

# Module - 1

## Elements of Quantum Mechanics

**Syllabus:** de-Broglie hypothesis - Matter waves and de-Broglie wavelength, Heisenberg's uncertainty principle, wave functions, their properties and physical significance normalization, time independent Schrodinger's wave equation in 1-dimension, particle in an one-dimensional infinite potential well, Numerical problems.

### Wave particle dualism:

While explaining the phenomenon's like, Interference, Diffraction, Polarization, etc., the radiation/ light is considered to have wave nature. While explaining the phenomenon's like, Black body spectrum, Photoelectric effect etc., the radiation/ light is considered to have particle nature.

This dual nature of matter/ radiation was observed by scientist de-Broglie. This double nature of matter/radiation is known as Wave particle dualism. The double nature of radiation cannot be observed simultaneously, i.e., both particle and wave nature cannot possible occur at the same time. During Propagation, the radiation behaves as Wave Nature and during Absorption or Emission, the radiation behaves as Particle nature. This is referred as de-Broglie hypothesis.

According to de-Broglie hypothesis, the wavelength associated with the material particle in motion is known as de-Broglie wavelength ( $\lambda$ ), given by the equation

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

Where,  $h$  – Planck's constant

$p$  – Momentum of particle.

For any particle moving with velocity  $v$ ,

$$\text{Eqn (1)} \Rightarrow \lambda = \frac{h}{mv}$$

For radiation having velocity  $c$ ,

$$\text{Eqn (1)} \Rightarrow \lambda = \frac{h}{mc}$$

**Matter wave:** It is the wave associated with material particle in motion.

The energy of moving particle is given by the equation,  $E = mc^2$ .

From Planck's law, the energy of a particle/Photon is given by the equation,  $E = h\nu = hc/\lambda$

From above two equations, we get,  $\lambda = \frac{h}{mc} = \frac{h}{p}$

Other forms of equations of de-Broglie wavelength ( $\lambda$ ):

i) **De-Broglie wavelength in terms of kinetic energy (E):**

$$\text{We know, } \lambda = \frac{h}{p}$$

$$\text{Kinetic Eenergy, } E = \frac{1}{2}mv^2 \text{ x } ^{ly} \text{ \& \div by 'm' on RHS}$$

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

$$\Rightarrow p^2 = 2Em$$

$$\Rightarrow p = \sqrt{2mE}$$

$$\text{Eqn(1)} \Rightarrow \lambda = \frac{h}{\sqrt{2mE}} \quad \text{----- (2)}$$

Where,  $m$  – mass of particle

$E$  – Kinetic energy of particle

ii) **De-Broglie wavelength in terms of Accelerating potential (V):**

(to show that the de-Broglie wavelength of electron is found to be equal to  $\frac{12.26}{\sqrt{V}}$  Å)

We know,  $\lambda = \frac{h}{p}$  ----- (1)

WKT, KE of an electron = Applied Potential

$\Rightarrow \frac{p^2}{2m} = eV$

$\Rightarrow p = \sqrt{2meV}$  ----- (2)

Put Eqn (2) in (1)

Eqn(1)  $\Rightarrow \lambda = \frac{h}{\sqrt{2meV}}$  ----- (3)

Where, m – mass of particle

e – Charge of particle (electron)

V- Applied potential

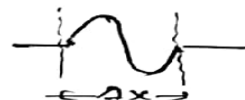
After substituting the values of h, m, e of an electron, we get  $\lambda = \frac{12.26}{\sqrt{V}}$  Å

**Uncertainty:**

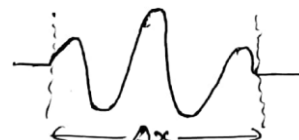
It is the inherent (inbuilt) property associated with the matter wave. i.e., in a matter wave the position of the particle can be located anywhere within the wave group but its exact location is not known. Therefore, we use the concept of probability of finding the particle.

Example:

- a) For narrower wave, there is a small uncertainty in the position and large uncertainty in the momentum (i. e.,  $\Delta x_{\min}$  &  $\Delta p_{\max}$  )



- b) For broader wave, there is a small uncertainty in the momentum and large uncertainty in the position (i. e.,  $\Delta p_{\min}$  &  $\Delta x_{\max}$  )



We can conclude, if the measurement of physical quantity is less uncertain then it is more accurate and if the measurement of physical quantity is more uncertain then it is less accurate.

**Heisenberg's uncertainty principle:**

Statement “It is impossible to determine both exact position and exact momentum of a particle simultaneously. The product of these two uncertainties is always greater than or equal to  $\frac{h}{4\pi}$  ”

If  $\Delta x$  is the uncertainty in the position and  $\Delta p$  is the uncertainty in the momentum for a particle moving along x-axis then from statement we can write,

$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi}$  along x-axis

Similarly,

$\Delta y \cdot \Delta p_y \geq \frac{h}{4\pi}$  along y-axis

$\Delta z \cdot \Delta p_z \geq \frac{h}{4\pi}$  along z-axis

Note: i) The uncertainty between Energy( $\Delta E$ ) & time ( $\Delta t$ ) is given by  $\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$

ii) The uncertainty between Angular momentum( $\Delta L$ ) & Angular displacement ( $\Delta \theta$ ) is given by  $\Delta L \cdot \Delta \theta \geq \frac{h}{4\pi}$

### **Physical significance of Heisenberg's uncertainty principle:**

It is not possible to find the exact position and exact momentum of a particle at the same time. If the momentum of a particle is measured accurately, then position of a particle become uncertain (less accurate) and vice-versa. Hence, concept of probability is used to find the particle.

### **Wave function:**

The quantity whose periodic variation makes up matter wave is called wave function. It is represented by the symbol ' $\psi$ ' (psi)

The value of  $\psi$  at a particular point (x,y,z) in space at time 't' is related to the probability of finding the particle at that time.

**Wave function has no direct physical significance. It is not a measurable and observable physical quantity.**

The wave function of the particle at a point (x,y,z) in space at time 't' is either positive, negative or complex. The value of probability lies between 0 and 1. If the probability is 0 (zero) then the particle not present and if the probability is 1 (one) then the particle is surely present.

The complex quantity of wave function is  $\psi = A + i B$

The complex conjugate of wave function is  $\psi^* = A - i B$

Where, A & B are real quantities.

To make the probability of the wave function always real and positive, we consider the product

$$\psi\psi^* = A^2 + B^2$$

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

**1. Probability density:** According to Max Born interpretation, the probability of finding the particle at a point (x,y,z) in space at time 't' is proportional to  $|\psi|^2$

- i) If  $|\psi|^2 dV = 1$ , Probability is large
- ii) If  $|\psi|^2 dV = 0$ , Probability is less or low

The square of the modulus of wave function in a certain volume element is known as Probability density.

### **2. Normalization of wave function:**

Definition: The integral of square of the modulus of wave function in a certain volume element is always equal to unity.

- (i) The normalization of wave function over entire space is given by

$$\int_{-\infty}^{\infty} |\psi|^2 dV = 1 \quad \text{For Open system}$$

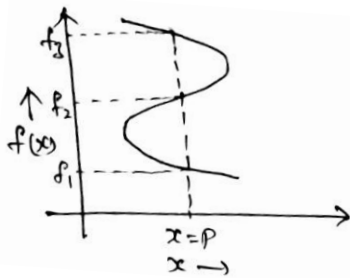
- (ii) The normalization of wave function in a given volume element is given by

$$\int_0^V |\psi|^2 dV = 1 \quad \text{For Bound state}$$

### **Properties of wave function:**

- 1.  $\Psi$  is Single valued.
- 2.  $\Psi$  is Finite everywhere.
- 3.  $\Psi$  and its first derivatives with respect to their variables are Continuous everywhere.
- 4. For bound system,  $\psi$  vanish at  $\infty$ . If  $\psi$  is complex function, then the product  $\psi\psi^*$  must vanish at  $\infty$ .

**(1)  $\psi$  is single valued everywhere:**



At point  $x = P$ , the wave function  $f(x)$  has three different values i.e.,  $f_1$ ,  $f_2$  and  $f_3$ .  $\therefore$  the function  $f(x)$  has a multiple values at  $x=P$  and  $f_1 \neq f_2 \neq f_3$ .

$\therefore f(x)$  is not an acceptable function because the probability of finding the particle has three different values at the same location which is not possible. Hence the  $f(x)$  wave function is not acceptable.

**(2)  $\psi$  is finite everywhere:**

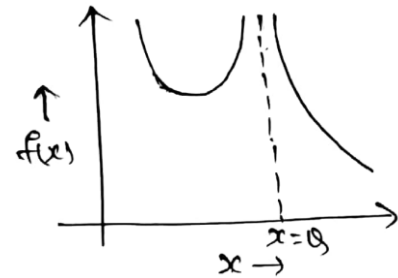
At  $x = Q$ , function  $f(x)$  is not having finite value i.e.,  $f(x)$  is infinity.

$\therefore f(x) = \infty$  at  $x = Q$ .

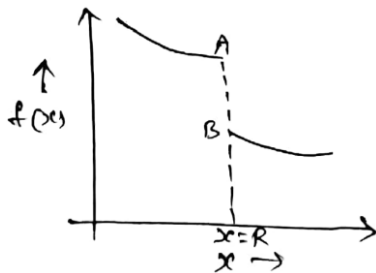
At point  $x = Q$ , the probability of finding the particle is large at a single location, which is against to the uncertainty principle.

$\therefore f(x)$  is not a wave function.

If  $f(x)$  is a wave function, it has to be finite everywhere.



**(3)  $\psi$  and its first derivatives with respect to its variable are continuous everywhere:**



At  $x = R$ , wave function  $f(x)$  is ended at point A & restarted at point B.  $\therefore f(x)$  is discontinuous between points A & B hence function  $f(x)$  is not defined between A & B.

$\therefore f(x)$  is not an acceptable wave function

If  $f(x)$  is a wave function, it has to be continuous everywhere.

**(1) For bound system,  $\psi$  vanish at  $\infty$ . If  $\psi$  is complex function, then the product  $\psi\psi^*$  must vanish at  $\infty$ .**

**Time Independent Schrödinger wave equation:**

The general differential equation of a wave travelling in  $x$ - direction with velocity  $v$  having the wave function is given by

$$\frac{d^2\Psi}{dx^2} = \frac{1}{v^2} \frac{d^2\Psi}{dt^2} \dots\dots\dots (1) \quad \left( \because \frac{d^2y}{dx^2} = \frac{1}{v^2} \frac{d^2y}{dt^2} \text{ and replacing } y \text{ with } \Psi \right)$$

The general solution of the eqn (1) is given by

$$\Psi = \Psi_0 e^{i(kx - \omega t)} \dots\dots\dots (2)$$

Where,  $\omega \rightarrow$  the angular frequency,

$k \rightarrow$  the wave number associated with the wave &

$\Psi_0 \rightarrow$  a constant.

Differentiating eqn (2) twice with respect to 't'

We get,  $\frac{d\Psi}{dt} = (-i\omega)\Psi_0 e^{i(kx - \omega t)}$

$$\frac{d^2\Psi}{dt^2} = (-i\omega)^2 \Psi_0 e^{i(kx - \omega t)}$$

$$\frac{d^2\Psi}{dt^2} = -\omega^2 \Psi_0 e^{i(kx - \omega t)} \quad (\text{Since } i^2 = -1)$$

$$\therefore \frac{d^2\Psi}{dt^2} = -\omega^2 \Psi$$

Substituting in eqn (1),

$$\text{We get } \frac{d^2\Psi}{dx^2} = -\frac{\omega^2}{v^2} \Psi \quad \dots\dots\dots (3)$$

$$\text{but } \omega = 2\pi\nu = \frac{2\pi v}{\lambda}$$

$$\Rightarrow \frac{\omega}{v} = \frac{2\pi}{\lambda}$$

$$\therefore \frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2}$$

Consider a particle of mass 'm' associated with a de-Broglie wave of wave length 'λ' and moving with a velocity 'v' then

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

$$\Rightarrow \lambda^2 = \frac{h^2}{m^2 v^2}$$

$$\therefore \frac{\omega^2}{v^2} = \frac{4\pi^2 m^2 v^2}{h^2} \quad \dots\dots\dots (4)$$

If E is the total energy of the particle and V is the potential energy associated with the particle then

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

$$E = \frac{1}{2} \frac{m^2 v^2}{m} + V \quad \text{(divide \& multiply by 'm')}$$

$$\therefore m^2 v^2 = 2m(E - V) \quad \dots\dots\dots (5)$$

Put eqn(5) in eqn(4)

$$\text{We get } \frac{\omega^2}{v^2} = \frac{4\pi^2 \times 2m(E-V)}{h^2}$$

$$\therefore \frac{\omega^2}{v^2} = \frac{8\pi^2 m(E-V)}{h^2} \quad \dots\dots\dots (6)$$

Substituting eqn(6) in eqn(3)

$$\text{eqn(3)} \Rightarrow \frac{d^2\Psi}{dx^2} = -\frac{8\pi^2 m(E-V)}{h^2} \Psi$$

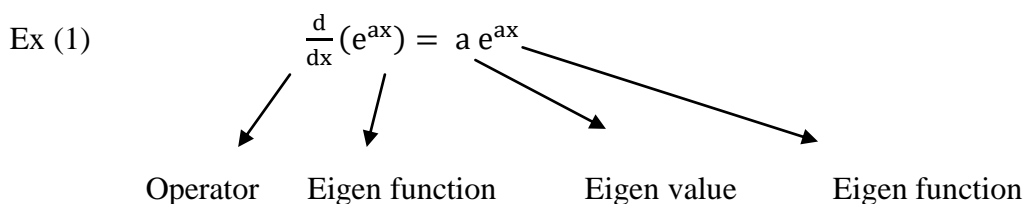
$$\Rightarrow \frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2} (E - V) \Psi = 0 \quad \dots\dots\dots (7)$$

Equation (7) is the expression for time independent Schrödinger wave equation.

### **Eigen Values and Eigen functions:**

Eigen functions are those functions in quantum mechanics which exhibits properties like Single valued, Finite everywhere and its first derivatives with respect their variables are continuous everywhere.

An Operator operated on a wave function will result in the wave function multiplied by a constant. This constant value is known as Eigen value.



Ex (2) In general,  $\hat{A} \Psi = \lambda \Psi$

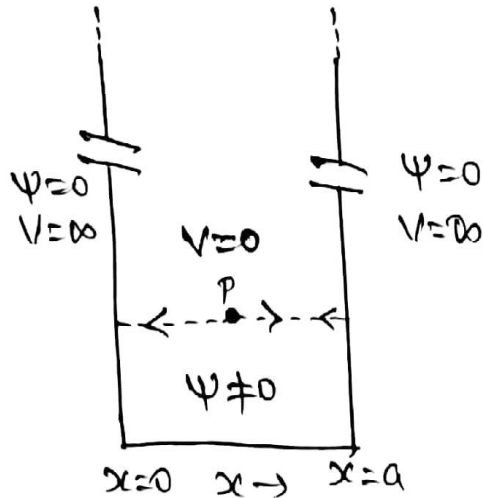
Where,  $\hat{A}$  = operator

$\Psi$  = Eigen function

$\lambda$  = Eigen value

### Application of Schrödinger wave equation:

#### Expression for Energy Eigen value for a Particle in 1 – Dimensional potential well of infinite depth:



Consider a particle of mass  $m$  confined to a 1- D box of width ' $a$ ' moving with a velocity ' $v$ ' along  $x$  - axis.

Let the box has two rigid walls at  $x = 0$  and  $x = a$  and has an infinite depth. The potential inside the box is zero and the particle will not lose energy when it collides with the rigid wall. The particle cannot be found on the wall.

The boundary conditions for a particle inside the box is given by

$$\Psi \neq 0 \text{ at } 0 < x < a$$

$$V = 0 \text{ at } 0 < x < a$$

Similarly, the boundary conditions for a particle outside the box is given by

$$\Psi = 0 \text{ at } 0 \leq x \text{ \& } x \geq a$$

$$V = \infty \text{ at } 0 \leq x \text{ \& } x \geq a$$

From Schrodinger's time independent wave equation,

$$\frac{d^2\Psi}{dx^2} + \left\{ \frac{8\pi^2m(E-V)}{h^2} \right\} \Psi = 0 \quad \dots\dots\dots (1)$$

For a particle inside the box  $V = 0$

$$\therefore \frac{d^2\Psi}{dx^2} + \left\{ \frac{8\pi^2mE}{h^2} \right\} \Psi = 0 \quad \dots\dots\dots (2)$$

Let  $\frac{8\pi^2mE}{h^2} = k^2 \quad \dots\dots\dots (3)$

Eqn (3)  $\Rightarrow \frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \quad \dots\dots\dots (4)$

The general solution of the eqn (4) is given by

$$\Psi = A \sin kx + B \cos kx \quad \dots\dots\dots (5)$$

Where  $A$  &  $B$  are arbitrary constants and its values can be calculated using boundary conditions.

First boundary condition is  $\Psi = 0$  at  $x = 0$

$$(5) \Rightarrow 0 = A \sin k0 + B \cos k0$$

$$\therefore B = 0$$

$$(5) \Rightarrow \Psi = A \sin kx \quad \dots\dots\dots (6)$$

Second boundary condition is  $\Psi = 0$  at  $x = a$

$$(6) \Rightarrow A \sin ka = 0 \quad \dots\dots\dots (7)$$

In Eqn(7),  $A \neq 0$ . If  $A \rightarrow 0$  then the particle does not exist inside the box.

$$\therefore \sin ka = 0$$

In general,  $ka = n\pi$

where  $n = 1, 2, 3, \dots$

$$\therefore k = \frac{n\pi}{a} \quad \dots\dots\dots (8)$$

Substituting value of  $k$  in Eqn (3),

For  $n^{\text{th}}$  state,

$$\begin{aligned} \text{Eqn (3)} \Rightarrow \quad & \frac{8\pi^2 m E_n}{h^2} = \left(\frac{n\pi}{a}\right)^2 \\ \Rightarrow \quad & E_n = \frac{n^2 h^2}{8ma^2} \end{aligned} \quad \dots\dots\dots (9)$$

Eqn (9) is the expression for Energy Eigen value.

When  $n = 1$ ,  $E_1 = \frac{h^2}{8ma^2}$

This is called **ground state energy or zero point energy**

When  $n = 2$ ,  $E_2 = \frac{4h^2}{8ma^2} = 4 E_1$

This is called **first excited energy state**

When  $n = 3$ ,  $E_3 = \frac{9h^2}{8ma^2} = 9 E_1$

This is called **second excited energy state**

For  $n^{\text{th}}$  state,

$$\text{Eqn (6)} \Rightarrow \quad \Psi_n = A \sin\left(\frac{n\pi}{a}\right) x \quad \dots\dots\dots (10)$$

Eqn (10) is the expression for Eigen wave function.

## Numerical on Elements of Quantum Mechanics

### Solved Numerical:

Standard conversion: 1 eV =  $1.6 \times 10^{-19}$  J

1. What is the de Broglie wavelength of a proton whose energy is 3eV? Given the mass of proton =  $1.67 \times 10^{-27}$  Kg.

Solution:

Given: Energy  $E = 3\text{eV} = 3 \times 1.6 \times 10^{-19} \text{ J} = 4.8 \times 10^{-19} \text{ J}$

Mass of proton  $m = 1.67 \times 10^{-27} \text{ kg}$

Formula: de Broglie wavelength  $\lambda = \frac{h}{\sqrt{2mE}}$

Substituting  $h = 6.626 \times 10^{-34} \text{ J-s}$ ,  $m$  and  $E$  value in the above equation, we get

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 4.8 \times 10^{-19}}}$$

$$\lambda = 1.655 \times 10^{-11} \text{ m}$$

The de Broglie wavelength of the proton is found to be  $1.655 \times 10^{-11} \text{ m}$

2. Calculate the de Broglie wavelength associated with an electron accelerated through a potential difference of 2kV.

Solution:

Given: Potential  $V = 2\text{kV} = 2000 \text{ V}$

Mass of an electron =  $9.1 \times 10^{-31} \text{ kg}$

Formula: de Broglie wavelength  $\lambda = \frac{h}{\sqrt{2meV}}$

Substituting  $h = 6.626 \times 10^{-34} \text{ J-s}$ , mass  $m$  and energy  $E$  value in the above equation, we get

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 2000}}$$

$$\lambda = 2.75 \times 10^{-11} \text{ m}$$

The de Broglie wavelength of the electron is found to be  $2.75 \times 10^{-11} \text{ m}$ .

3. Calculate the kinetic energy of an electron of wavelength 18nm.

Solution:

Given: wavelength of the electron =  $18 \text{ nm} = 18 \times 10^{-9} \text{ m}$

Mass of an electron =  $9.1 \times 10^{-31} \text{ kg}$

Formula: de Broglie wavelength  $\lambda = \frac{h}{\sqrt{2mE}}$

$$\text{On rearranging, we get, } E = \frac{h^2}{2m\lambda^2}$$

Substituting  $h = 6.626 \times 10^{-34} \text{ J-s}$ ,  $m$  and  $\lambda$  value in the above equation, we

$$\text{get } E = \frac{(6.626 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times (18 \times 10^{-9})^2}$$

$$E = 7.445 \times 10^{-22} \text{ J} = (7.445 \times 10^{-22} / 1.6 \times 10^{-19}) \text{ eV} = 0.0046 \text{ eV}$$

The kinetic energy of an electron of wavelength 18nm is 0.0046 eV



4. Calculate the de Broglie wavelength of an electron moving with  $1/10^{\text{th}}$  part of the velocity of the light.

Solution:

Given: Velocity of the electron,  $v = \frac{1}{10} c = \frac{3 \times 10^8}{10} = 3 \times 10^7 \text{ m/s}$

Mass of an electron =  $9.1 \times 10^{-31} \text{ kg}$

Formula: de Broglie wavelength  $\lambda = \frac{h}{mv}$

Substituting  $h = 6.626 \times 10^{-34} \text{ Js}$ , mass  $m$  and velocity  $v$  value in the above equation, we get;

$$\lambda = \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^7}$$

$$\lambda = 2.43 \times 10^{-11} \text{ m}$$

The de Broglie wavelength of an electron is  $2.43 \times 10^{-11} \text{ m}$

5. An electron has a speed of  $4.8 \times 10^5 \text{ m/s}$  accurate to 0.012%. With what accuracy can the position of electron be located?

Given:  $v = 4.8 \times 10^5 \text{ m/s}$ ,  $\Delta v = 0.012\%$  of  $4.8 \times 10^5 \text{ m/s} = \frac{0.012}{100} \times 4.8 \times 10^5 = 57.6 \text{ m/s}$

Mass of an electron =  $9.1 \times 10^{-31} \text{ kg}$

Formula: Heisenberg uncertainty principle:  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$

To find  $\Delta p$ , we know that  $p = mv$ , then  $\Delta p = m\Delta v$ .

Then  $\Delta x$  is given by  $\Delta x \geq \frac{h}{4\pi\Delta p}$  (from formula)

Substituting  $h = 6.626 \times 10^{-34} \text{ J-s}$  and  $\Delta p$  value in the above equation, we get

$$\Delta x \geq \frac{6.626 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times 57.6}$$

$$\Delta x \geq 10^{-6} \text{ m}$$

6. An electron has a speed of 100m/s. The inherent uncertainty in its measurement is 0.005%. What will be the uncertainty that arises in the measurement of its position?

Solution:

Given: speed of an electron  $v = 100 \text{ m/s}$ , mass of an electron =  $9.1 \times 10^{-31} \text{ kg}$ .

Uncertainty in measurement  $\Delta v = 0.005\%$  of  $100 \text{ m/s} = \frac{0.005 \times 100}{100} = 0.005 \text{ m/s}$ .

Formula: Heisenberg uncertainty principle:  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$

To find  $\Delta p$ : We know that  $p = mv$ , then  $\Delta p = m\Delta v$ .

Then  $\Delta x$  is given by  $\Delta x \geq \frac{h}{4\pi\Delta p}$  (from formula)

Substituting  $h = 6.626 \times 10^{-34} \text{ Js}$  and  $\Delta p$  value in the above equation, we get

$$\Delta x \geq \frac{6.626 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times 0.005} \Rightarrow \Delta x \geq 0.0116 \text{ m}$$

7. In a measurement of position and velocity of an electron moving with the speed of  $6 \times 10^5 \text{ m/s}$ , calculate the highest accuracy with which its position could be determined if the inherent error in the measurement of its velocity is 0.01% for the speed stated.

Solution:

Given: speed of an electron  $v = 6 \times 10^5$  m/s, mass of an electron  $= 9.1 \times 10^{-31}$  kg.

Uncertainty in measurement  $\Delta v = 0.01\%$  of  $6 \times 10^5$  m/s  $= \frac{0.01 \times 6 \times 10^5}{100} = 0.06 \times 10^3$  m/s

Formula: Heisenberg uncertainty principle:  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$

To find  $\Delta p$ : We know that  $p = mv$ , then  $\Delta p = m\Delta v$ .

Then  $\Delta x$  is given by  $\Delta x \geq \frac{h}{4\pi\Delta p}$  (from formula)

Substituting  $h = 6.626 \times 10^{-34}$  Js and  $\Delta p$  value in the above equation, we get

$$\Delta x \geq \frac{6.626 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times 0.06 \times 10^3}$$

$$\Delta x \geq 9.65 \times 10^{-7} \text{ m}$$

**8. Calculate the energy in eV for the first excited state of an electron in an infinite potential well of width 2 Å.**

Solution:

Given: width of the potential well 'a' = 2 Å =  $2 \times 10^{-10}$  m

Mass of an electron =  $9.1 \times 10^{-31}$  kg.

Formula: Energy of a particle in an infinite potential well in  $n^{\text{th}}$  state  $E_n = \frac{n^2 h^2}{8ma^2}$

Where  $n=1, 2$  and  $3$  corresponds to ground, first excited and second excited state respectively.

Energy of an electron in first excited state ( $n=2$ ) is  $E_2 = \frac{2^2 h^2}{8ma^2}$

$$E_2 = \frac{4 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2 \times 10^{-10})^2} = 6.03 \times 10^{-18} \text{ J}$$

$$E_2 = 37.69 \text{ eV}$$

**9. Calculate the zero-point energy for an electron in a box of width 10 Å.**

Solution:

Given: width of the potential well 'a' = 10 Å =  $10 \times 10^{-10}$  m

Mass of an electron =  $9.1 \times 10^{-31}$  kg.

Formula: Energy of a particle in an infinite potential well in  $n^{\text{th}}$  state  $E_n = \frac{n^2 h^2}{8ma^2}$

Where  $n=1, 2$  and  $3$  corresponds to ground/zero-point, first excited and second excited state respectively.

Zero-point energy for an electron ( $n=1$ )  $E_0$  or  $E_1 = \frac{h^2}{\pi m a^2}$

$$E_1 = \frac{1 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10 \times 10^{-10})^2} = 6.03 \times 10^{-20} \text{ J} = 0.376 \text{ eV}$$

**10. An electron is bound in 1-D potential well of width 0.18nm, find its energy value in eV in the second excited state.**

Solution:

Given: width of the potential well 'a' = 0.18 nm =  $0.18 \times 10^{-9}$  m

Mass of an electron =  $9.1 \times 10^{-31}$  kg.

Formula: Energy of a particle in an infinite potential well in  $n^{\text{th}}$  state  $E_n = \frac{n^2 h^2}{8ma^2}$

Where  $n=1, 2$  and  $3$  corresponds to ground/zero-point, first excited and second excited state respectively.

Energy of an electron in second excited state ( $n = 3$ )  $E_3 = \frac{3^2 h^2}{8ma^2}$

$$E_3 = \frac{9 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.18 \times 10^{-9})^2} = 1.675 \times 10^{-17} \text{ J}$$

$$E_3 = 104.7 \text{ eV}$$

**11. The ground state energy of an electron in an infinite well is  $5.6 \times 10^{-3} \text{ eV}$ . What will be the ground state energy if the width of the well is doubled?**

Solution:

Energy of a particle in an infinite potential well in  $n^{\text{th}}$  state  $E_n = \frac{n^2 h^2}{8ma^2}$

In ground state  $n=1$ ,  $E_1 = \frac{h^2}{8ma^2}$

If width of the potential well changes from  $a$  to  $2a$ , then the new energy  $E_1^1$

becomes  $E_1^1 = \frac{h^2}{8m(2a)^2} = \frac{h^2}{8m \cdot 4a^2} = \frac{E_1}{4} = \frac{5.6 \times 10^{-3}}{4} = 1.4 \times 10^{-3} \text{ eV}$

### Exercise Problems:

1. Calculate the de Broglie wavelength of a neutron whose energy is  $5 \text{ eV}$ .
2. Calculate the kinetic energy of an electron with a wavelength of  $15 \text{ nm}$ .
3. An electron has a speed of  $3.2 \times 10^5 \text{ m/s}$  accurate to  $0.01\%$ . What is the accuracy with which its position can be measured?
4. Calculate the energy in  $\text{eV}$  for the first excited state of an electron in an infinite potential well of width  $1.5 \text{ \AA}$ .
5. Find the ground state energy of an electron in a box of width  $8 \text{ \AA}$ .
6. Calculate the energy in  $\text{eV}$  for the second excited state of an electron in an infinite potential well of width  $30 \text{ \AA}$ .