QUANTUM MECHANICS

Q. What is de Broglie's hypothesis? Derive an expression for electron wave if it is moving under potential difference of V volt OR Discuss concept of matter wave and derive equation for wavelength of matter wave in terms of kinetic energy.

Ans. de Broglie's hypothesis :

According to de Broglie's hypothesis a particle of mass m moving with velocity v has a wave associated with it, known as matter wave or de Broglie wave or pilot wave. The wavelength of de Broglie wave is,

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

The following observations led him to put forward this theory.

- Nature manifests herself in the form of energy and matter. Nature loves symmetry. Since radiation has dual nature, by analogy matter must possess dual nature.
- Einstein's expression E = mc2 is followed both by energy and matter. If energy has dual nature, matter must have dual nature.
- The principle of least action in mechanics and the principle of least time in optics imply similar conditions. This close parallelism between mechanics and optics also indicates similarity between matter and radiation. i.e. if radiation has dual nature, matter must also have dual nature.

Thus there is wave associated with particle in motion.

Wavelength of matter wave:

Einstein's mass - energy relation

$$E = mc^2 \quad \text{................. (Eq. 1)}$$

Where m is mass and c is velocity of light.

According to Planck's quantum theory, $E = h\nu$ .... (Eq. 2)

Equating equations (1) and (2)

$$h\nu = mc^2$$

$$h\frac{c}{\lambda} = mc^2 \qquad (\because \text{Velocity} = \text{frequency} \times \text{wavelength})$$

$$\therefore \lambda = \frac{h}{mc} = \frac{h}{P}$$

Where P = mc is momentum of photon and λ is its wavelength. If it is applied to particle of mass m moving with velocity v,

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

Kinetic energy of particle,

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

$$\therefore P = \sqrt{2mE}$$

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

For electron,

$$E = \frac{1}{2}m_0 v^2 = eV \quad \text{where V is accelerating potential.}$$

$$\therefore \lambda_e = \frac{h}{\sqrt{2m_0 eV}}$$

$$\therefore \lambda = \frac{12.25}{\sqrt{V}} A^0$$

Q. Show that matter waves are faster than light

Ans.

Wave velocity is $u = \nu \lambda$

From Einstein – Planck equation,

$E = h\nu = mc^2$

$$\therefore \nu = \frac{mc^2}{h} \quad \text{and} \quad \lambda = \frac{h}{mv}$$

$$\therefore u = \frac{mc^2}{h} \cdot \frac{h}{mv}$$

$$\therefore u = \frac{c^2}{v}$$

As v < c; u > c hence, Matter waves are faster than light.

Q. State the properties of matter wave.

Ans.

Properties of matter wave :

1) Wavelength of matter wave is $\lambda = h/mv$. Thus lighter the particle, greater is its de Broglie wavelength. Faster the particle, smaller is the wavelength.

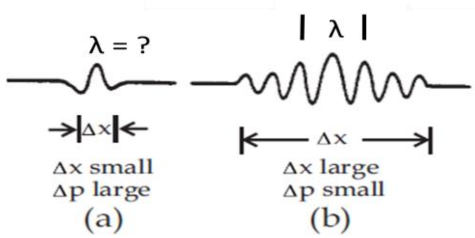
2) If particle is at rest, $\lambda = \infty$ i.e wavelength becomes indeterminate. That means matter waves are produced by motion of particle.

3) The de Broglie wavelength is independent of charge and nature of the particle. Therefore they are neither electromagnetic nor acoustic waves.

4) The velocity of matter wave depends on the velocity of particle and is not constant.
5) Matter wave travels faster than light ($u = c^2/v$)
6) A wave can not be localized at any point and it introduces certain uncertainty in the position of the particle.
7) It is the wave of probability. It is symbolic representation of particle.

Q. State and explain Heisenberg's uncertainty principle OR show that position and momentum of particle can not be determined simultaneously and accurately.

Ans. 1) According classical mechanics position and momentum of particle can be determined simultaneously and accurately.
2) According to wave mechanics a moving particle has a wave packet associated with it and particle may be positioned anywhere within the wave packet. It puts limit on accuracy of measurement of position and momentum of particle.
3) If the wave group is narrow (fig. a) the position of the particle is precisely found, but its wavelength and hence momentum ($\lambda=h/p$) is difficult to measure. On the contrary, if a wave group is wide (fig. b) the wavelength and hence momentum can be measured accurately, but location of the particle can not be found. Thus the certainty in position involves uncertainty in momentum and vice versa. Thus it is impossible to simultaneously measure the position and momentum of a particle.



"The product of uncertainty in the measurement of position (ΔX) and uncertainty in the measurement of momentum (ΔP) would always be of the order of Planck's constant."

$\Delta X \cdot \Delta P \geq h/2\pi$

Similarly, $\Delta E \cdot \Delta t \geq h/2\pi$; E is the Energy and t is time.

Q. Electron can not be present in the nucleus, justify the statement.

Ans. The radius of nucleus is of the order of 10^{-14} m. If electron is to be present in the nucleus, uncertainty in its position $\Delta x = 2 \times 10^{-14}$ m

Applying uncertainty principle, $\Delta p = \dfrac{\hbar}{\Delta x} = 5.2\times10^{-21}\ kgm/s$

It implies, the minimum required energy of the electron is about 96 MeV.
But, experimental result shows that, maximum K.E. of β particle (electron) is about 4 MeV.
Hence, electrons are not present in the nucleus.

Radius of Bohr's first orbit:

Using Heisenberg's uncertainty principle, equation for Bohr's first orbit can be obtained as,

$$r = \frac{\varepsilon_0 h^2}{\pi m z e^2}$$

Ground state energy of linear harmonic oscillator:

$$E_{\min} = \frac{1}{2}\hbar\omega$$

Q. Explain the concept of wave function and its probability interpretation.

Ans. Wave represents the propagation of disturbance through medium. In sound waves the quantity that varies periodically is pressure and in light waves it is electromagnetic field. In matter waves associated with moving particle, the quantity that varies periodically is wave function (ψ).

The wave function ψ itself has no physical significance as it is not observable quantity. But square of its absolute magnitude $|\psi|^2$ over a particular region of space at particular time is proportional to probability of finding the particle in that region at that time. Since ψ is complex,

$|\psi|^2 = \psi^*\psi$ where ψ^* is complex conjugate of ψ.

$|\psi|^2$ must be finite and real.

(e.g if $\psi = x + iy$, $\psi^* = x - iy$

$\therefore$ $|\psi|^2 = \psi^*\psi = x^2+y^2$ ----- a real quantity.)

Since particle must exist somewhere in space,

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 1$$

If $\int_{-\infty}^{\infty} |\psi|^2 dv = 0$ particle does not exist at all

And $\int_{-\infty}^{\infty} |\psi|^2 dv = \infty$ particle is present everywhere simultaneously.

Both these conditions are meaningless. Hence $|\psi|^2$ must be finite, single valued and real.

The wave describing a particle of momentum p and energy E has wavelength $\lambda = h/p$ and frequency $\nu = E/h$.

Let's define wave propagation number $k = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$ and the angular frequency, $\omega = \frac{E}{\hbar}$

Q. Derive Schrodinger time dependent wave equation for matter wave.

Ans.

The wave function for a moving particle in positive X – direction is given by,

$\Psi(x,t) = A \exp[- i(\omega t - kx)]$ where $\omega = \frac{E}{\hbar}$ and $k = \frac{p}{\hbar}$

$\therefore \Psi(x,t) = A \exp[- \frac{i}{\hbar} (Et - px)]$ ----------------(1)

Differentiating w.r.t. x twice,

$$\frac{\partial\psi}{\partial x} = \frac{i}{\hbar} p\psi$$

And $\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi$ ----------------(2)

Differentiating equation (1) w.r.t. time,

$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi$ ----------------(3)

From equations (2) and (3),

$E \to i\hbar\frac{\partial}{\partial t}$ and $p^2 \to -\hbar^2 \frac{\partial^2}{\partial x^2}$ ----------------(4)

E and p are termed as energy and momentum operators respectively.

$\therefore E\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$ ----------------(5)

And $p^2\psi(x,t) = -\hbar^2 \frac{\partial^2\psi(x,t)}{\partial x^2}$ ----------------(6)

We know that, If V is potential energy, total energy is,

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

Above equation becomes,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t)$$

$\therefore \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi = i\hbar\frac{\partial\psi(x,t)}{\partial t}$ ----------------(7)

This is Schrodinger time dependent wave equation in one dimension. In three dimensions,

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$\therefore H\psi = E\psi$$

$H = \frac{-\hbar^2}{2m}\nabla^2 + V$ - Hamiltonian operator.

Q. Derive Schrödinger Time independent wave equation.

Ans. If potential energy V is time independent and varies only with position, the field is said to be stationary. Wavefunction ψ is

$$\psi(x,t) = A\exp\left[-\frac{i}{\hbar}(Et - px)\right]$$

$$= A\exp\left(\frac{-iE}{\hbar}\right)t\exp\left(\frac{ip}{\hbar}\right)x$$

$$\therefore \psi(x,t) = \left[A \exp\left(\frac{ip}{\hbar}\right) x \right] \exp\left(\frac{-iE}{\hbar}\right) t$$

$$= \psi(x) \exp\left(\frac{-iE}{\hbar}\right) t \qquad \text{-------------------------------------(1)}$$

We know that, total energy $E = \frac{p^2}{2m} + V$

$$\therefore E\psi(x,t) = \frac{p^2}{2m}\psi(x,t) + V(x)\psi(x,t)$$

From eq. (1),

$$\therefore E\psi(x,t)\exp\left(\frac{-iE}{\hbar}\right)t = \frac{p^2}{2m}\psi(x,t)\exp\left(\frac{-iE}{\hbar}\right)t + V(x)\psi(x,t)\exp\left(\frac{-iE}{\hbar}\right)t$$

We know that, $p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$

$$\therefore E\psi(x)\exp\left(\frac{-iE}{\hbar}\right)t = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\exp\left(\frac{-iE}{\hbar}\right)t + V(x)\psi(x)\exp\left(\frac{-iE}{\hbar}\right)t$$

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

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

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

This is steady state or time independent equation.

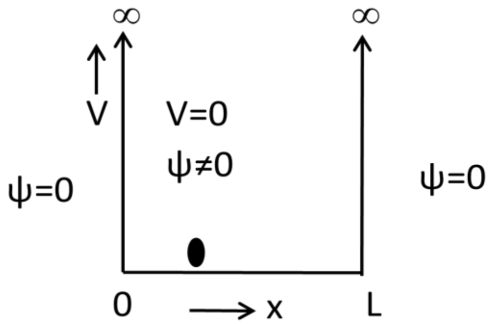
In three dimensions,

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

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

Q. Obtain Energy levels of a particle in infinite square well potential (particle in a box).

Ans. A potential well is a potential energy function V(x) that has minimum value (say zero) and no maximum limit. If the particle is left in the well, it can vibrate back and forth with periodic motion but cannot leave the well. Thus the particle is trapped in the well and it is called bound state.



Consider a potential well as shown in figure. The particle is trapped in the region 0<x<L.

V=0 for 0<x<L and V=∞ at x=0 and x=L; the situation is called as one-dimensional potential box.

Then the Schrodinger time independent equation for particle becomes,

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}E\psi(x)=0 \qquad\qquad 0 < x < L$$

Substituting $\frac{2mE}{\hbar^2} = k^2$

$$\frac{\partial^2\psi}{\partial x^2}+k^2\psi(x)=0 \qquad \text{------------------------------(1)}$$

As the particle can move back and forth freely between x=0 and x= L, the solution of equation (1) is,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{------------------------------(2)}$$

(+X and -X direction)

Applying boundary condition,

At x= 0, ψ (x)= A+B = 0

$\therefore A = -B$

$\therefore \psi(x) = A\left(e^{ikx} - e^{-ikx}\right) = 2iA\sin kx$

& At x=L, ψ(x)=0

$\therefore \psi(L) = 2iA\sin kL$

But 2iA $\neq$ 0, $\therefore$ sin kL=0

$\therefore$ kL = nπ ------------------------------(3)

As $k = \frac{2\pi}{\lambda}$; $\frac{2\pi L}{\lambda} = n\pi$

$$\therefore \lambda = \frac{2L}{n} \qquad \text{------------------------------(4)}$$

Where, n =1,2,3,…..

Thus the particle waves form standing wave pattern within potential box.

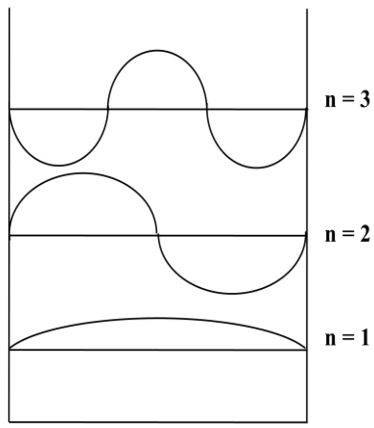
(i) Possible values of momentum

p=ħk

$$\therefore\ p = \hbar\frac{n\pi}{L} = \frac{h}{2\pi}\frac{n\pi}{L} = \frac{nh}{2L} \qquad \text{------------------------------(5)}$$

(ii) Possible values of energy

$$E = \frac{p^2}{2m} = \frac{n^2h^2}{4L^2.2m} = \frac{n^2h^2}{8mL^2} \qquad \text{-----------------------------(6)}$$



Thus the particle has certain allowed values for energy. Zero energy is not allowed. The lowest energy that the particle can have in 1-D potential box is,

$E_1 = \frac{h^2}{8mL^2}$ ------- Zero point energy level and it is first energy level

$E_2 = \frac{h^2}{2mL^2}$ ------- Second energy level

$E_3 = \frac{9h^2}{8mL^2}$ ------- Third energy level and so on….

5.16 Applications of quantum mechanics:

5.16.1 Quantum tunneling:

Quantum tunneling is the phenomenon where a wave function can propagate through a potential barrier. For example, consider a potential barrier of height V_0 and width L as shown in fig. 5.9. The region around the barrier is divided into three regions.

Region I – $x < 0$ and $V = 0$

Region II – $0 < x < L$ and $V = V_0$

Region III – $x > L$ and $V = 0$

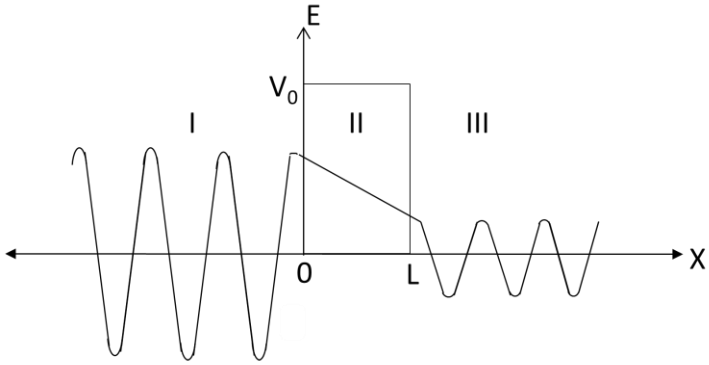


Fig. 5.9

In region I and III, the total energy of particle is only kinetic energy while in region II, it is kinetic and potential energy. Let a particle of energy E is incident from region I on potential barrier. If E < V_0, it can not cross the barrier and enter region III. However, according quantum mechanics, there is finite probability for the electron to penetrate the barrier and enter region III as shown in figure. This phenomenon is called tunneling. Tunneling occurs with barriers of thickness around 1–3 nm and smaller. It has applications in the tunnel diode, quantum computing and scanning tunneling microscope.

5.16.2 Quantum computation:

Quantum computing is a type of computation that utilizes collective properties of quantum states viz, superposition, entanglements to perform calculations. The devices that perform quantum computation are called quantum computers. Quantum computer works differently from the traditional computers. The traditional computers based on classical mechanics can work on and compute only one transaction at a time while the quantum computers can perform multiple transactions at the same time which increase their speed. Quantum computers have applications in cryptography and security computers. The best feature of quantum computers is their security. Theoretically it is not possible to hack the quantum computer system. Quantum computers use observer effect. If anyone tries to measure one parameter of a micro-particle, it will alter another parameter. This phenomenon, should resolve the main issue of classical communications. Thus an attempt to spy on a communication will modify the transmitted message. There are three main reasons which make the Quantum cryptography much more secure than the classical computation. Due to quantum entanglement, the unknown quantum state cannot be copied. Any attempt to calculate and measure the quantum state will disturb the system and alter the message. The altered message is of no use.

The fundamental building block of a quantum computer is Qubit as shown in the fig. 5.10. An ordinary bit can compute or store 0 or 1 but a Qubit can work and operate in between the values of 0 and 1. Qubits can take many forms, like atoms, ions, photons, and individual electrons. They are measured using binary system 1s and 0s. But qubits can be both 1 and 0 at the same time. This is possible due to superposition and entanglement of quantum states. In superposition, a qubit can be in multiple states at the same time, with value 0, 1, both and any numbers in between 0 and 1

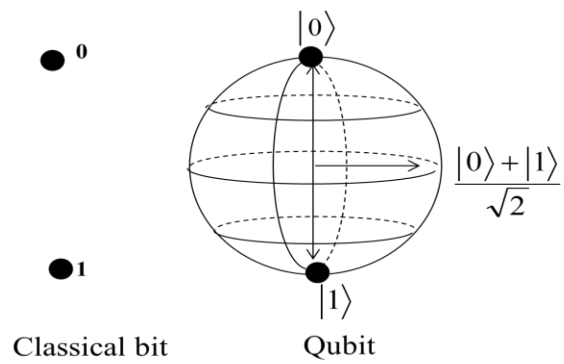


Fig.

Qubit contains large amount of information that can be extracted by measurement. Though qubit can be in multiple states between 0 and 1, the result of measurement is a ordinary bit 0 or 1 and probability of each outcome depends on latitude. Qubits can be entangled that enables more parallel computations.

EXERCISE

Q.1 State the de Broglie's hypothesis of matter wave. Derive an expression for wavelength of matter wave in terms of kinetic energy of particle.

Q.2 Give different properties of matter wave.

Q.3 State and explain Heisenberg's uncertainty principle.

Q.4 Illustrate Heisenberg’s uncertainty principle using electron diffraction.

Q.5 ‘If an electron is localized in space, its momentum becomes uncertain.’ Explain this statement.

Q.6 Define a wave function. Show that it represents probability density of finding the particle at a given position and given time.

Q.7 Explain the concept of wave function and give its physical significance.

Q.8 Derive Schrodinger’s time dependent wave equation.

Q.9 Derive Schrodinger’s time independent wave equation.

Q.10 Apply the Schrodinger’s time independent equation for a particle confined to a rigid box and find its energy levels..

Q.11 Show that the energy of electron confined in one dimensional potential well of length L and infinite depth is quantized. Is the electron trapped in infinite potential well allowed to take zero value? Elaborate the answer.

Q.12 Show that the energy of particle confined in one dimensional potential well of length L is given by

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

Q.13. Explain applications of quantum mechanics.

PROBLEMS FOR PRACTICE

1) What is de Broglie wavelength of an electron travelling at a speed of 10^7m/s?

(0.727 A^0)

2) Calculate the ratio of de Broglie wave associated with a proton and an electron each having the kinetic energy 20 MeV. [mp=1.67×10^{-27} kg and me = 9.1×10^{-31} kg]

($\lambda p : \lambda e$ = 1: 43)

3) A proton and a deuteron have the same kinetic energy. Which particle has longer wavelength? Justify your answer.

4) Uncertainty in measurement of position of particle is 0.1μm and mass is of 1.6×10^{-27} kg, calculate uncertainty in velocity of particle. (0.659 m/s)

5) An electron and a 150 gm baseball are traveling at a speed of 220 m/s, measured to an accuracy of 0.065%. Calculate uncertainty in position of each.

(ΔXe = 0.81mm, $\Delta Xb = 4.92 \times 10^{-33}$m)

6) An electron is confined to move between two rigid walls separated by distance 1 nm. Find de Broglie wavelength representing first allowed state and corresponding energy. (λ = 2 nm, E = 6.038×10^{-20} J)

7) Calculate energy required to excite an electron from ground state to second excited state in one dimensional potential box of length 2 A^0. (75.2 eV)