jan-2025-22S-CSE STREAM)

Data: Width of the potential well,  $L = 0.1 \text{ nm} = 0.1 \times 10^{-9} \text{ m}$

To find: Values of energy of the electron in the ground and the first two excited states  
i.e  $E_1 = ?$  i.e., Ground state,  $E_2 = ?$  (First excited state),  $E_3 = ?$  (Second excited state)

Solution: The energy of the electron in a one dimensional infinite potential well is given by,

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

$$\therefore \text{First energy state, } E_1 = \frac{n^2 h^2}{8mL^2} = \frac{1^2 (6.63 \times 10^{-34})^2}{8(9.11 \times 10^{-31})(0.1^{-9})^2}$$

$$\therefore E_0 = E_1 = 6.0314 \times 10^{-18} J = 37.64 \text{ eV}$$

$$\text{First Excited State Energy } n=2, E_2 = 4 E_1 = 24.115 \times 10^{-18} J = 150.72 \text{ eV}$$

$$\text{First Excited State Energy } n=2, E_3 = 9 E_1 = 54.260 \times 10^{-18} J = 339.12 \text{ eV}$$