Unit - III
Quantum Mechanics

Syllabus : De-Broglie hypothesis - Concept of phase velocity and group velocity (qualitative) - Heisenberg Uncertainty Principle - Wave-function and its physical significance - Schrodinger's equations : time independent and time dependent - Application of Schrodinger's time independent wave equation - Particle enclosed in infinitely deep potential well (Particle in RigidBox) - Particle in Finite potential well (Particle in Non Rigid box) (qualitative) - Tunneling effect, Tunneling effect examples (principle only): Alpha Decay, Scanning Tunneling Microscope, Tunnel diode - Introduction to quantum computing.

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6 Quantum Mechanics

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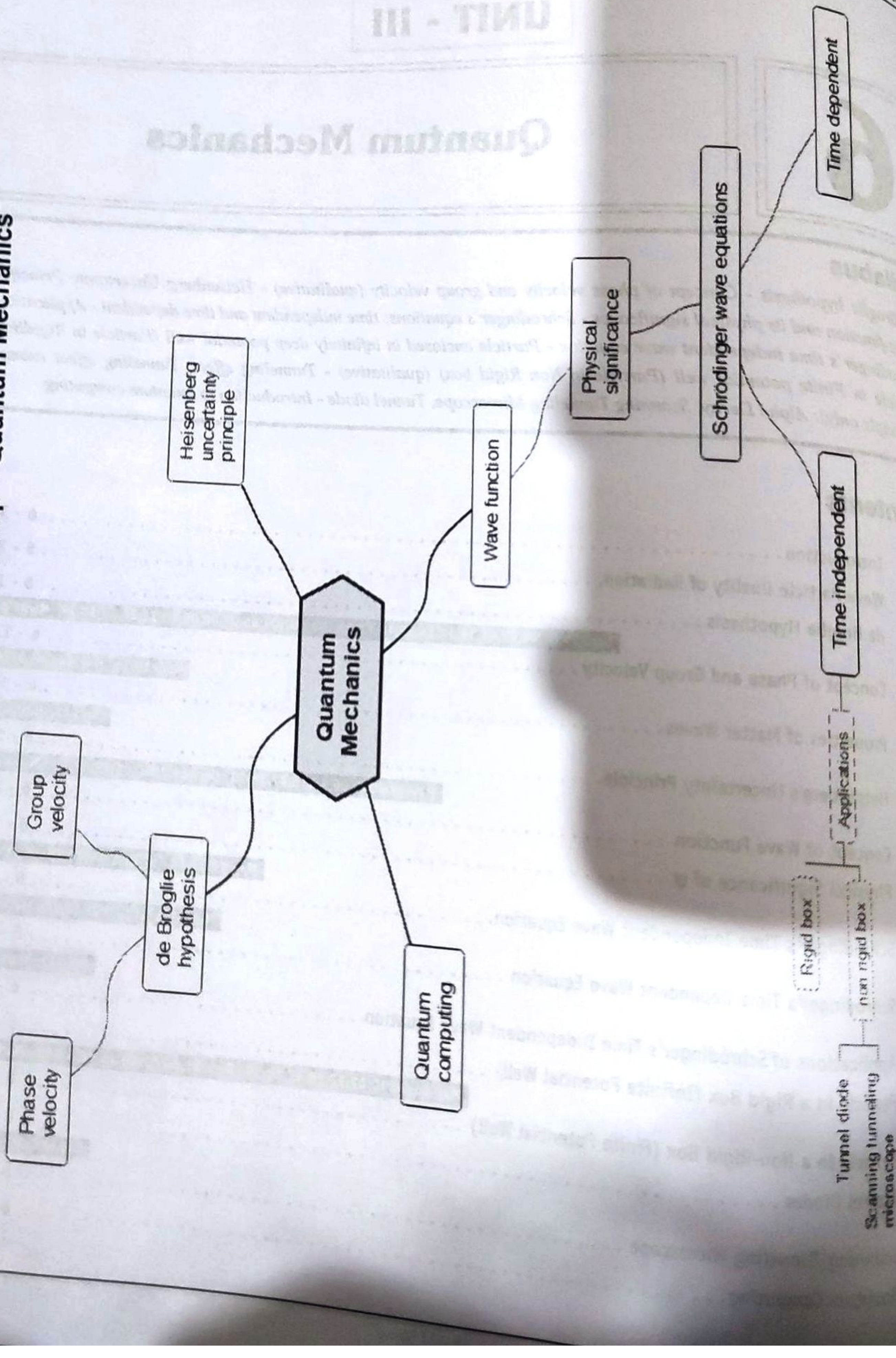
Mind Map – Quantum Mechanics



6.1 : Introduction

- Louis de Broglie's hypothesis of matter waves in 1924 laid the foundation on which Schrödinger, Heisenberg and others developed quantum mechanics.
- Application of quantum mechanics to molecules, atoms and nuclei led to accurate predictions of molecular, atomic and nuclear phenomena.
- The basic concepts involved in the development of quantum mechanics are discussed in this chapter.

6.2 : Wave Particle Duality of Radiation

- Some phenomena exhibited by radiation like interference and diffraction can be explained only on the basis of wave theory whereas phenomena like photoelectric effect and compton effect can be explained only by considering radiation to be made up of particles.
- Hence it can be concluded that radiation behaves like waves in certain situations and like particles in certain other situations.
- The wave and particle properties are never exhibited simultaneously.

6.3 : de Broglie Hypothesis

SPPU : Dec.-99,01,04,07,09,10,11,14,15,16,17,18, May-02,04,05,07,08,09,10,11,16,17,18,19

- Louis de Broglie proposed in 1924 that just like radiation, matter also possesses wave as well as particle characteristics i.e., matter exhibits particle properties in certain situations and wave properties in others.
- The particle and wave properties are not exhibited simultaneously.
- According to **de Broglie's hypothesis**, every moving particle is associated with a wave, called the **matter wave** or **de Broglie wave**, whose wavelength (λ) is given by,

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad \text{... (6.3.1)}$$

where, h = Planck's constant,

m = Mass of the particle

and v = Particle velocity.

- Note that 'm' is the relativistic mass of the particle which is related to its rest mass 'm_0' by the formula.

$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$$

where, c = Velocity of light in vacuum.

- For velocities small compared to velocity of light,

$$m \approx m_0$$

6.3.1 de Broglie Wavelength by Analogy with Radiation

- From theory of relativity, the momentum (p) of a massless particle like photon is related to its energy (E) by the formula.

$$E = pc \quad \text{... (6.3.2)}$$

- By Planck's quantum theory, the energy of photon is given by,

$$E = h\nu = \frac{hc}{\lambda} \quad \dots (6.3.3)$$

where ν = Frequency.

- From equations (6.3.2) and (6.3.3),

$$pc = \frac{hc}{\lambda}$$

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

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

- de Broglie suggested that the above equation, which is valid for a photon, applies to material particles also.
- As, for material particles, $p = mv$

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

6.3.2 de Broglie Wavelength for a Free Particle in terms of its Kinetic Energy

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

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

- Multiplying and dividing by 'm',

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

But $$p = mv$$

$$\therefore \quad E = \frac{p^2}{2m}$$

$$\therefore \quad p = \sqrt{2mE}$$

- By de Broglie hypothesis,

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

$$\therefore \quad \lambda = \frac{h}{\sqrt{2mE}} \quad \dots (6.3.4)$$

6.3.3 de Broglie Wavelength of an Electron Accelerated through Some Potential Difference

- If an electron is accelerated through a potential difference of 'V' volts, the work done on the electron is eV which is converted into kinetic energy.

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

$$\therefore \quad \frac{p^2}{2m} = eV$$

$\therefore$ $p = \sqrt{2meV}$

- The de Broglie wavelength is given by,

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

$\therefore$ $$\lambda = \frac{h}{\sqrt{2meV}} \quad \dots (6.3.5)$$

- As

$$h = 6.63\times 10^{-34} \text{ J-s,}$$

$$m = 9.1\times 10^{-31} \text{ kg}$$

$$e = 1.6\times 10^{-19} \text{ C}$$

(Neglecting relativistic correction)

$\therefore$ $$\lambda = \frac{6.63\times 10^{-34}}{\sqrt{2\times 9.1\times 10^{-31}\times 1.6\times 10^{-19}\ V}} = \frac{12.27\times 10^{-10}}{\sqrt{V}} \text{ m}$$

$\therefore$ $$\lambda = \frac{12.27}{\sqrt{V}} \text{ A°} \quad \dots (6.3.6)$$

Ex. 6.3.1 : *Determine the velocity and kinetic energy of a neutron having de Broglie wavelength 1 A°. Mass of neutron = 1.67×10^{-27} kg.*

SPPU : Dec.-99,09, May-04

Sol. : Given data

$$h = 6.63\times 10^{-34} \text{ J-s}$$

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

$$\lambda = 1 \text{ A°} = 1\times 10^{-10} \text{ m}$$

Formula : $\lambda = \dfrac{h}{mv}$, $\lambda = \dfrac{h}{\sqrt{2\,mE}}$

$\therefore$ $$v = \frac{h}{m\lambda}$$

$\therefore$ $$v = \frac{6.63\times 10^{-34}}{1.67\times 10^{-27}\times 1\times 10^{-10}}$$

$\therefore$ $$\boxed{v = 3970 \text{ m/s}}$$

Also, $$\lambda = \frac{h}{\sqrt{2mE}}$$

$\therefore$ $$E = \frac{h^2}{2m\lambda^2} = \frac{(6.63\times 10^{-34})^2}{2\times 1.67\times 10^{-27}\times (1\times 10^{-10})^2}$$

$\therefore$ $$E = 1.316\times 10^{-20} \text{ J} = \frac{1.316\times 10^{-20}}{1.6\times 10^{-19}} \text{ eV}$$

$\therefore$ $$\boxed{E = 8.225\times 10^{-2} \text{ eV}}$$

Ex. 6.3.2 : *Find the de Broglie wavelength of*
i) An electron accelerated through a potential difference of 182 volts and
ii) 1 kg object moving with a speed of 1 m/s.
Comparing the results, explain why the wave nature of matter is not more apparent in daily observations.

SPPU : Dec.-01

Sol. : i) Given data :

$$V = 182 \text{ V}$$

Formula :

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ A}^\circ$$

$$\therefore \quad \lambda = \frac{12.27}{\sqrt{182}}$$

$$\therefore \quad \boxed{\lambda = 0.91 \text{ A}^\circ}$$

ii) Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}, \; m = 1 \text{ kg}, \; v = 1 \text{ m/s}.$$

Formula :

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

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34}}{1 \times 1} = 6.63 \times 10^{-34} \text{ m}$$

$$\therefore \quad \boxed{\lambda = 6.63 \times 10^{-24} \text{ A}^\circ}$$

This wavelength is too small and hence is not measurable whereas the wavelength of electron is measurable. Hence wave nature of matter is not apparent in daily observations.

Ex. 6.3.3 : *If electron had existed inside the nucleus, then its de Broglie wavelength would be roughly of order of nuclear distance, i.e. 10^{-14} m. How much momentum corresponds to this wavelength ? How much energy corresponds to this momentum ? Express this energy in MeV and explain how this result proves that the electron cannot exist inside the nucleus. (The maximum nuclear binding energy is 8.8 MeV per nuclear particle.) Given : Planck's constant = 6.63×10^{-34} J-s.*

Sol. : Given data :

SPPU : May

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$\lambda = 10^{-14} \text{ m}$$

Formula :

$$\lambda = \frac{h}{p}, \quad E = \frac{p^2}{2m}$$

$\therefore$ The momentum of electron is

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

$$\therefore \quad p = \frac{6.63 \times 10^{-34}}{10^{-14}}$$

$$\therefore \quad \boxed{p = 6.63\times 10^{-20} \text{ kg-m/s}}$$

The corresponding energy is,

$$E = \frac{p^2}{2m} = \frac{(6.63\times 10^{-20})^2}{2\times 9.1\times 10^{-31}}$$

$$\therefore \quad E = 2.415\times 10^{-9} \text{ J}$$

As

$$1 \text{ MeV} = 1.6\times 10^{-13} \text{ J},$$

$$E = \frac{2.415\times 10^{-9}}{1.6\times 10^{-13}} \text{ MeV}$$

$$\therefore \quad \boxed{E = 15093.75 \text{ MeV}}$$

This energy of the electron is much larger than the 8.8 MeV energy required to keep the electron inside the nucleus. Hence, the electron cannot exist inside the nucleus.

Ex. 6.3.4 : ***An electron initially at rest is accelerated through a potential difference of 3000 V. Calculate for the electron wave the following parameters :***

i) The momentum. ii) The de Broglie wavelength.

SPPU : May-19, Marks 3

Sol. : Given data :

$$V = 3000 \text{ V}$$

Formula :

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ A°}$$

$$\therefore \quad \lambda = \frac{12.27}{\sqrt{3000}}$$

$$\therefore \quad \boxed{\lambda = 0.224 \text{ A°}}$$

ii) Formula :

$$\lambda = \frac{h}{p} \quad \text{where } p \text{ is the momentum}$$

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

$$= \frac{6.63\times 10^{-34}}{0.224\times 10^{-10}}$$

$$\therefore \quad \boxed{p = 2.96\times 10^{-23} \text{ kg-m/s}}$$

Ex. 6.3.5 : ***An electron is accelerated through a potential difference of 10 kV. Calculate the de Broglie wavelength and momentum of electron.***

SPPU : Dec.-04

Sol. : Given data :

$$V = 10 \text{ kV} = 10\times 10^3 \text{ V}$$

Formula : $\lambda = \frac{12.27}{\sqrt{V}}$ A° $\quad p = \frac{h}{\lambda}$

$$\therefore \quad \lambda = \frac{12.27}{\sqrt{10\times 10^3}}$$

$$\therefore \quad \boxed{\lambda = 0.1227 \text{ A}^\circ}$$

The momentum of electron is,

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

$$= \frac{6.63\times 10^{-34}}{0.1227\times 10^{-10}}$$

$$\therefore \quad \boxed{p = 5.403\times 10^{-23} \text{ kg - m/s}}$$

Ex. 6.3.6 : ***A proton and an α-particle are accelerated by the same potential difference. Show that the ratio of the de Broglie wavelengths associated with them is $2\sqrt{2}$. Assume the mass of α-particle to be 4 times the mass of proton.*** SPPU : May-05,18, Marks 3

Sol. : Given data : The charge of proton is 'e' and that of an α-particle is $2e$. Also,

$$m_\alpha = 4\,m_p$$

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

For proton, $$\lambda_p = \frac{h}{\sqrt{2m_p eV}} \quad \dots (1)$$

For α-particle, $$\lambda_\alpha = \frac{h}{\sqrt{2(4m_p)\,(2e)\,V}} \quad \dots (2)$$

From equations (1) amd (2),

$$\frac{\lambda_p}{\lambda_\alpha} = \frac{h}{\sqrt{2m_p eV}} \times \frac{\sqrt{2(4m_p)\,(2e)\,V}}{h}$$

$$= \sqrt{8}$$

$$\therefore \quad \boxed{\frac{\lambda_p}{\lambda_\alpha} = 2\sqrt{2}}$$

6.3.7 : ***Calculate the velocity and de Broglie wavelength of an α-particle of particle of energy 1 keV.*** SPPU : May-07

en : Mass of α-particle = 6.68×10^{-27} kg.

: Given data :

$$h = 6.63\times 10^{-34} \text{ J-s}$$

$$m = 6.68\times 10^{-27} \text{ kg}$$

$$E = 1 \text{ keV} = 1.6 \times 10^{-16} \text{ J}$$

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

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 6.68 \times 10^{-27} \times 1.6 \times 10^{-16}}}$$

$$\therefore \quad \lambda = 4.535 \times 10^{-13} \text{ m}$$

$$\therefore \quad \boxed{\lambda = 4.535 \times 10^{-3} \text{ A}^\circ}$$

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

$$\therefore \quad v = \frac{h}{m\lambda}$$

$$= \frac{6.63 \times 10^{-34}}{6.68 \times 10^{-27} \times 4.535 \times 10^{-13}}$$

$$\therefore \quad \boxed{v = 2.19 \times 10^5 \text{ m/s}}$$

Ex. 6.3.8 : ***Which has a shorter wavelength - 1 eV photon or 1 eV electron ? Calculate the value and explain.***

SPPU : May-07, Dec.-11

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$c = 3 \times 10^8 \text{ m/s}$$

$$E = 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

Formula : $$\lambda_{ph} = \frac{hc}{E}, \quad \lambda = \frac{h}{\sqrt{2mE}}$$

$$\therefore \quad \lambda_{ph} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19}}$$

$$= 1.2431 \times 10^{-6} \text{ m}$$

$$\therefore \quad \boxed{\lambda_{ph} = 12431 \text{ A}^\circ}$$

For an electron with energy 'E'

$$\lambda_e = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}}$$

$$= 1.229 \times 10^{-9} \text{ m}$$

$\therefore \quad \boxed{\lambda_e = 12.29 \text{ A}^\circ}$

The wavelength of electron is shorter than the photon. This is because of the larger momentum of electron (mv or $\sqrt{2mE}$) compared to photon $\left(\frac{hv}{c} \text{ or } \frac{E}{c}\right)$.

Ex. 6.3.9 : ***An electron has kinetic energy equal to its rest mass energy. Claculate de Broglie's wavelength associated with it.***

SPPU : Dec.-17

Sol. : Given data :

$$m_0 = 9.1 \times 10^{-31} \text{ kg}$$

$$c = 3 \times 10^8 \text{ m/s}$$

$$\therefore \quad E = 9.1 \times 10^{-31} \times (3 \times 10^8)^2$$

$$\therefore \quad E = 8.19 \times 10^{-14} \text{ J}$$

Formula : $E = m_0 c^2 \text{ , } \lambda = \frac{h}{\sqrt{2mE}}$

$$= \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 8.19 \times 10^{-14}}}$$

$$= 1.717 \times 10^{-12} \text{ m}$$

$$\therefore \quad \boxed{\lambda = 1.717 \times 10^{-2} \text{ A}^\circ}$$

Ex. 6.3.10 : ***In a T.V. set, electrons are accelerated by a potential difference of 10 kV. What is the wavelength associated with these electrons ?***

SPPU : May-08, Dec.-18 Marks 3

Sol. : Given data :

$$V = 10 \text{ kV} = 10^4 \text{ V}$$

Formula : $\lambda = \frac{12.27}{\sqrt{V}} \text{ A}^\circ$

$$\therefore \quad \lambda = \frac{12.27}{\sqrt{10^4}}$$

$$\therefore \quad \boxed{\lambda = 0.1227 \text{ A}^\circ}$$

Ex. 6.3.11 : ***Find the De-Broglie wavelength associated with monoenergetic electron beam having momentum 10^{-23} kg m/s.***

SPPU : May-04

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$p = 10^{-23} \text{ kg-m/s}$$

Formula :

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

$$\therefore \quad \lambda = \frac{6.63\times 10^{-34}}{10^{-23}}$$

$$\therefore \quad \lambda = 6.63\times 10^{-11}\ \text{m}$$

$$\therefore \quad \boxed{\lambda = 0.663\ \text{A}^\circ}$$

Ex. 6.3.12 : *Calculate De-Broglie wavelength of 10 keV protons in A°.* **SPPU : May-10,11, Dec.-17, Marks 3**

Sol. : Given data :

$$h = 6.63 \times 10^{-34}\ \text{J-s.}$$

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

$$E = 10\ \text{keV} = 10 \times 1.6 \times 10^{-16}\ \text{J}$$

$$\therefore \quad E = 1.6 \times 10^{-15}\ \text{J}$$

Formula :

$$\lambda = \frac{h}{\sqrt{2\,mE}}$$

$$\therefore \quad \lambda = \frac{6.63\times10^{-34}}{\sqrt{2\times1.67\times10^{-27}\times1.6\times10^{-15}}}$$

$$= 2.868 \times 10^{-13}$$

$$\therefore \quad \boxed{\lambda = 2.868 \times 10^{-3}\ \text{A}^\circ}$$

Ex. 6.3.13 : *At what kinetic energy an electron will have a wavelength of 5000 A° ?* **SPPU : Dec.-10**

Sol. : Given data :

$$\lambda = 5000\ \text{A}^\circ = 5000 \times 10^{-10}\ m$$

Formula

$$\lambda = \frac{h}{\sqrt{2\,mE}}$$

$$\therefore \quad E = \frac{h^2}{2\,m\lambda^2} = \frac{(6.63\times10^{-34})^2}{2(9.1\times10^{-31})\,(5000\times10^{-10})^2}$$

$$= 9.66 \times 10^{-25}\ \text{J} = \frac{9.66\times10^{-25}}{1.6\times10^{-19}}\ \text{eV}$$

$$\therefore \quad \boxed{E = 6.038 \times 10^{-6}\ \text{eV}}$$

Ex. 6.3.14 : *Calculate the De Broglie wavelength of electron having kinetic energy 1 keV.* **SPPU : Dec.-14,15 Marks 3**

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J s}, \; m = 9.1 \times 10^{-31} \text{ kg}$$

$$E = 1 \text{ keV}$$

Formula :

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-16}}}$$

$$= 3.89 \times 10^{-11} \text{ m}$$

$$\therefore \quad \boxed{\lambda = 0.39 \text{ A°}}$$

Ex. 6.3.15 : ***Calculate de Broglie wavelength for a proton moving with velocity 1 percent of velocity of light.***

SPPU : May-16, Marks

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ Js}, \; m = 1.673 \times 10^{-27} \text{ kg}$$

$$V = \frac{1}{100} \times 3 \times 10^{8} = 3 \times 10^{6} \text{ m/s}$$

Formula :

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

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34}}{1.673 \times 10^{-27} \times 3 \times 10^{6}}$$

$$\therefore \quad \boxed{\lambda = 1.32 \times 10^{-13} \text{ m}}$$

Ex. 6.3.16 : ***An electron beam is accelerated from rest through a potential difference of 200 V. Calculate the associated wavelength.***

SPPU : Dec.-16, Marks

Sol. : Given data :

$$V = 200 \text{ V}$$

Formula :

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

$$\therefore \quad \lambda = \frac{12.27}{\sqrt{200}}$$

$$\therefore \quad \boxed{\lambda = 0.868 \text{ A°}}$$

Ex. 6.3.17 : ***Calculate the energy (in eV) with which a proton has to acquire de-Broglie wavelength of 0.1 Å***

SPPU : May-17, Marks

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ Js}, \quad m = 1.673 \times 10^{-27} \text{ kg}$$

$$\lambda = 0.1\ \mathring{A} = 0.1 \times 10^{-10}\ m$$

Formula :

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$E = \frac{h^2}{2m\lambda^2}$$

$$\therefore \quad E = \frac{(6.63\times10^{-34})^2}{2\times1.673\times10^{-27}\times(0.1\times10^{-10})^2}$$

$$\therefore \quad = 1.314\times10^{-18}\ J$$

$$= \frac{1.314\times10^{-18}}{1.6\times10^{-19}}\ eV$$

$$\therefore \quad \boxed{E = 8.2\ eV}$$

Review Questions

1. *What is De-Broglie's hypothesis of matter waves. Shown that the De-Broglies's wavelength of a charged particle is inversely proportional to the square root of the accelerating potential.* **SPPU : Dec.-16, Marks 6**
2. *What is de-Broglie hypothesis. Derive an expression for de-Broglie wavelength for an electron when it is accelerated by potential difference 'V'.* **SPPU : May-17, Marks 4**
3. *State de-Broglie hypothesis of matter waves. Derive the expression for matter waves for an accelerating particle in terms of its kinetic energy.* **SPPU : May-18, Marks 4**
4. *What is De-Broglie hypothesis ? Derive an expression for de-Broglie wavelength for an electron when it is accelerated by potential difference V.* **SPPU : May-19, Marks 4**

6.4 : Concept of Phase and Group Velocity

SPPU : Dec.-15,16, May-16

- **Phase velocity** (also known as **wave velocity**) is the velocity with which a particular phase of the wave propagates in a medium.
- The equation of a wave travelling in 'x'-direction with vibrations in 'y'-direction is

$$y = A \sin(\omega t - kx) \quad \text{... (6.4.1)}$$

where, A = Amplitude of vibrations,

k = Propagation constant

and ω = Angular frequency.

- $\omega = 2\pi\nu$ and $k = \frac{2\pi}{\lambda}$

$\therefore\ \nu = \frac{\omega}{2\pi}$ and $\lambda = \frac{2\pi}{k}$

The phase velocity v_p is,

$$v_p = \nu\lambda = \frac{\omega}{2\pi}\times\frac{2\pi}{k}$$

$\therefore$ $$v_p = \frac{\omega}{k} \quad \text{... (6.4.2)}$$

- For de Broglie waves,

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

$\therefore$ $$k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} \quad \text{... (6.4.3)}$$

- To find the frequency ν, we equate the energy '$h\nu$' with relativistic total energy 'mc^2'.

$$h\nu = mc^2$$

$\therefore$ $$\nu = \frac{mc^2}{h}$$

As $$\omega = 2\pi\nu$$

$\therefore$ $$\omega = \frac{2\pi\, mc^2}{h} \quad \text{... (6.4.4)}$$

- Substituting equation (6.4.3) and (6.4.4) in equation (6.4.2),

$$v_p = \frac{\left(\dfrac{2\pi mc^2}{h}\right)}{\left(\dfrac{2\pi\, mv}{h}\right)}$$

$\therefore$ $$v_p = \frac{c^2}{v} \quad \text{... (6.4.5)}$$

- As the particle velocity 'v' is always less than the velocity of light 'c',

$$v_p = \frac{c}{v} \cdot c$$

As $$v < c, \quad \frac{c}{v} > 1$$

$\therefore$ $$v_p > c$$

i.e., velocity of de Broglie waves is always greater than the velocity of light.

- Hence de Broglie waves cannot be represented simply by an equation of the type of equation (6.4.1). Instead, we represent the moving body by a **wave group or wave packet.**
- Mathematically, a wave group can be described in terms of a superposition of individual waves of different wavelengths.
- The interference of these waves gives variation in amplitude defining the shape of the wave group.
- If velocities of the waves are same, the wave group travels with this same velocity.
- But, if the wave velocity changes with wavelength the wave group has different velocity from those of the individual waves.
- If the two waves have angular velocities differing by $d\omega$ and propagation constants differing by dk (due to difference $d\lambda$ in their wavelengths) their equations can be written as,

$$y_1 = A \sin(\omega t - kx)$$

and
$$y_2 = A \sin [(\omega + d\omega)t - (k + dk)x]$$

- The resultant displacement 'y' at time 't' is

$$y = y_1 + y_2$$

- Using
$$\sin C + \sin D = 2 \sin\left(\frac{C+D}{2}\right) \cos\left(\frac{C-D}{2}\right)$$

$$y = 2A \sin\left(\frac{2\omega + d\omega}{2} t - \frac{2k+dk}{2} x\right) \cos\left(\frac{d\omega}{2} \cdot t - \frac{dk}{2} \cdot x\right)$$

- As $d\omega$ and dk are very small compared to ω and k respectively,

$$2\omega + d\omega \approx 2\omega$$

$$2k + dk \approx 2k$$

$\therefore$
$$y = 2A \sin(\omega t - kx) \cos\left(\frac{d\omega}{2} t - \frac{dk}{2} \cdot x\right)$$

- The sine term in the above equation represents a wave of angular frequency ω and propagation constant k.
- The cosine term in the equation modulates this wave with angular frequency $\frac{d\omega}{2}$ and propagation constant $\frac{dk}{2}$ to produce wave groups (like phenomenon of 'beats' in sound waves) travelling with a velocity

$$v_g = \frac{dw}{dk}$$

which is the group velocity.

$\therefore$
$$v_g = \frac{dw/dv}{dk/dv} \qquad \dots (6.4.6)$$

- From equation (6.4.4),

$$\omega = \frac{2\pi mc^2}{h}$$

- As
$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$\omega = \frac{2\pi m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$\frac{d\omega}{dv} = \frac{2\pi m_0}{h} v \left(1 - \frac{v^2}{c^2}\right)^{-3/2} \qquad \dots (6.4.7)$$

- From equation (6.4.3),

$$k = \frac{2\pi mv}{h}$$

$$\therefore \quad k = \frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}}$$

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-3/2} \quad \text{... (6.4.8)}$$

- Substituting equation (6.4.7) and (6.4.8) in equation (6.4.6),

$$v_g = v \quad \text{... (6.4.9)}$$

i.e., the de Broglie wave group associated with moving particle travels with the same velocity as the particle.

Relation between Phase Velocity and Group Velocity

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

- From equation (6.4.2)

$$\omega = v_p k$$

- Substituting in equation (6.4.6),

$$v_g = \frac{d}{dk}(v_p k)$$

$$\therefore \quad v_g = v_p + k\frac{dv_p}{dk} = v_p + k\frac{dv_p}{d\lambda}\cdot\frac{d\lambda}{dk}$$

$$\therefore \quad v_g = v_p + k\frac{dv_p}{d\lambda}\times\frac{1}{\left(\frac{dk}{d\lambda}\right)} \quad \text{... (6.4.10)}$$

As

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

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

- Substituting in equation (6.4.10),

$$v_g = v_p + \frac{2\pi}{\lambda}\frac{dv_p}{d\lambda}\times\frac{1}{\left(\frac{-2\pi}{\lambda^2}\right)}$$

$$\therefore \quad v_g = v_p - \lambda\frac{dv_p}{d\lambda}$$

Review Questions

1. *Define phase (wave) velocity. Show that the phase velocity of matter wave is greater than the velocity of light.*
   SPPU : Dec.-15, Marks 4
2. *Define phase velocity and group velocity. Show that group velocity is equal to particle velocity.*
   SPPU : May-16, Marks 6
3. *Define phase velocity and group velocity. Derive the relation between them.*
   SPPU : Dec.-16, Marks 4

Properties of Matter Waves

- Matter particles moving with velocity 'v' exhibit wave nature for which the wavelength is given by,

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

- The properties of these waves are as follows :

1. If m = Constant, $\lambda \propto \frac{1}{v}$ i.e., for particles having same mass, the particles moving with smaller velocities will have longer wavelengths associated with them.
2. If v = Constant, $\lambda \propto \frac{1}{m}$, i.e., for particles of different masses moving with the same velocities the lighter particles will have longer wavelengths associated with them.
3. For particles at rest, $v = 0$

   $\therefore \lambda = \infty$

   i.e., particles at rest do not exhibit wave nature.
4. Matter waves are associated with charged as well as uncharged particles. Hence they are not electromagnetic in nature. In fact, they cannot be classified into any of the types which we have encountered so far, i.e., transverse or longitudinal, electromagnetic or mechanical etc.
5. The phase velocity of matter waves is,

$$v_p = \frac{c^2}{v}$$

   which is greater than 'c', the velocity of light as the particle velocity 'v' is always less than 'c'. Also, this velocity depends on the particle velocity 'v' and hence, is not constant.
6. For waves in a string, the position of particles varies with time. In sound waves pressure varies with time. In electromagnetic waves the electric and magnetic fields vary with time. Similarly, the quantity whose variations consitute matter waves is called the wave function (represented by ψ). However, the wave function ψ has no direct physical significance. The value of the wavefunction at any point in space at any time is related to the probability of finding the particle there at that time.
7. A particle is localized in space whereas wave is spread out. Hence wave nature of matter introduces uncertainty in position of the particle.
8. The wave and particle properties are not exhibited simultaneously.

Review Question

1. *State and explain de-Broglie hypothesis of matter waves. Explain in brief any two properties of matter waves.* **SPPU : Dec.-17, Marks 4**

Heisenberg's Uncertainty Principle

SPPU : May-99,2000,06,12,16,17,18,19, Dec.-99,2000,06,15,17,18

- Describing a moving particle as a wave group introduces uncertainty in the measurement of particle properties like position and momentum.
- This uncertainty is not due to any inadequacy in the measuring instruments but is inherent in wave nature.

- As described earlier, in properties of matter waves, the position of particle becomes uncertain when it is described as a wave group.
- The particle may be located any where within the wave group but its exact location within the wave group is not known.
- Narrower the wave group, smaller is the uncertainty in its position as illustrated in Fig. 6.6.1 (a) and (b).

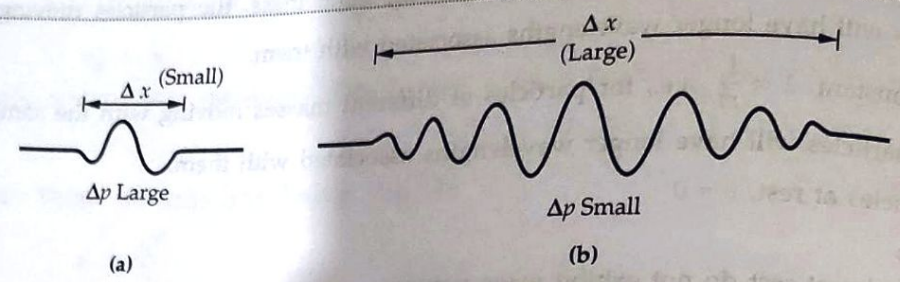


Fig. 6.6.1

- To understand the uncertainty in wavelength and hence the momentum, we use the Fourier transform which gives the amplitudes of different frequencies present in a given waveform.

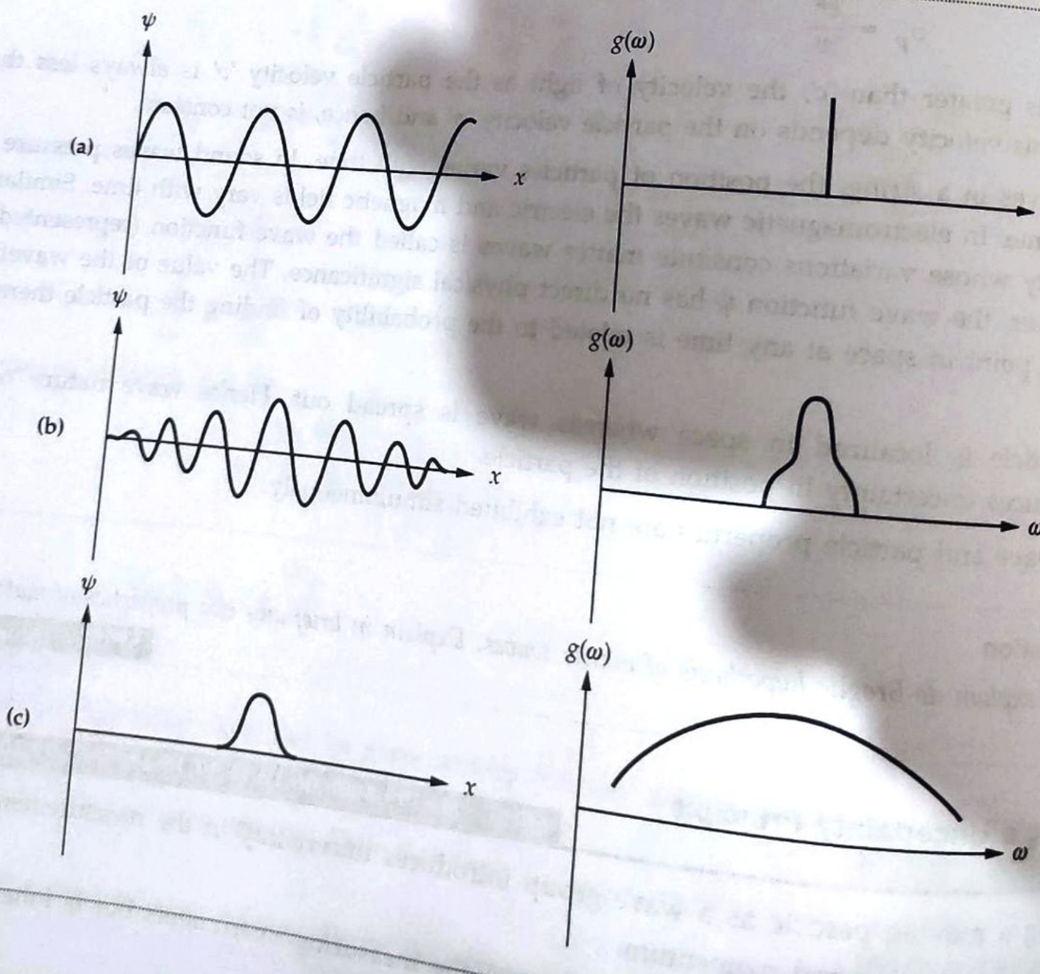


Fig. 6.6.2

- For a purely sinusoidal wave $\psi(x)$, the Fourier transform $g(\omega)$ gives amplitude only at a single frequency as shown in Fig. 6.6.2 (a).
- For a wavegroup a broader range of frequencies are present as shown in Fig. 6.6.2 (b) and for a narrow pulse shown in Fig. 6.6.2 (c), a very large number of frequencies are present.
- Hence, if the wave group is narrower, it will consist of larger number of frequencies and hence wavelengths due to which the wavelength becomes more uncertain.
- As $\lambda = \frac{h}{p}$, an uncertainty in wavelength leads to uncertainty in momentum.
- Thus for broader wave groups, there is smaller uncertainty in wavelength and momentum, whereas for narrower wavegroups there is larger uncertainty in wavelength and momentum.
- From the above discussion, we can conclude that for a narrow wave group there is small uncertainty in position but large uncertainty in momentum, whereas for a broader wave group there is larger uncertainty in position and smaller uncertainty in momentum.
- The Heisenberg's uncertainty principle states that it is impossible to determine both the exact position and the exact momentum of a particle at the same time. The product of uncertainties in these quantities is always greater than or equal to the Planck's constant 'h'.

$$\Delta x \, \Delta p_x \geq h \quad \ldots (6.6.1)$$

Note More precise equation relating these uncertainties is,

$$\Delta x \, \Delta p_x \geq \frac{h}{4\pi}$$

- For the present syllabus, we will use equation (6.6.1).

6.6.1 Uncertainty Principle Applied to Energy and Time

- The kinetic energy of particles can be written as

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

- The uncertainty in energy ΔE can be obtained by differentiating the above equation.

$$\Delta E = \frac{1}{2} m \cdot 2v \, \Delta v$$

$$= v \cdot (m \Delta v)$$

- As

$$p = mv$$

$$\Delta p = m \Delta v$$

$\therefore$

$$\Delta E = v \Delta p$$

- As

$$v = \frac{\Delta x}{\Delta t},$$

$$\Delta E = \frac{\Delta x}{\Delta t} \Delta p$$

$\therefore$

$$\Delta E \, \Delta t = \Delta x \, \Delta p$$

- By Heisenberg's uncertainty principle,

$$\Delta x \, \Delta s \geq h$$

$$\therefore \quad \Delta E \, \Delta t \geq h \qquad \text{... (6.6.2)}$$

6.6.2 Illustration of Heisenberg's Uncertainty Principle by Single Slit Electron Diffraction

- Consider hypothetical experiment in which a parallel beam of electrons is incident on a narrow slit as shown in Fig. 6.6.3.
- The diffraction pattern is formed by the electrons which pass through the slit, but from which position in the slit a particular electron passes is unknown. Hence the uncertainty in position of electron in the y-direction is equal to the width of the slit, say Δy.
- From single slit diffraction pattern, we know that, most of the intensity is concentrated in the central maximum which lies between the two first order minima.
- An electron which passes through the slit, hits the screen somewhere between A and B.
- For the first minimum intensity formed at angle θ,

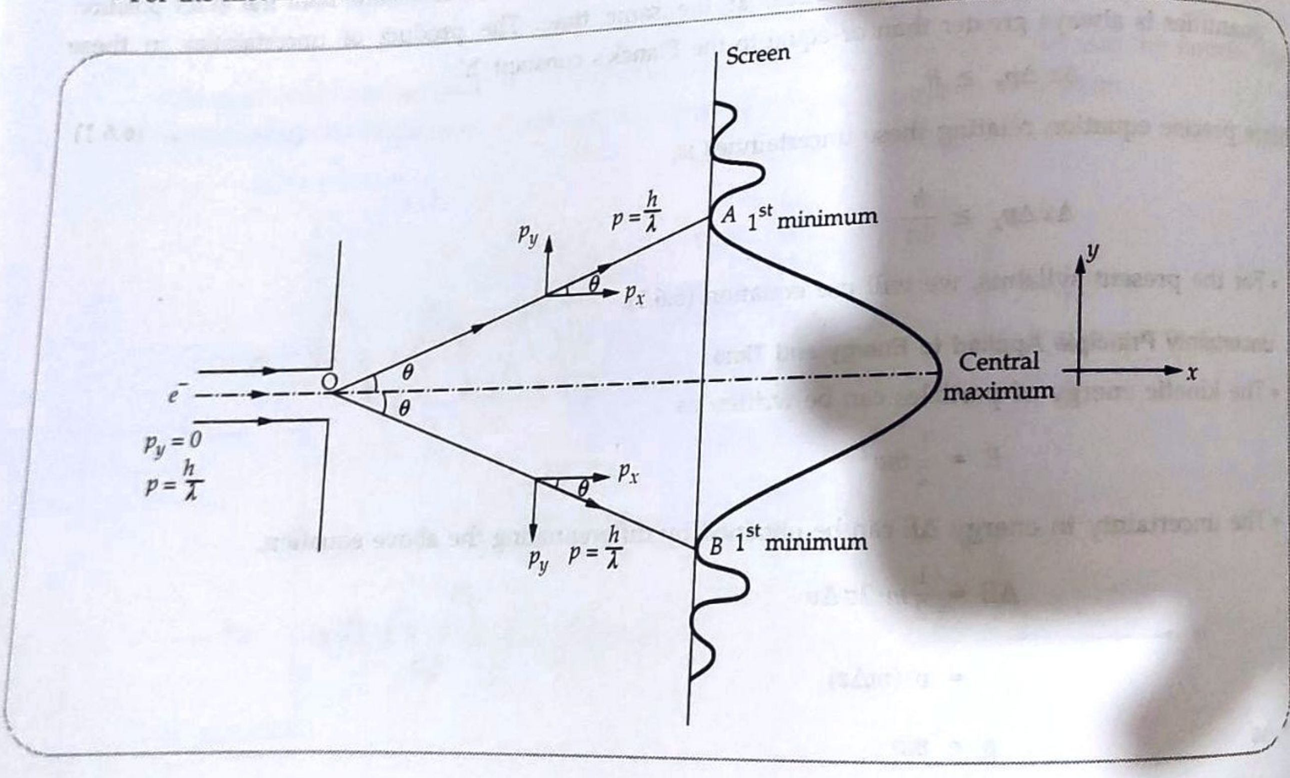


Fig. 6.6.3

$$\Delta y \sin\theta = 1 \cdot \lambda$$

where, λ is the de Broglie wavelength of electrons.

$$\therefore \quad \Delta y = \frac{\lambda}{\sin\theta} \qquad \text{... (6.6.3)}$$

- The momentum of electrons is $p = \frac{h}{\lambda}$ which is along the x-direction before the electrons pass through the slit.

$$\Delta x \, \Delta s \geq h$$

$$\therefore \quad \Delta E \, \Delta t \geq h \qquad \ldots (6.6.2)$$

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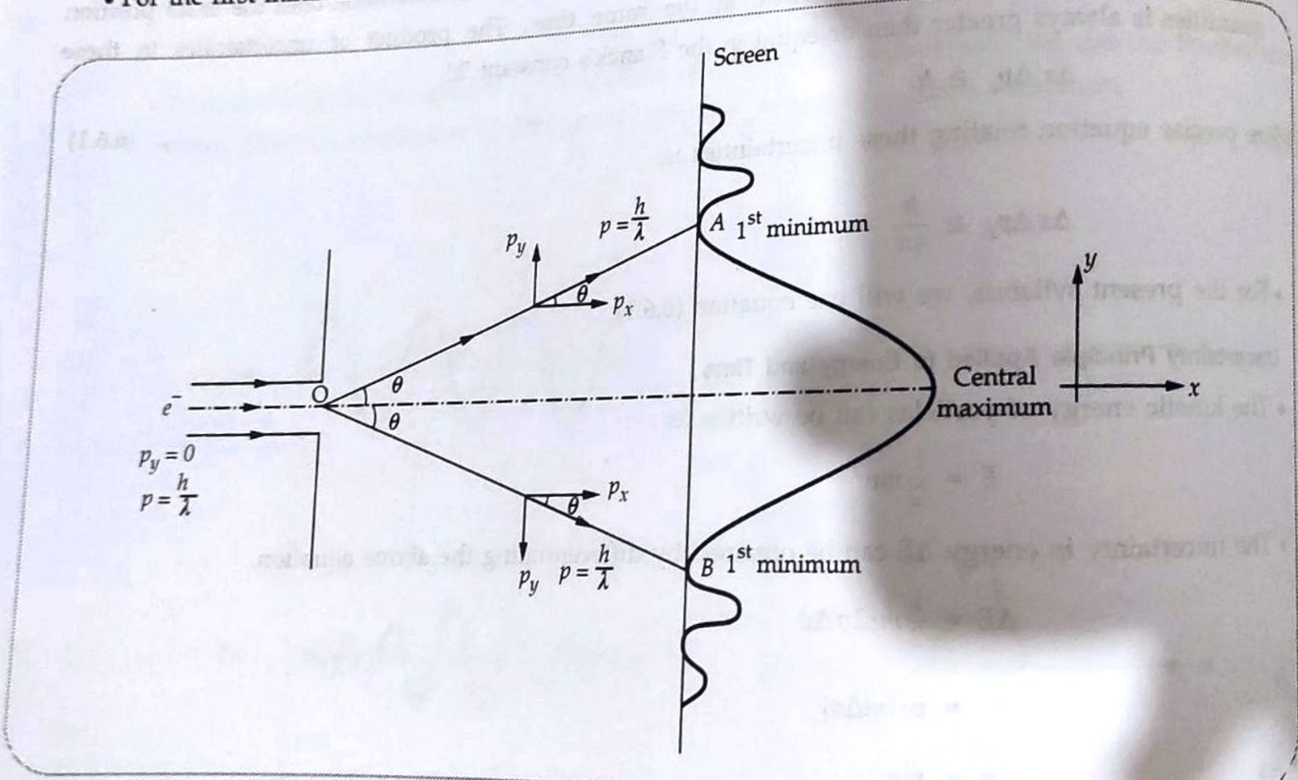

Fig. 6.6.3

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where, λ is the de Broglie wavelength of electrons.

$$\therefore \quad \Delta y = \frac{\lambda}{\sin\theta} \qquad \ldots (6.6.3)$$

- The momentum of electrons is $p = \frac{h}{\lambda}$ which is along the x-direction before the electrons pass through the slit.

- After diffraction, wavelength remains same and hence the momentum is also of the same magnitude but is now directed any where between OA and OB.
- The y-component of momentum, therefore, lies between $+\frac{h}{\lambda}\sin\theta$ and $-\frac{h}{\lambda}\sin\theta$. Hence the uncertainty in momentum along y-direction is

$$\Delta p_y = \frac{h}{\lambda}\sin\theta - \left(-\frac{h}{\lambda}\sin\theta\right)$$

$$\therefore \quad \Delta p_y = \frac{2h}{\lambda}\sin\theta \qquad \text{... (6.6.4)}$$

- From equations (6.6.3) and (6.6.4),

$$\Delta y\,\Delta p_y = 2h$$

$$\therefore \quad \Delta y\,\Delta p_y \geq h$$

which is Hiesenberg's uncertainty principle.

Non-existence of Electron in the Nucleus

- If an electron is confined to the nucleus which has a radius of the order of 10^{-14} m, the maximum uncertainty in position of the electron will be of the order of the radius.

$$\therefore \quad (\Delta x)_{max} = 10^{-14}\ m$$

- By Heisenberg uncertainty principle,

$$(\Delta x)_{max}\,(\Delta p)_{min} = h$$

$$\therefore \quad (\Delta p)_{min} = \frac{h}{(\Delta x)_{max}} = \frac{6.63 \times 10^{-34}}{10^{-14}}$$

$$\therefore \quad (\Delta p)_{min} = 6.63 \times 10^{-20}\ \text{kg}\cdot\text{m/s}$$

- The momentum of electron has to be atleast comparable in magnitude to this uncertainty.

$$\therefore\ p_{min} \simeq (\Delta p)_{min} = 6.63 \times 10^{-20}\ \text{kg}\cdot\text{m/s}$$

- The equation for energy from theory of relativity is

$$E = \sqrt{p^2c^2 + m_0^2 c^4}$$

- Here, $m_0^2 c^4 << p^2c^2$

$$\therefore \quad E = pc$$

$$\therefore \quad E_{min} = 6.63 \times 10^{-20} \times 3 \times 10^{8} = 1.989 \times 10^{-11}\ J$$

$$\therefore \quad E_{min} = 124.3\ \text{MeV}$$

- Thus, for an electron to exist in the nucleus, its energy must be atleast 124.3 MeV.
- Experimentally, it has been observed during beta decay that the β-particles (electrons emitted by the nucleus) never have energy exceeding about 4 MeV.
- As the minimum energy of an electron in a nucleus is 124.3 MeV, the electron can never exist in a nucleus. In fact the β-particles are electrons which are produced in the nucleus due to decay of neutrons.

Ex. 6.6.1 : ***Compute the minimum uncertainty in the location of a 2 gm mass moving with a speed of 1.5 m/s and the minimum uncertainty in the location of an electron moving with a speed of 0.5×10^8 m/s, given that the uncertainty in the momentum is $\Delta p = 10^{-3}\, p$ for both.*** **SPPU : May**

Sol. : Given data :

$$h = 6.63\times10^{-34}\ \text{J-s}$$

$$\Delta p = 10^{-3}p = 10^{-3}\,mv$$

For the 2 gm mass, $m = 2\ \text{gm} = 2\times10^{-3}\ \text{kg}$

$$v = 1.5\ \text{m/s}$$

For the electron, $m = 9.1\times10^{-31}\ \text{kg}$

$$v = 0.5\times10^{8}\ \text{m/s}$$

Formula : $\Delta x\,\Delta p = h$

$$\therefore \quad \Delta x = \frac{h}{\Delta p}$$

$$\therefore \quad \Delta x = \frac{h}{10^{-3}\,mv}$$

$$\therefore \quad \Delta x = \frac{6.63\times10^{-34}}{10^{-3}\times2\times10^{-3}\times1.5}$$

$$\therefore \quad \boxed{\Delta x = 2.21\times10^{-28}\ \text{m}}$$

$$\therefore \quad \Delta x = \frac{6.63\times10^{-34}}{10^{-3}\times9.1\times10^{-31}\times0.5\times10^{8}}$$

$$\therefore \quad \boxed{\Delta x = 1.46\times10^{-8}\ \text{m}}$$

Ex. 6.6.2 : ***An electron has a speed of 600 m/s with an accuracy of 0.005 %. Calculate the uncertainty with which we can locate the position of the electron.*** **SPPU : Dec-99**

Sol. : Given data :

$$\Delta v = \frac{0.005}{100}\times600 = 0.03\ \text{m/s}$$

$$h = 6.63\times10^{-34}\ \text{J-s}$$

$$m = 9.1\times10^{-31}\ \text{kg}$$

Formula : $\Delta x\,\Delta p = h$

$$\therefore \quad \Delta x = \frac{h}{\Delta p} = \frac{h}{m\Delta v}$$

$$\therefore \quad \Delta x = \frac{6.63\times10^{-34}}{9.1\times10^{-31}\times0.03}$$

$$\therefore \quad \boxed{\Delta x = 0.0243 \text{ m}}$$

Ex. 6.6.3 : *A bullet of mass 25 grams is moving with a speed of 400 m/s. The speed is measured accurate upto 0.02 %. Calculate the certainty with which the position of the bullet can be located.*

SPPU : May-2000

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 25 \text{ gm} = 25 \times 10^{-3} \text{ kg}$$

$$\Delta v = \frac{0.02}{100} \times 400 = 0.08 \text{ m/s}$$

Formula : $$\Delta x \, \Delta p = h$$

$$\therefore \quad \Delta x = \frac{h}{\Delta p} = \frac{h}{m \Delta v}$$

$$\Delta x = \frac{6.63 \times 10^{-34}}{25 \times 10^{-3} \times 0.08}$$

$$\therefore \quad \boxed{\Delta x = 3.315 \times 10^{-31} \text{ m}}$$

Ex. 6.6.4 : *Calculate the minimum uncertainty in the velocity of an electron confined to a box of length 10 A°.*

SPPU : Dec.-2000

Sol. : Given data :

The maximum uncertainty in position of electron is equal to the length of the box.

$$(\Delta x)_{max} = 10 \text{ A°} = 10 \times 10^{-10} \text{ m}$$

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

Formula : $$\Delta x \, \Delta p = h$$

$$\therefore \quad \Delta x \cdot m \Delta v = h$$

$$\Delta v = \frac{h}{m \Delta x}$$

For minimum uncertainty in velocity, the uncertainty in position is maximum.

$$\therefore \quad (\Delta v)_{min} = \frac{h}{m (\Delta x)_{max}}$$

$$\therefore \quad (\Delta v)_{min} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 10 \times 10^{-10}}$$

$$\therefore \quad \boxed{(\Delta v)_{min} = 7.286 \times 10^{5} \text{ m/s}}$$

Ex. 6.6.5 : *If the uncertainty in location of a particle is equal to its de Broglie wavelength, show that the uncertainty in its velocity is equal to its velocity.*

SPPU : May

Sol. : Given data :

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

Formula :

$$\Delta x \, \Delta p = h$$

$$\Delta p = m\Delta v$$

$$\therefore \quad \frac{h}{mv} \cdot m\Delta v = h$$

$$\therefore \quad \boxed{\Delta v = v}$$

Ex. 6.6.6 : *What potential difference must be applied to an electron microscope to obtain electrons of wavelength 0.3 A° ?*

SPPU : May

Sol. : Given data :

$$\lambda = 0.3 \text{ A°}$$

Formula :

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ A°}$$

$$\therefore \quad V = \frac{12.27^2}{\lambda^2}$$

$$\therefore \quad V = \frac{12.27^2}{0.3^2}$$

$$\therefore \quad \boxed{V = 1672.81 \text{ V}}$$

Ex. 6.6.7 : *An electron is confined to a box of length 2A°. Calculate the minimum uncertainty in its velocity.*

SPPU : Dec

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$(\Delta x)_{max} = 2 \text{ A°} = 2 \times 10^{-10} \text{ m}$$

Formula :

$$(\Delta v)_{min} = \frac{h}{m(\Delta x)_{max}}$$

$$\therefore \quad (\Delta v)_{min} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 2 \times 10^{-10}}$$

$$\therefore \quad \boxed{(\Delta v)_{min} = 3.643 \times 10^{6} \text{ m/s}}$$

Review Questions

1. *State Heisenberg's uncertainty principle and prove it by thought experiment of electron diffraction at a single slit.* **SPPU : Dec.-15, Marks 6**
2. *State and explain Heisenberg's uncertainty principle.* **SPPU : May-16, Marks 4**
3. *State and explain Heisenberg's uncertainty principle. Illustrate the principle by electron diffraction at a single silt.* **SPPU : May-17, Marks 6**
4. *State and explain Heisenberg's Uncertainty Principle. Show that it is also applicable for energy and time.* **SPPU : Dec.-17, Marks 6**
5. *State and explain Heisenberg's uncertainty principle. Illustrate it by an experiment of diffraction at a single slit.* **SPPU : May-18, Marks 6**
6. *Obtain an expression for Heisenberg's uncertainty principle for energy and time.* **SPPU : Dec.-18, Marks 4**
7. *State and explain Heisenberg's uncertainty principle. Show that it is also applicable for energy and time.* **SPPU : Dec.-18, Marks 6**
8. *State and explain Heisenberg's uncertainty principle. Illustrate the principle of electron diffraction at a single silt.* **SPPU : May-19, Marks 6**

6.7 : Concept of Wave Function

- Every wave is characterized by periodic variation in some physical quantity. For example, pressure varies periodically in sound waves whereas electric and magnetic fields vary periodically in an electromagnetic wave.
- Similarly, the quantity whose periodic variations make up the matter wave is called wave function ψ.
- The value of ψ at a particular point (x, y, z) in space at time '*t*' is related to the probability of finding the particle there at that time. ψ itself does not have any direct physical significance and is not an experimentally measurable quantity.
- The probability of finding a particle at some point in space at time '*t*' is a positive value between 0 and 1. But ψ can be positive, negative or complex. Hence ψ is not an observable quantity.
- In general, the wave function ψ is a complex quantity and can be written as,

$$\psi = A + iB$$

where A and B are real.

- Complex conjugate of ψ is

$$\psi^* = A - iB$$

- The product $\psi\psi^* = |\psi|^2 = A^2 + B^2$ is a real and positive quantity.
- Although $|\psi|^2$ is a positive and real quantity, it need not be less than 1. Hence we still cannot say that the probability of finding the particle is equal to $|\psi|^2$. We can only say that the probability is proportional to $|\psi|^2$.

SPPU : May-16,17,18,19, Dec.-15,16,18

6.8 : Physical Significance of ψ

- According to Max Born's interpretation, the probability of finding the particle described by the wave function ψ at a point (x, y, z) in space at time '*t*' proportional to the value of $|\psi|^2$ at that point at time '*t*'.
- A large value of $|\psi|^2$ represents larger probability of finding the particle.

- The probability of finding the particle is zero at a point only if ...
- Even if there is a small value of $|\psi|^2$ at a point, there will be some probability of detecting the particle there.
- The probability of finding the particle in a certain volume element $dv = dx\ dy\ dz$ is $|\psi|^2\ dv$ which is called the probability density if $|\psi|^2$ represents probability.
- As the particle has to exist somewhere in space, the total probability of finding the particle is 1. i.e,

$$\int_{-\infty}^{\infty} |\psi|^2\ dv = 1 \qquad \cdots (6.8.1)$$

- The above condition is satisfied only if $|\psi|^2$ represents probability.
- But, in general, the wave functions obtained as solutions of differential equations do not satisfy equation (6.8.1). Instead, on integrating over the whole volume, yield a finite positive and real quantity, say N^2 i.e.,

$$\int_{-\infty}^{\infty} |\psi|^2\ dv = N^2$$

- Normalized wave function ψ_N is then constructed from ψ as,

$$\psi_N = \frac{\psi}{N}$$

and

$$\psi_N^* = \frac{\psi^*}{N}$$

- The normalized wave function satisfies equation (6.8.1) so that $|\psi_N|^2$ represents probability.
- The process of constructing ψ_N from ψ is called **normalization** of the wave function.
- Physically acceptable wave function ψ should satisfy the following conditions :
  i) ψ should be normalized wave function so that $|\psi|^2$ will represent probability and satisfy equation (8.9.1).
  ii) As probability is a single valued function, ψ must also be a single valued function at every point in space.
  iii) ψ must be finite at each and every point in space.
  iv) ψ must be continuous in the region where it is defined.
  v) The first order derivatives of ψ, i.e., $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}$ and $\frac{\partial \psi}{\partial z}$ must be continuous in the region where ψ is defined.

Review Question

1. *What is wave function ? Explain what is normalization of wave function.*
2. *Explain why probability of finding of a particle cannot be predicted by the interpretation of wave function Ψ. Explain physical significance of $|\Psi|^2$.* **SPPU : Dec.-15, Marks 4**
3. *Write down the conditions which are to be satisfied by well behaved wave function.* **SPPU : May-16, Marks 4**
4. *Explain physical significance of wave function Ψ and $(\Psi)^2$. State the mathematical conditions that wave function Ψ should satisfy.* **SPPU : Dec.-16, Marks 4**
5. *Explain wave-function ψ. Give the physical significance of $|\psi^2|$* **SPPU : May-17, Marks 4**

SPPU : May-18, Marks 4

6. *Explain wave-function ψ. Give the physical significance of $|\psi^2|$* **SPPU : Dec.-18, Marks 4**
7. *Write down the conditions which are to be satisfied by well behaved wave function.* **SPPU : May-19, Marks 4**

6.9 : Schrödinger's Time Independent Wave Equation

SPPU : May-16,17,19, Dec.-15,17

- The general differential equation for a wave with wave function 'ψ', travelling with velocity 'u' in three dimensions is

$$\frac{\partial^2 \psi}{\partial t^2} = u^2\left[\frac{\partial^2 \psi}{\partial x^2}+\frac{\partial^2 \psi}{\partial y^2}+\frac{\partial^2 \psi}{\partial z^2}\right]$$

i.e.,

$$\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi \quad \ldots (6.9.1)$$

where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is called the Laplace operator.

- The general solution of equation (6.9.1) is of the form

$$\psi(x, y, z, t) = \psi_0 (x, y, z) e^{-i\omega t} \quad \ldots (6.9.2)$$

where $\psi_0(x, y, z)$ is the amplitude of the wave at point (x, y, z). The above equation can also be written as

$$\psi(\vec{r}, t) = \psi_0(\vec{r}) e^{-i\omega t} \quad \ldots (6.9.3)$$

where $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ is the position vector of the point (x, y, z).

- Differentiating equation (6.9.3) partially with respect to 't' twice,

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega)\psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi_0 e^{-i\omega t}$$

- But

$$\psi = \psi_0 e^{-i\omega t}$$

$\therefore$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi$$

- Substituting in equation (6.9.1),

$$-\omega^2 \psi = u^2 \nabla^2 \psi \quad \ldots (6.9.4)$$

$$\nabla^2 \psi + \frac{\omega^2}{u^2}\psi = 0$$

$$\omega = 2\pi\nu = 2\pi \frac{u}{\lambda}$$

$\therefore$

$$\frac{\omega}{u} = \frac{2\pi}{\lambda}$$

$$\frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2} \qquad \dots (6.9.5)$$

- From De Broglie hypothesis for matter waves,

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

$$\therefore \quad \lambda^2 = \frac{h^2}{p^2} \qquad \dots (6.9.6)$$

- The total energy (E) of particle is a sum of kinetic energy $\left(\frac{1}{2}mv^2\right)$ and potential energy V.

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

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

$$\therefore \quad E = \frac{p^2}{2m} + V$$

$$\therefore \quad p^2 = 2m(E-V)$$

- Substituting in equation (6.9.6),

$$\lambda^2 = \frac{h^2}{2m(E-V)}$$

- Substituting in equation (6.9.5),

$$\frac{\omega^2}{u^2} = 4\pi^2 \times \frac{2m(E-V)}{h^2}$$

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

- Substituting in equation (6.9.4),

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \qquad \dots (6.9.7)$$

- The quantity $\frac{h}{2\pi}$ appears very frequently in quantum mechanics and hence is substituted as $\hbar$.

$$\therefore \quad \nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \qquad \dots (6.9.8)$$

- Equation (6.9.7) or (6.9.8) is the Schrödinger's time independent wave equation.

Review Questions

1. *Deduce Schrodinger's time independent wave equation.* **SPPU : Dec.-15, May-16,17,19, Marks 6**
2. *Starting from de-Broglie hypothesis, derive Schrodinger's time independent wave equation.* **SPPU : Dec.-17, Marks 6**

6.11 : Schrödinger's Time Dependent Wave Equation

SPPU : May-11

- The general differential equation for a wave with wave function ψ, travelling with velocity 'u' in three dimensions is,

$$\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi \qquad \dots (6.10.1)$$

where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplace operator.

- The general solution of equation (6.10.1) is of the form,

$$\psi(x, y, z, t) = \psi_0(x, y, z)\, e^{-i\omega t} \qquad \dots (6.10.2)$$

where $\psi_0(x, y, z)$ is the amplitude of the wave at point (x, y, z). The above equation can also be written as,

$$\psi(\vec{r}, t) = \psi_0(\vec{r})\, e^{-i\omega t} \qquad \dots (6.10.3)$$

where $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ is the position vector of the point (x, y, z).

- Differentiating equation (6.10.3) partially with respect to 't',

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0\, e^{-i\omega t}$$

$$\therefore \quad \frac{\partial \psi}{\partial t} = -i\omega\psi \qquad \dots (6.10.4)$$

- As $\omega = 2\pi\nu$ and $E = h\nu$,

$$\omega = 2\pi \frac{E}{h}$$

- From equation (6.10.4),

$$\frac{\partial \psi}{\partial t} = \frac{-i\, 2\pi E}{h}\psi$$

$$\therefore \quad E\psi = \frac{-h}{i 2\pi}\frac{\partial \psi}{\partial t}$$

$$\therefore \quad E\psi = \frac{ih}{2\pi}\frac{\partial \psi}{\partial t} \qquad \dots (6.10.5)$$

- Schrödinger's time independent equation is

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

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

$$\frac{-h^2}{8\pi^2 m}\nabla^2\psi + V\psi = E\psi$$

- Substituting for $E\psi$ from equation (6.10.5),

$$\frac{-h^2}{8\pi^2 m}\nabla^2\psi + V\psi = \frac{ih}{2\pi}\frac{\partial \psi}{\partial t} \qquad \dots (6.10.6)$$

- The above equation is known as Schrödinger's time dependent wave equation.

Review Question **SPPU : May-11, Marks 7**

1. *Deduce Schrödinger's time dependent wave equation.*

6.11 : Applications of Schrödinger's Time Independent Wave Equation

- In many situations, particles are bound to a certain region in space by a potential distribution which does not depend on time.
- For example, an electron is bound by the potential distribution of nucleus.
- Similarly, the nucleons (i.e., protons and neutrons) are bound to the nucleus because of the potential distribution arising from the nuclear force.
- In such situations, the potential function 'V' is substituted in Schrödinger's time independent equation and steady state solutions can be then obtained for the wave function ψ which describe the particle.
- The equations are solved using boundary conditions which satisfy the physical restrictions on wave function ψ which are described in section 6.9.
- Real practical problems are three dimensional and analysis of such problems require advanced mathematical techniques and are beyond the scope of this book.
- However, two applications are discussed which are one dimensional and require limited mathematical background.
- Even such vastly simplified problems give results which are strikingly different from classical mechanics which is observed in day-to-day life.

6.12 : Particle in a Rigid Box (Infinite Potential Well)

SPPU : May-05,06,10,11,12,16,17,18,19, Dec.-03,04,05,10,15,16,17,18

- Consider a one dimensional problem in which a particle of mass 'm' moving with speed 'v' along x-axis is confined to a box of length 'L' with perfectly rigid walls at $x = 0$ and $x = L$ as shown in Fig. 6.12.1 (a).
- The particle does not lose energy when it collides with the walls so that its total energy remains constant.
- This physical problem of particle confined between two rigid walls can be converted into a problem of potential distribution by specifying the potential energy of the particle to be infinite at and beyond the walls. i.e.,

$$V = \infty \quad \text{for } x \leq 0 \text{ and for } x \geq L$$

- The potential energy of the particle is constant within the box which can be taken to be zero for convenience i.e.,

$$V = 0 \quad \text{for } 0 < x < L$$

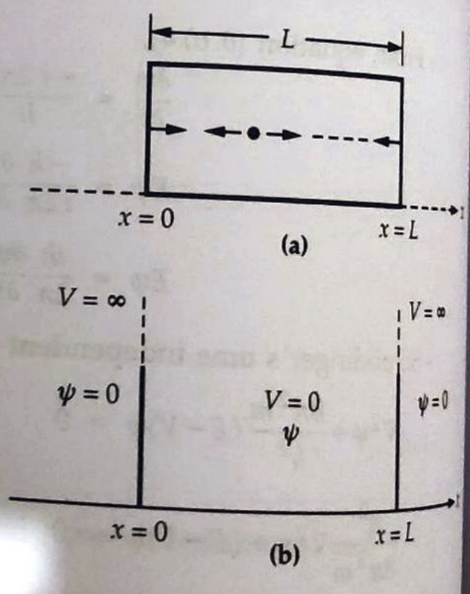

Fig. 6.12.1

- The potential energy distribution is shown in Fig. 6.12.1 (b). It is as if the particle is inside an infinite potential well.
- As the particle does not exist at the walls and beyond them,

$$\psi = 0 \quad \text{for } x \leq 0 \text{ and } x \geq L$$

- The wave function ψ exists only for $0 < x < L$.

- Schrödinger's time independent wave equation is

$$\nabla^2\psi+\frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \qquad \dots (6.12.1)$$

- As it is a problem in one dimension along x-axis, $\nabla^2\psi$ can be replaced by $\frac{\partial^2\psi}{\partial x^2}$ which in turn can be replaced by $\frac{d^2\psi}{dx^2}$ as ψ is a function of x only.
- Also, substituting $V = 0$ for $0 < x < L$ in equation (6.12.1),

$$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}E\psi = 0$$

Let

$$K^2 = \frac{8\pi^2 mE}{h^2} \qquad \dots (6.12.2)$$

$\therefore$

$$\frac{d^2\psi}{dx^2}+K^2\psi = 0 \qquad \dots (6.12.3)$$

- The general solution of equation (6.12.3) is

$$\psi = A\sin Kx + B\cos Kx \qquad \dots (6.12.4)$$

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

- The first boundary condition is

$\psi = 0$ at $x = 0$

$\therefore$ From equation (6.12.4),

$$0 = A\sin 0 + B\cos 0$$

$$B = 0$$

$\therefore$ From equation (6.12.4)

$$\psi = A\sin Kx \qquad \dots (6.12.5)$$

- The second boundary condition is

$\psi = 0$ at $x = L$

$\therefore$ From equation (6.12.5),

$$0 = A\sin KL$$

- $A \neq 0$ as for $A = 0$, $\psi = 0$ for all values of x which will mean that the particle does not exist inside the box.

$\therefore$

$$\sin KL = 0$$

$\therefore$

$$KL = n\pi\ ;\ n = 1, 2, 3, \dots \qquad \dots (6.12.6)$$

- $n \neq 0$ as $n = 0 \Rightarrow \psi = 0$ for all values of x which is not possible.

$\therefore$

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

From equations (6.12.2) and (6.12.5),

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

- As energy 'E' depends on 'n', we use suffix 'n' for 'E'.

$$\therefore \qquad E_n = \frac{n^2 h^2}{8mL^2} \qquad \ldots (6.12.7)$$

where, $\qquad n = 1, 2, 3, \ldots$

- From the above equation, the smallest value of energy that the particle can have is

$$E_1 = \frac{h^2}{8mL^2}$$

which is non-zero. This contradicts classical mechanics, according to which the particle can have zero energy.

- The other possible values of energy are $E_2 = \frac{4h^2}{8mL^2}$, $E_3 = \frac{9h^2}{8mL^2}$, etc.
- These energy values are discrete. They are not continuous as expected from classical mechanics.
- Thus, according to quantum mechanics, the particle inside a rigid box cannot have all values of energy, but only those discrete values which are given by equation (6.12.7). These discrete energy values are known as **energy eigen values.** These energy levels are shown in Fig. 6.12.2.
- In a similar situation in three dimensions, an electron in an atom has descrete energy levels. During transition from higher level to lower level, the energy difference is given out and for transition from lower level to higher, energy equivalent to the energy difference is absorbed.

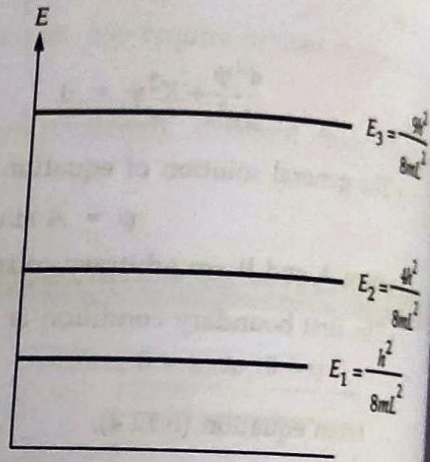

Fig. 6.12.2

Wave function :

- Substituting equation (6.12.6) in equation (6.12.5), we get,

$$\psi = A \sin\left(\frac{n\pi x}{L}\right) \qquad \ldots (6.12.8)$$

- The complex conjugate of ψ is

$$\psi^* = A \sin\left(\frac{n\pi x}{L}\right)$$

- To normalize the wave function, we find $\int_0^L \psi\psi^* dx$

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

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

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

$$= \frac{A^2}{2}[L - 0]$$

$$\int_0^L \psi\psi^* dx = \frac{A^2 L}{2}$$

• Let the R.H.S. be N^2 i.e.,

$$N^2 = \frac{A^2 L}{2}$$

or

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

• The normalized wave function ψ_n is obtained using

$$\psi_n = \frac{\psi}{N}$$

$\therefore$

$$\psi_n = \frac{A\sin\left(\frac{n\pi x}{L}\right)}{\left(A\sqrt{\frac{L}{2}}\right)}$$

$\therefore$

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \ldots (6.12.9)$$

• These normalized wave functions are called eigen functions.

$$\psi_n^* = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

The probability function is

$$P(x) = |\psi_n|^2 = \psi_n\psi_n^* = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \quad \ldots (6.12.10)$$

• The wave function and probability functions for $n = 1, 2, 3$ are shown in Fig. 6.12.3.

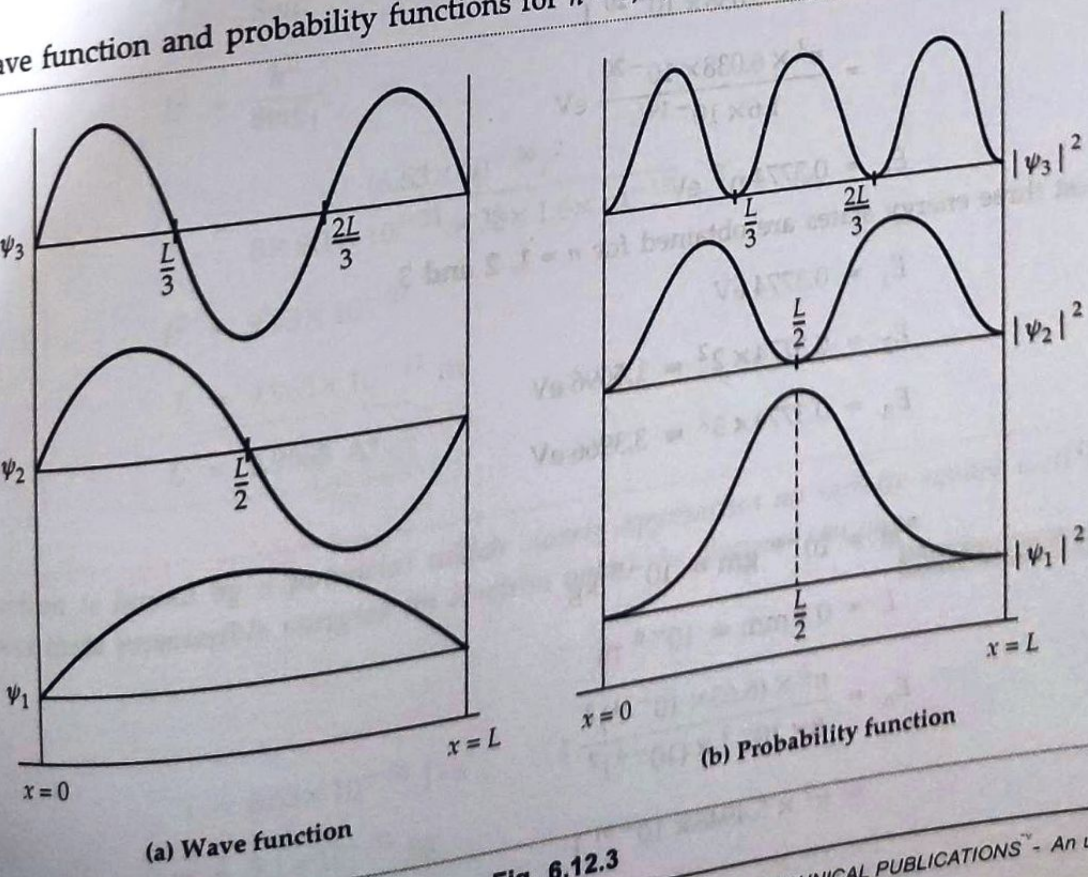

Fig. 6.12.3

- A particle having the lowest energy E_1 has wave function ψ_1 for which the probability of finding the particle is maximum at the centre of the box. For a particle of energy E_2, the probability of finding the particle is zero at the centre.
- Thus quantum mechanics predicts certain forbidden regions for the particle with a certain energy.
- Such situations are encountered with electrons in atoms. This is not predicted by classical mechanics in which there is same probability of finding the particle throughout the region.

Ex. 6.12.1 : ***Compare the lowest three energy states for (i) An electron confined in a potential well of width 10 A° and (ii) A grain of dust with mass 10^{-6} gm in an infinite potential well of width 0.1 mm. What can you conclude from this comparison ?*** **SPPU : Dec-03**

Sol. : For a particle of mass 'm' in an infinite potential well, the energy levels are given by,

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

i) Given :

$$m = 9.1\times 10^{-31} \text{ kg}$$

$$L = 10 \text{ A}^{\circ} = 10\times 10^{-10} \text{ m}$$

$$\therefore \quad L = 10^{-9} \text{ m}$$

$$h = 6.63\times 10^{-34} \text{ J-s}$$

$$\therefore \quad E_n = \frac{n^2\times(6.63\times 10^{-34})^2}{8\times 9.1\times 10^{-31}\times(10^{-9})^2} \text{ J}$$

$$= n^2\times 6.038\times 10^{-20} \text{ J}$$

$$= \frac{n^2\times 6.038\times 10^{-20}}{1.6\times 10^{-19}} \text{ eV}$$

$$E_n = 0.3774\, n^2 \text{ eV}$$

The lowest three energy states are obtained for n = 1, 2 and 3.

$$E_1 = 0.3774 \text{ eV}$$

$$E_2 = 0.3774\times 2^2 = 1.5096 \text{ eV}$$

$$E_3 = 0.3774\times 3^2 = 3.3966 \text{ eV}$$

ii) Given :

$$m = 10^{-6} \text{ gm} = 10^{-9} \text{ kg}$$

$$L = 0.1 \text{ mm} = 10^{-4} \text{ m}$$

$$E_n = \frac{n^2\times(6.63\times 10^{-34})^2}{8\times 10^{-9}\times(10^{-4})^2} \text{ J}$$

$$= n^2\times 5.4946\times 10^{-51} \text{ J}$$

$$= \frac{n^2 \times 5.4946 \times 10^{-51}}{1.6 \times 10^{-19}} \text{ eV}$$

$$E_n = 3.434 \times 10^{-32} \, n^2 \text{ eV}$$

∴ The lowest three energy states are,

$$E_1 = 3.434 \times 10^{-32} \text{ eV}$$

$$E_2 = 3.434 \times 10^{-32} \times 2^2 = 1.37365 \times 10^{-31} \text{ eV}$$

$$E_3 = 3.434 \times 10^{-32} \times 3^2 = 3.091 \times 10^{-31} \text{ eV}$$

The energy levels of dust are very close to each other and hence will appear continuous whereas the energy difference is larger for electrons due to which the energy levels will appear discrete. Hence the quantization of energy will be observed more easily for the smaller particle, i.e., electron, compared to the larger dust particles.

Ex. 6.12.2 : *Lowest energy of an electron trapped in a potential well is 38 eV. Calculate the width of the well.*

SPPU : Dec.-04,17, May-05,19

Sol. : Given :

$$E_1 = 38 \text{ eV} = 38 \times 1.6 \times 10^{-19} \text{ J}$$

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

Formula :

$$E_1 = \frac{h^2}{8mL^2}$$

$$L^2 = \frac{h^2}{8mE_1}$$

$$= \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 38 \times 1.6 \times 10^{-19}}$$

$$L^2 = 9.93 \times 10^{-21}$$

$$\therefore \quad L = 9.965 \times 10^{-11} \text{ m}$$

$$\boxed{L = 0.9965 \text{ A}^\circ}$$

Ex. 6.12.3 : *An electron is bound by a potential which closely approaches an infinite square well of width 1 A°. Calculate the lowest three permissible energies (in electron volts) the electron can have.*

SPPU : Dec.-05, May-10,11,18

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$L = 1 \text{ A}^\circ = 10^{-10} \text{ m}$$

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

$$\therefore \quad E_n = \frac{n^2 \times (6.63\times 10^{-34})^2}{8\times 9.1\times 10^{-31}\times (10^{-10})^2} \text{ J}$$

$$= n^2 \times 6.038\times 10^{-18} \text{ J}$$

$$= \frac{n^2 \times 6.038\times 10^{-18}}{1.6\times 10^{-19}} \text{ eV}$$

$$\therefore \quad E_n = 37.74\, n^2 \text{ eV}$$

The lowest three permissible energies are

$$E_1 = 37.74 \text{ eV}$$

$$E_2 = 37.74\times 2^2 = 150.96 \text{ eV}$$

$$E_3 = 37.74\times 3^2 = 339.66 \text{ eV}$$

Ex. 6.12.4 : ***An electron is trapped in a rigid box of width 2 A°. Find its lowest energy level and momentum. Hence find energy of the third energy level.*** **SPPU : May-06,12, Dec-18**

Sol. : Given :

For lowest energy, $n = 1$

$$h = 6.63\times 10^{-34} \text{ J-s}$$

$$m = 9.1\times 10^{-31} \text{ kg}$$

$$L = 2 \text{ A}^\circ = 2\times 10^{-10} \text{m}$$

Formula : $E_n = \frac{n^2h^2}{8mL^2}$, $p = \sqrt{2mE}$

$$E_1 = \frac{(6.63\times 10^{-34})^2}{8\times 9.1\times 10^{-31}\times (2\times 10^{-10})^2} \text{ J}$$

$$= 1.5095\times 10^{-18} \text{ J}$$

$$= \frac{1.5095\times 10^{-18}}{1.6\times 10^{-19}} \text{ eV}$$

$$\therefore \quad \boxed{E_1 = 9.434 \text{ eV}}$$

The corresponding momentum is,

$$p_1 = \sqrt{2\text{m}\,\text{E}_1}$$

$$= \sqrt{2\times 9.1\times 10^{-31}\times 1.5095\times 10^{-18}}$$

$$\therefore \quad \boxed{p_1 = 1.66\times 10^{-24} \text{ kg-m/s}}$$

The third energy level is

$$E_3 = E_1 \times 3^2$$

$$= 9.434 \times 3^2$$

$$\therefore \quad \boxed{E_3 = 84.906 \text{ eV}}$$

Ex. 6.12.5 : ***An electron is confined in an infinite potential well of width 5 A°. Calculate the energy and wavelength of the emitted photon if the electron makes a transition from its n = 2 energy level to n = 1.***

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$L = 5 \text{ A}° = 5 \times 10^{-10} \text{ m}$$

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

For $n = 1$,

$$E_1 = \frac{h^2}{8mL^2}$$

For $n = 2$,

$$E_2 = \frac{4h^2}{8mL^2}$$

The energy of emitted photon is $E_2 - E_1$, i.e.,

$$E_2 - E_1 = \frac{3h^2}{8mL^2}$$

$$\therefore \quad E_2 - E_1 = \frac{3 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (5 \times 10^{-10})^2}$$

$$= 7.246 \times 10^{-19} \text{ J}$$

$$= \frac{7.246 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV}$$

$$\therefore \quad \boxed{E_2 - E_1 = 4.53 \text{ eV}}$$

The energy of photon in terms of wavelength is $\frac{hc}{\lambda}$

$$\therefore \quad \frac{hc}{\lambda} = 7.246 \times 10^{-19} \text{ J}$$

$$c = 3 \times 10^8 \text{ m/s}$$

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{7.246 \times 10^{-19}}$$

The third energy level is

$$E_3 = E_1 \times 3^2$$

$$= 9.434 \times 3^2$$

$$\therefore \quad \boxed{E_3 = \mathbf{84.906\ eV}}$$

Ex. 6.12.5 : *An electron is confined in an infinite potential well of width 5 A°. Calculate the energy and wavelength of the emitted photon if the electron makes a transition from its n = 2 energy level to n = 1.*

Sol. : Given data :

$$h = 6.63 \times 10^{-34}\ \text{J-s}$$

$$m = 9.1 \times 10^{-31}\ \text{kg}$$

$$L = 5\ \text{A}° = 5 \times 10^{-10}\ \text{m}$$

Formula :

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

For $n = 1$,

$$E_1 = \frac{h^2}{8mL^2}$$

For $n = 2$,

$$E_2 = \frac{4h^2}{8mL^2}$$

The energy of emitted photon is $E_2 - E_1$, i.e.,

$$E_2 - E_1 = \frac{3h^2}{8mL^2}$$

$$\therefore \quad E_2 - E_1 = \frac{3 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (5 \times 10^{-10})^2}$$

$$= 7.246 \times 10^{-19}\ \text{J}$$

$$= \frac{7.246 \times 10^{-19}}{1.6 \times 10^{-19}}\ \text{eV}$$

$$\therefore \quad \boxed{E_2 - E_1 = \mathbf{4.53\ eV}}$$

The energy of photon in terms of wavelength is $\frac{hc}{\lambda}$

$$\therefore \quad \frac{hc}{\lambda} = 7.246 \times 10^{-19}\ \text{J}$$

$$c = 3 \times 10^8\ \text{m/s}$$

$$\therefore \quad \lambda = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{7.246 \times 10^{-19}}$$

$$\therefore \quad \boxed{\lambda = 2.745 \times 10^{-7} \text{ m}}$$

Ex. 6.12.6 : *Compute energy diffrence between the ground state and first excited state for an electron in a one-dimensional rigid box of length 10^{-8} cm.* **SPPU : Dec.-10, Marks 4**

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ J-s}$$
$$m = 9.1 \times 10^{-31} \text{ kg}$$
$$L = 10^{-8} \, cm = 10^{-10} \text{ m}$$

Formula :

$$E_1 = \frac{h^2}{8 \, mL^2}$$

and in first excited state,

$$E_2 = \frac{4 \, h^2}{8 \, mL^2}$$

The difference in energy is,

$$E_2 - E_1 = \frac{3h^2}{8 \, mL^2}$$

$$= \frac{3 \times (6.63 \times 10^{-34})^2}{8(9.1 \times 10^{-31})\,(10^{-10})^2}$$

$$= 1.8114 \times 10^{-17} \text{ J}$$

$$= \frac{1.8114 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV}$$

$$\therefore \quad \boxed{E_2 - E_1 = 113.21 \text{ eV}}$$

Ex. 6.12.7 : *The lowest energy of an electron trapped in a rigid box is 4.19 eV. Find the width of the box in A.U.* **SPPU : Dec.-15, Marks 3**

Sol. : Given data :

$$E_1 = 4.19 \text{ eV} = 4.19 \times 1.6 \times 10^{-19} \text{ J}$$

$$h = 6.63 \times 10^{-34} \text{ Js}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

Formula :

$$E_1 = \frac{h^2}{8 \, m \, L^2}$$

$$\therefore \quad 4.19 \times 1.6 \times 10^{-19} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times L^2}$$

$$\boxed{L = 3 \times 10^{-10} \text{ m}}$$

Ex. 6.12.8 : A neutron is trapped in an infinite potential well of width 10^{-14} m. Calculate its first energy value in eV.

SPPU : May-16, Marks

Sol. : Given data :

$$h = 6.63\times10^{-34}\ Js$$

$$m = 1.675\times10^{-27}\ kg$$

$$L = 10^{-14}\ m$$

Formula : $$E_1 = \frac{h^2}{8mL^2}$$

$$E_1 = \frac{(6.63\times10^{-34})^2}{8\times1.675\times10^{-27}\times(10^{-14})^2}$$

$$= 3.28\times10^{-13}\ J$$

$$= \frac{3.28\times10^{-13}}{1.6\times10^{-19}}\ eV$$

$$\therefore \quad \boxed{E_1 = 2.05\times10^{6}\ eV}$$

Ex. 6.12.9 : Calculate the energy required to excite the electron from its ground state to fourth excited state in rigid box of length 0.1 nm.

SPPU : Dec.-16, Marks 3

Sol. : Given data :

$$h = 6.63\times10^{-34}\ J\ s$$

$$m = 9.1\times10^{-31}\ kg$$

$$L = 0.1\ nm = 0.1\times10^{-9}\ m$$

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

For ground state, $$E_1 = \frac{h^2}{8mL^2}$$

For fourth excited state,

$$E_5 = \frac{5^2h^2}{8mL^2} = \frac{25h^2}{8mL^2}$$

Energy required to excite the electron is

$$E_5 - E_1 = \frac{25h^2}{8mL^2} - \frac{h^2}{8mL^2} = \frac{3h^2}{8mL^2}$$

$$E_5 - E_1 = \frac{3\times(6.63\times10^{-34})^2}{8\times9.1\times10^{-31}\times(0.1\times10^{-9})^2}$$

$$= 1.81 \times 10^{-17} \text{ J}$$

$$= \frac{1.81 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV}$$

$$\therefore \quad \boxed{E_5 - E_1 = 113.125 \text{ eV}}$$

Ex. 6.12.10 : ***A neutron is trapped in an infinite potential well of width 1 A. Calculate the values of energy and momentum in its ground state.*** **SPPU : May-17, Marks 3**

Sol. : Given data :

$$h = 6.63 \times 10^{-34} \text{ Js}, \quad m = 1.675 \times 10^{-27} \text{ kg}$$

$$L = 1 \text{ Å} = 1 \times 10^{-10} \text{ m}$$

Formula :

$$E = \frac{h^2}{8mL^2}, \; p = \sqrt{2mE}$$

$$E = \frac{(6.63 \times 10^{-34})^2}{8 \times 1.675 \times 10^{-27} \times (1 \times 10^{-10})^2}$$

$$\therefore \quad \boxed{E = 3.28 \times 10^{-21} \text{ J}}$$

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

$$= \sqrt{2 \times 1.675 \times 10^{-27} \times 3.28 \times 10^{-21}}$$

$$\therefore \quad \boxed{p = 3.315 \times 10^{-24} \text{ kg-m/s}}$$

Review Questions

1. *Derive an expression for energy of a particle trapped in an infinite potential well.* **SPPU : Dec.-16, Marks 6**
2. *Derive equation of energy when a particle is confined to an infinite potential well. Draw first three energy levels for an electron confined in it.* **SPPU : May-18, Marks 6**
3. *Derive expression for the energy and wave function of a particle enclosed in an infinite potential well (rigid box).* **SPPU : Dec.-18, Marks 6**

13 : Particle in a Non-Rigid Box (Finite Potential Well)

- Consider another one dimensional problem of a particle of mass 'm' confined to a non-rigid box of length 'L'.
- As the walls are not rigid, which is the case in a real world, the potential energy of the particle would be finite, say V_0 outside the box.
- Inside the box, the potential energy is constant, taken to be zero for convenience.
- The potential energy distribution is shown in Fig. 6.13.1.

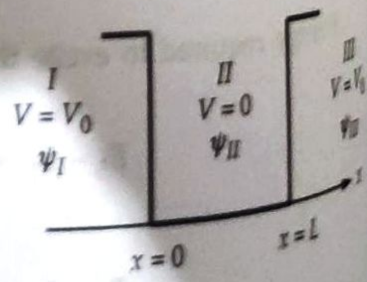

Fig. 6.13.1

- We consider a particular case of interest where $E < V_0$, i.e. the particle energy is less than the energy required to overcome the barrier represented by the walls.
- According to classical mechanics, in such a case, the particle will never be able to come out of the box.
- Schrödinger's time independent wave equation in one dimension is

$$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \qquad \text{... (6.13.1)}$$

- In region I, $V = V_0$ and $\psi = \psi_I$

$$\therefore \quad \frac{d^2\psi_I}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V_0)\psi_I = 0$$

- As $E < V_0$, $E-V_0 < 0$

$$\therefore \text{ Let } \quad \frac{8\pi^2 m}{h^2}(E-V_0) = -K'^2$$

$$\therefore \quad \frac{d^2\psi_I}{dx^2}-K'^2\psi_I = 0$$

- The general solution of this equation is,

$$\psi_I = Ae^{K'x}+Be^{-K'x} \qquad \text{... (6.13.2)}$$

- In region II, $V = 0$ and $\psi = \psi_{II}$

$$\therefore \quad \frac{d^2\psi_{II}}{dx^2}+\frac{8\pi^2 m}{h^2}E\psi_{II} = 0$$

- Let $\quad K^2 = \dfrac{8\pi^2 mE}{h^2}$

$$\therefore \quad \frac{d^2\psi_{II}}{dx^2}+K^2\psi_{II} = 0$$

- The general solution of this equation is,

$$\psi_{II} = Ce^{iKx}+De^{-iKx} \qquad \text{... (6.13.3)}$$

- In region III, $V = V_0$, $\psi = \psi_{III}$

$$\therefore \quad \frac{d^2\psi_{III}}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V_0)\psi_{III} = 0$$

$$\therefore \quad \frac{d^2\psi_{III}}{dx^2}-K'^2\psi_{III} = 0$$

- The general solution of this equation is

$$\psi_{III} = Fe^{K'x}+Ge^{-K'x} \qquad \text{... (6.13.4)}$$

- The condition in region I is

$$\psi_I \to 0 \text{ as } x \to -\infty$$

∴ From equation (6.13.2),

$$B = 0 \qquad \cdots (6.13.5)$$

∴ $$\psi_I = Ae^{K'x}$$

- Similarly in region III,

$\psi_{III} \to 0$ as $x \to \infty$

∴ $$F = 0 \qquad \cdots (6.13.6)$$

∴ $$\psi_{III} = Ge^{-K'x}$$

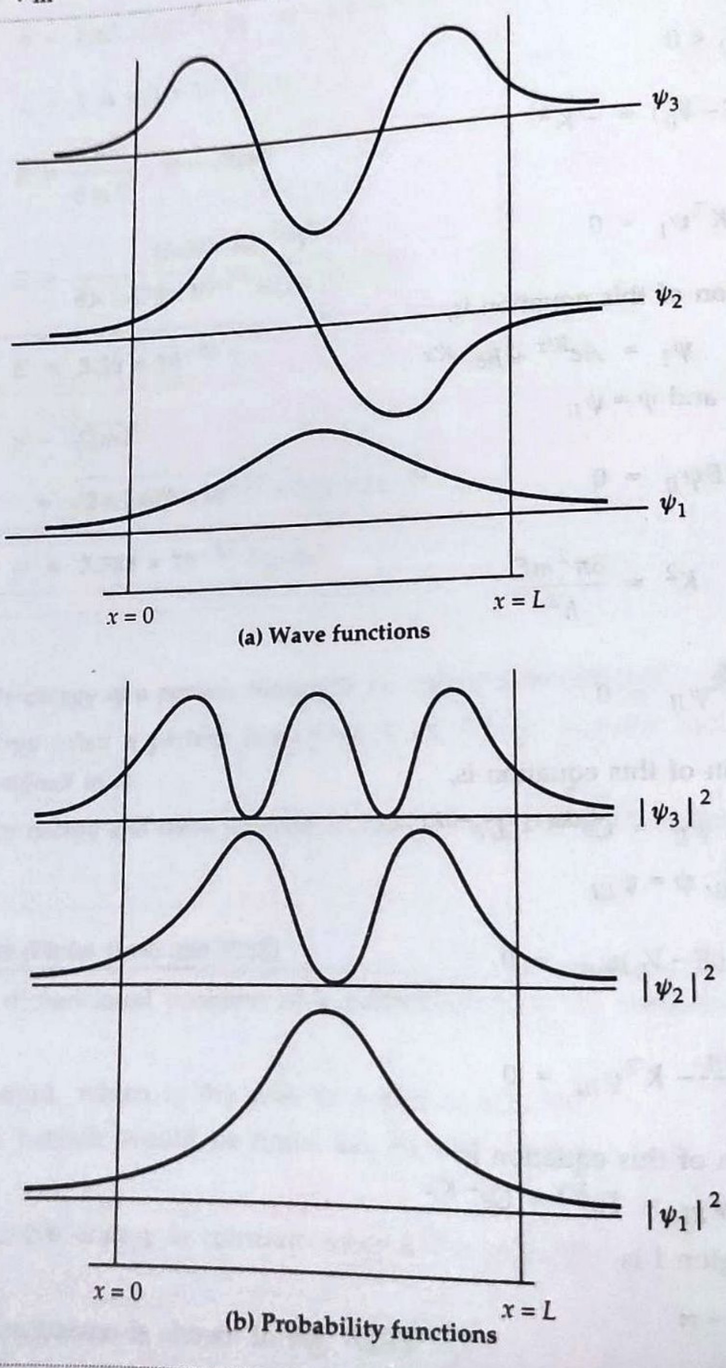

Fig. 6.13.2

- The boundary conditions to be imposed on the wave function are :

i) Continuity of wave function at $x = 0$:

$$[\psi_I]_{x=0} = [\psi_{II}]_{x=0}$$

ii) Continuity of wave function at $x = L$:

$$[\psi_{II}]_{x=L} = [\psi_{III}]_{x=L}$$

iii) Continuity of first order derivative of wave function at $x = 0$:

$$\left[\frac{d\psi_I}{dx}\right]_{x=0} = \left[\frac{d\psi_{II}}{dx}\right]_{x=0}$$

iv) Continuity of first order derivative of wave function at $x = L$

$$\left[\frac{d\psi_{II}}{dx}\right]_{x=L} = \left[\frac{d\psi_{III}}{dx}\right]_{x=L}$$

- Using these four boundary conditions, the four arbitrary constants A, C, D and G in equations (6.13.3), (6.13.5) and (6.13.6) can be evaluated to obtain solution for ψ_I, ψ_{II} and ψ_{III}.
- The nature of ψ_{II} is similar to the wave function in a rigid box, except that the values at $x = 0$ and $x = L$ are not zero. ψ_I has a non-zero value at $x = 0$ and decreases exponentially to zero as $x \rightarrow -\infty$. ψ_{III} has a non-zero value at $x = L$ and decreases exponentially to zero as $x \rightarrow +\infty$.
- The energy eigen values are discrete.
- The eigen functions and the corresponding probability functions are shown in Fig. 6.13.2.
- In addition to the discrete energy values and prediction of certain forbidden regions, like in the case of a rigid box, another significant result is the finite probability of finding the particle outside the box (as shown in Fig. 6.13.2 (b)).
- Even though the particle does not have sufficient energy to overcome the barrier, still there is some finite probability of the particle escaping from the box.
- This explains the phenomenon of α- decay where α-particles do not have sufficient energy to come out of the nucleus but still do escape from the nucleus.
- The tunnel diode and scanneling tunneling microscope work on the same principle of particles being able to 'tunnel' through a barrier even though they do not have sufficient energy.

Review Question

1. *Explain the results obtained from quantum mechanics for particle in a non-rigid box and state their significance.*

6.14 : Tunnel Diodes

SPPU : Dec.-17

- When impurity concentration in an n-type semiconductor is small. The donor levels are discrete as there is negligible interaction amongst the donor atoms.
- As the donor impurity concentration is increased the interaction amongst donor atoms increases.
- Due to this the donor levels which are just below the conduction band spread to form an energy band and overlap with the bottom of the conduction band.
- As a result the fermilevel for n-type semiconductors with high doping concentration lies in the conduction band.

- Similarly, the fermi level in a heavily doped p-type semiconductor lies in the valence band.
- The tunnel diode is formed by heavily doped p and n-type semiconductors.
- The depletion region in these diodes is very thin.
- The conduction band of n-type overlaps with the valence band of p-type so as to equalize the fermi levels as shown in Fig. 6.14.1 (a).
- Under equilibrium conditions when no voltage is applied across the diode, the electrons from conduction band of n-type tunnel across the potential barrier in the depletion layer into valence band of p-type and the electrons from valence band of p-type tunnel into conduction band of n-type in equal numbers. Hence there is no current through the diode.

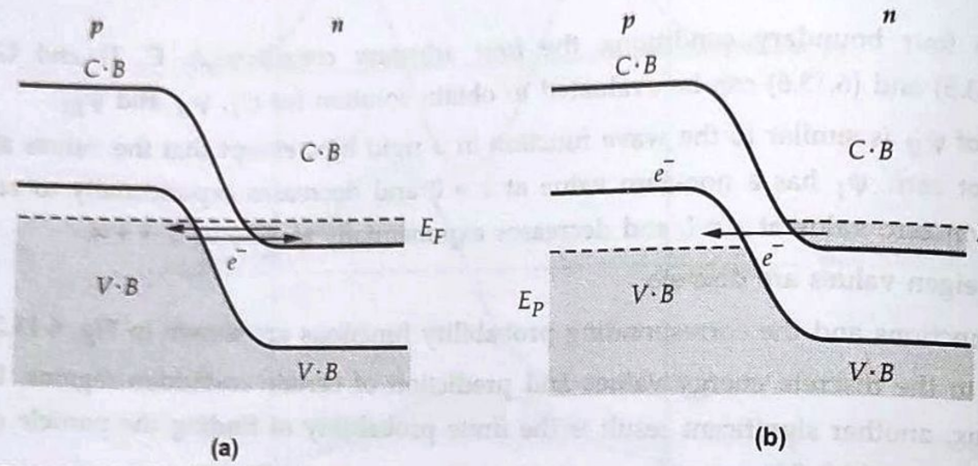

Fig. 6.14.1 (a)

- When a small forward biased voltage is applied to the diode, the conduction band and fermi level in n-type is slightly raised with respect to valence band in p-type as shown in Fig. 6.14.1 (b).
- The lower part of the n-type conduction band containing electrons is just next to the upper part of the valence band in p-type which is empty.
- As a result the electrons from the higher energy levels in conduction band of n-type tunnel into the lower energy levels in valence band of p-type.
- Tunnelling of electrons is not possible from p-type to n-type as the filled energy levels of p-type are at lower level compared to empty levels of n-type.
- As the electrons tunnel from n-type to p-type, it constitutes a current from p-type to n-type.
- If the forward baised voltage is increased the conduction band of n-type is raised further with respect to valence band and the two bands no longer overlap as shown in Fig. 6.14.1 (c) as a result the tunnelling current decreases. (See Fig. 6.14.1 (c) on next page)
- For further increase in voltage, the diffussion current starts due to injected charge carriers and the current increases exponentially as in any other p-n junction diode.
- The tunnel diode voltage-current characteristics are as shown in Fig. 6.14.2.

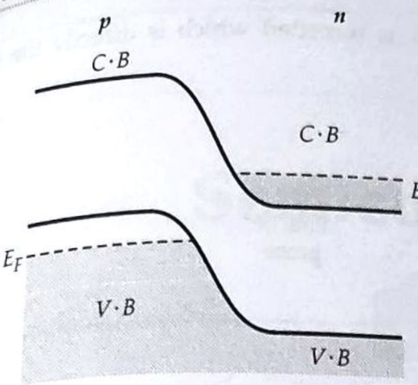

Fig. 6.14.1 (c)

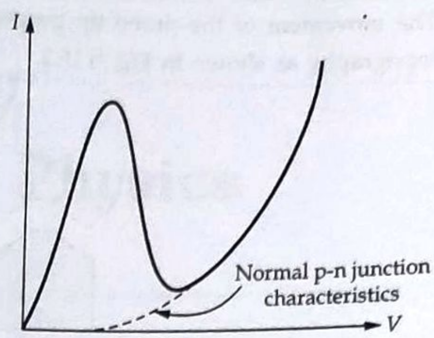

Fig. 6.14.2

- The response time of tunnel diodes to small changes in voltage is very small. Hence they are used in high frequency oscillators and fast switching circuits.

Review Question

1. *Explain tunneling effect. How is this principle used in a tunnel diode.* **SPPU : Dec.-17, Marks 4**

6.15 : Scanning Tunneling Microscope

- The scanning tunneling microscope consists of a probe with a fine tip that is made to move on a surface which is to be studied.
- The probe is kept at a positive potential with respect to that surface and kept at a distance of about 1 nm above the surface.
- The microscope can be used in either constant height mode or the constant current mode.

Constant height mode :

- In this mode, the probe is maintained at a constant height above the surface.
- Due to the positive potential of the probe tip, electrons on the surface tunnel through to the probe tip giving rise to a small current.
- As the tip moves on the surface at a constant height, the distance of the tip from the surface changes due to the irregularities on the surface.
- As a result, the probe current changes.
- It increases when the distance of the probe tip from the surface decreases.
- Thus the probe current gives an indication of the surface topography when the probe tip is scanned on the surface as shown in Fig. 6.15.1.

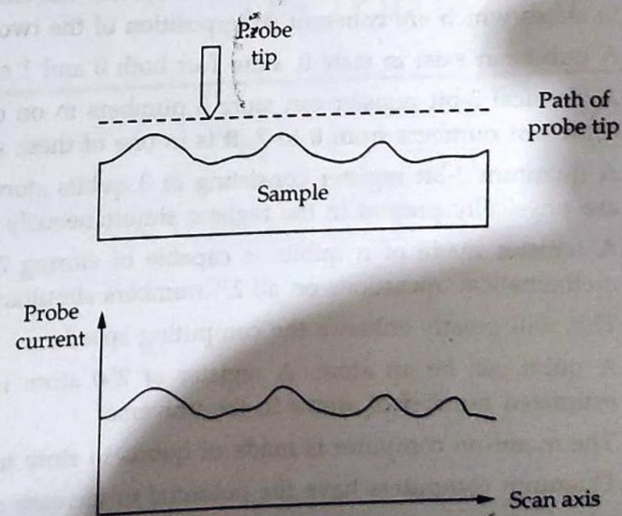

Fig. 6.15.1

Constant current mode :

- In this mode, the distance of the probe tip from the surface is varied so as to get a constant current.