

UNIT-I: Quantum Mechanics

Introduction:

The nineteenth century was a very eventful period, particularly in the realm of physics. The pioneering work on dynamics by Newton, on electromagnetic theory by Maxwell, the laws of thermodynamics, and kinetic theory were successful in explaining a wide variety of phenomena. Inability of the classical concepts to explain certain experimental observations, especially those involving subatomic particles, led to the formulation and development of modern physics in the early twentieth century. Quantum theory and the theory of relativity are the two important concepts that led to the development of modern physics. The quantum theory was first proposed by Max Planck to explain and overcome the inadequacies of classical theories of black body radiation. The pioneering work of Einstein, Planck, Compton, Roentgen, Born, and others formed the basis of modern physics. The dual nature of matter proposed by de Broglie was confirmed by experiments.

Matter waves and de Broglie's hypothesis:

The phenomena such as interference, diffraction, and polarization show the wave nature of light. The phenomena such as the photoelectric effect and the Compton effect show the particle nature of light. This property of light to exhibit both wave and particle nature is known as the **dual nature of light**.

Louis de Broglie (in 1924) suggested that, if radiation can behave as a particle under certain circumstances, then one can even expect that entities which ordinarily behave as particles to exhibit wave properties under appropriate circumstances and hence exhibit a dual nature. **The waves associated with the moving particles are called matter waves or de Broglie waves. And the wavelength of these matter waves is called the de Broglie wavelength.** This hypothesis is called the de-Broglie hypothesis. The de-Broglie hypothesis opened up new thinking in almost all fields of Physics. In fact, it can be treated as the new beginning of Modern Physics.

The light, believed to be a wave, exhibited particle properties and electrons, believed to be particles, exhibited wave properties. The particle nature of waves and wave nature of particles is known as **wave-particle dualism**.

De Broglie's hypothesis was based on the following arguments:

Light behaves as a particle, and this has been evident from Einstein's explanation of the photoelectric effect in 1905. Now, "converse also holds true?" In 1923, de Broglie postulated that if waves can behave like particles, then particles should be able to behave like waves. According to de Broglie, a moving particle can be associated with a wave, or in other words, a wave can guide the motion of the particle. Such waves associated with the moving particles are known as de Broglie waves or matter waves.

Suppose a particle of mass m is moving with the velocity v , the de Broglie wavelength associated with the particle is given by

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

where $h = 6.62 \times 10^{-34} \text{ Js}$ is Planck's constant.

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Proof: According to Planck's hypothesis, the energy associated with a photon of frequency ν is $E = h\nu$. Further relativistic mass-energy relation given by Einstein, for the particle of rest mass m_0 and momentum p is $E = \sqrt{p^2 c^2 + m_0^2 c^4}$, where c is the speed of light. Since the rest mass m_0 of the photon is zero, the energy of the photon is $E = pc$. Therefore, we can write

$$\nu = p c \text{ OR } p = \frac{h\nu}{c} = \frac{h}{\lambda} \quad \text{OR} \quad \lambda = \frac{h}{p}$$

As de Broglie has stated that matter particle behaves as photons, so the same expression can be used for the matter particles moving with velocity v and momentum $p = mv$ as

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

The above relation is known as the de Broglie relation, which connects the momentum/velocity of the particle to the wavelength of a wave associated with the particle.

Important points:

- i. In everyday life, the de Broglie wavelength comes out to be very small for massive particles.
- ii. de Broglie wavelength is charge independent.
- iii. It was found that the velocity of de Broglie waves is always greater than the velocity with which the particle travels.

De-Broglie wavelength of an accelerated electron:

The de Broglie wavelength can be calculated for any particle using the above relation. In case of charged particles like electrons, a beam of high-energy particles can be obtained by accelerating them in an electric field. For example, an electron with charge e starting from rest when accelerated with a potential difference V , the kinetic energy acquired by the electron is given by

$$E = \frac{1}{2}mv^2 = eV, \text{ where } m \text{ is mass and } v \text{ is the velocity of the electron.}$$

The momentum may be calculated as

$$p = mv = (2meV)^{1/2} = \sqrt{2meV}$$

Using the de Broglie equation, the wavelength associated with the accelerated electron can be calculated as

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2meV}}$$

This equation suggests that, at a given speed, the de Broglie wavelength associated with the particle varies inversely as the mass of the particle.

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Characteristics of matter waves:

1. Matter waves are associated with a moving body. All particles having mass m and moving with a velocity \mathbf{v} will be associated with a wave of wavelength λ given by, $\lambda = h/mv$, where h is the Planck's constant.
2. The wavelength ($\lambda = h/mv$) of different matter waves may differ depending on the mass and velocity of the particle. The wavelength of matter waves is inversely proportional to the velocity with which the body is moving. Hence, a body at rest has an infinite wavelength and the one travelling with a high velocity has a lower wavelength.
3. Wavelength of matter waves also depends on the mass of the body and decreases with increase in mass. Due to this reason, the wavelike behavior of heavier bodies is not very evident whereas wave nature of subatomic bodies could be observed experimentally.
4. A wave is normally associated with some quantity that varies periodically with the frequency of the wave. For example, in a water wave, it is the height of the water surface; in a sound wave it is the pressure and in an electromagnetic wave, it is the electric and magnetic fields that vary periodically. But in matter waves, there is no physical quantity that varies periodically. We use a wave function to define matter waves and this wave function is related to the probability of finding the particle at any place at any instant.
5. Matter waves are represented by a wave packet made up of a group of waves of slightly differing wavelengths. Hence, we talk of group velocity of matter waves rather than the phase velocity. The group velocity can be shown to be equal to the particle velocity.
6. Matter waves show properties similar to other waves. For example, a beam of accelerated electrons produces interference and diffraction effects similar to an electromagnetic wave of same wavelength.

Phase velocity and Group velocity:

Phase velocity:

A wave is represented by $y = A \cos (\omega t - kx)$

where y is the displacement at any instant t , A is the amplitude of vibration, ω is the angular frequency equal to $2\pi\nu$ and k is the propagation constant or wave number, equal to $(2\pi/\lambda)$.

The phase velocity of such a wave is the velocity with which a particular phase (or phase point) of the wave travels.

This corresponds to the phase being constant.

i.e., $(\omega t - kx) = \text{constant}$

or, $x = \text{constant} + \omega t/k$

Phase velocity $v_p = dx/dt = \omega/k$

Thus, the phase velocity is the velocity with which a non-localised wave travels and is velocity with which a particular phase point moves.

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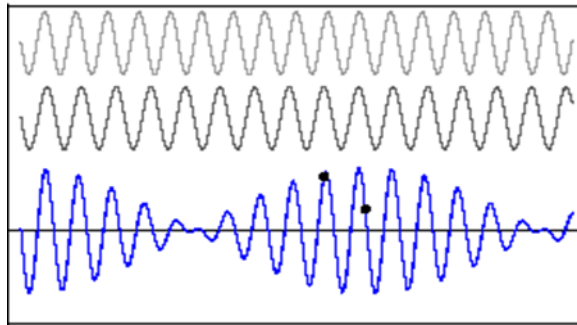
Group velocity:

The de Broglie waves are represented by a wave packet and hence we have **group velocity** associated with them. **Group velocity is the velocity with which the wave packet** (or group of waves) **travels**.

In order to understand the concept of group velocity, consider the combination of two waves represented by the formula

$$y_1 = A \cos (\omega t - kx) \text{----- (1)}$$

$$y_2 = A \cos \{(\omega + \Delta\omega)t - (k + \Delta k)x\} \text{----- (2)}$$



The resultant displacement is given by

$$\begin{aligned} y &= y_1 + y_2 = A \cos (\omega t - kx) + A \cos \{(\omega + \Delta\omega)t - (k + \Delta k)x\} \\ &= 2A \cos \{[(\omega + \omega + \Delta\omega)t - (k + k + \Delta k)x]/2\} \cos [(\Delta\omega t - \Delta kx)/2] \\ &\approx 2A \cos(\omega t - kx) \cos(\Delta\omega t/2 - \Delta kx/2) \\ y &= 2A \cos(\Delta\omega t/2 - \Delta kx/2) \cos(\omega t - kx) \text{----- (3)} \end{aligned}$$

Comparing equations (1) and (3), the coefficient of $\cos(\omega t - kx)$ in both equations is the amplitude. The velocity of the resultant wave is given by the velocity with which a reference point, say the maximum amplitude point, moves.

Taking the amplitude of the resultant wave as constant, we have

$$2A \cos(\Delta\omega t/2 - \Delta kx/2) = \text{constant}$$

$$\text{or} \quad (\Delta\omega t/2 - \Delta kx/2) = \text{constant}$$

$$\text{or} \quad x = \text{constant} + (\Delta\omega/\Delta k)t$$

$$\text{Group velocity } v_g = dx/dt = (\Delta\omega/\Delta k)$$

Instead of two discrete values for ω and k , if the group of waves has a continuous spread from ω to $(\omega + \Delta\omega)$ and k to $(k + \Delta k)$, then the **group velocity** is given by

$$v_g = d\omega/dk$$

Relation between group velocity and phase velocity:

We have the equation for group velocity and phase velocity are given by,

$$v_g = \frac{d\omega}{dk} \quad \text{and} \quad v_{ph} = \frac{\omega}{k}$$

where ω is angular frequency and k is wave vector

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

$$\therefore v_g = \frac{d\omega}{dk} = \frac{d}{dk} (k v_{ph})$$

$$v_g = v_{ph} + k \cdot \frac{dv_{ph}}{dk}$$

$$v_g = v_{ph} + \frac{2\pi}{\lambda} \cdot \frac{dv_{ph}}{d\lambda} \cdot \frac{d\lambda}{dk}$$

$$\text{Since } k = \frac{2\pi}{\lambda}, \quad \frac{dk}{d\lambda} = \frac{-2\pi}{\lambda^2}$$

$$v_g = v_{ph} + \frac{2\pi}{\lambda} \cdot \frac{dv_{ph}}{d\lambda} \left[\frac{-\lambda^2}{2\pi} \right]$$

$$v_g = v_{ph} - \lambda \left[\frac{dv_{ph}}{d\lambda} \right]$$

This is the relation between group velocity and phase velocity

Relation between group velocity (V_g) and particle velocity (V or $V_{particle}$):

Group velocity is given by,

$$v_g = \frac{d\omega}{dk} \quad \text{--- (1)}$$

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

$$d\omega = \frac{2\pi}{h} dE \quad \text{--- (2)}$$

Also, we have,

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

$$dk = \left(\frac{2\pi}{h}\right) dp \quad \text{--- (3)}$$

Divide (2) by (3),

$$\frac{d\omega}{dk} = \frac{dE}{dp} \quad \text{--- (4)}$$

But We Know that,

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

Where p is the momentum of the particle.

$$\frac{dE}{dp} = \frac{2p}{2m} = \frac{p}{m}$$

Using the above in equation (4), we have,

$$\frac{d\omega}{dk} = \frac{p}{m}$$

But, $p = mv_{\text{particle}}$ where 'v' is the velocity of the particle.

$$\frac{d\omega}{dk} = \frac{mv_p}{m} = v_{\text{particle}} \quad \text{--- (5)}$$

Therefore from (1) and (5)

$$\mathbf{v_{group} = v_{particle}}$$

The de Broglie wave group associated with a particle, travels with a velocity equal to the velocity of the particle itself.

Relation between velocity of light, group velocity and phase velocity:

We know, $v_{\text{ph}} = \frac{\omega}{k}$

By substituting for ω and k ,

$$v_{\text{ph}} = \frac{E}{p} = \frac{mc^2}{mv_{\text{particle}}} = \frac{c^2}{v_{\text{particle}}}$$

But $v_{\text{group}} = v_{\text{particle}}$

$$\mathbf{v_{ph} v_{group} = c^2}$$

Heisenberg's Uncertainty principle:

This principle was given by Heisenberg in 1927 and is the fundamental principle of Quantum Mechanics. In classical physics the position and momentum of an object can be measured to a high accuracy simultaneously. But in case of Quantum Mechanics, sub atomic (micro) particles like atoms, molecules, protons, electrons, neutrons, nuclei, group of atoms, group of molecules and nanoparticles etc., it is impossible to measure position and momentum of an object to a high accuracy simultaneously. Because the moving particle is treated as a de Broglie wave packet.

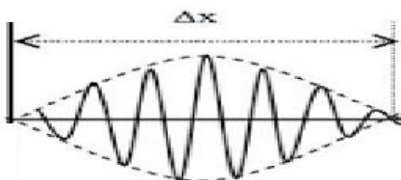
Statement: It is impossible to determine both the position (x) and momentum (p) of a particle precisely and simultaneously. The product of inherent uncertainties involved in the measurements of position and momentum simultaneously is greater than or equal to $h/4\pi$.

$$\text{i.e. } \Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

The Uncertainty principle can also be stated to another pair of conjugate variables such as energy and time as follows.

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

When we assign wave properties to particles there is a limitation to the accuracy with which we can measure the properties like position and momentum. Consider a wave packet as shown in figure. The particle associated with this wave packet can be found anywhere within the region Δx . This means that the accuracy of finding the exact position of the particle is limited. That is the probability of finding the particle is maximum at the middle of the wave packet and it falls to zero at its ends.



This means that there is always uncertainty inherently involved in the measurements of position and momentum of quantum particles. These uncertainties can be related by the principle known as Heisenberg's Uncertainty Principle.

Mathematically it can be expressed as $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$

The above uncertainties arise as a direct consequence of the wave nature of the associated particles and is not related to limitations of measuring techniques or instruments.

The principle can also be stated to another pair of conjugate variables such as energy and time as follows.

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

The Heisenberg uncertainty principle applies to electrons and states that we cannot determine the exact position of an electron. Instead, we could determine the probability of finding an electron at a particular position.

Wave packet:

A wave packet is a superposition of a large number of waves with different wavelengths such that the resultant amplitude of the wave packet is finite only in a narrow time interval or space and the amplitude is zero everywhere else. A wave packet is used to describe matter waves. The wavelengths of the different waves are slightly varying from each other and the average wavelength is equal to the de Broglie wavelength.

Application of Heisenberg's uncertainty principle:***Non-existence of electrons inside the atomic nucleus:***

Heisenberg's Uncertainty principle states that,

$$\Delta x \cdot \Delta p \geq h/4\pi$$

The typical size of the nucleus is approximately $5 \times 10^{-15} \text{m}$. If the electron exists inside the nucleus, then the uncertainty in its position Δx must not exceed the size of the nucleus i.e. $\Delta x \leq 10^{-15} \text{m}$.

Therefore, uncertainty in momentum is,

$$\Delta p \geq \frac{h}{4\pi \Delta x}$$

$$\Delta p \geq \frac{6.63 \times 10^{-34}}{4\pi \times 5 \times 10^{-15}}$$

$$\Delta p \geq 1.055 \times 10^{-20} \text{kg.m.s}^{-1}$$

which is the uncertainty in the momentum of the electron.

According to the theory of relativity, the energy E of a particle is:

$$E^2 \geq p^2 c^2 + m_0^2 c^4$$

An electron whose momentum is $1.055 \times 10^{-20} \text{kg.m.s}^{-1}$ has an energy many times greater than its rest mass energy $m_0 c^2$. That means $\text{K.E.} \gg m_0 c^2$. Neglecting the second term, as it is much smaller compared to the first term, we can use the relativistic formula as

$$E = pc$$

$$E = (1.055 \times 10^{-20})(3 \times 10^8)$$

$$= 3.2 \times 10^{-12} \text{ J}$$

$$= (3.2 \times 10^{-12} / 1.6 \times 10^{-19}) \text{ eV}$$

$$= 20 \text{ MeV}$$

This shows that if an electron exists inside the nucleus, the kinetic energy of the electron must be more than 20 MeV. But electrons of such large energy have never been found to be emitted during beta decay. The maximum energy of a beta particle emitted is only 2 to 3 MeV. Hence, we conclude that electrons cannot be present within the nucleus and the electrons observed in Beta-decay are created at the instant of decay.

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Wave Mechanics:

Quantum theory is based on the quantization of energies. It deals with the particle nature of radiation. It implies that addition or liberation of energy will be between discrete energy levels. It assigns particle status to a packet of energy by calling it 'quantum of energy' or 'photon' and treats the interaction of radiation with matter as a two-body problem. On the other hand, de Broglie's hypothesis and the concept of matter waves led to the development of a different formulation called 'Wave mechanics'. This deals with the wave properties of material particles. It was shown later that quantum mechanics and wave mechanics are mathematically identical and lead to the same conclusion.

Wave function and its physical significance:

The matter waves are represented by the wave function, denoted by the symbol Ψ . Wave function Ψ is itself a complex quantity and is denoted in complete form as

$\Psi = \psi(x, y, z) e^{-i\omega t}$, where $\psi(x, y, z)$ represents the space-dependent part and $e^{-i\omega t}$ represents the time-dependent part.

Even though the wave function Ψ itself has no physical interpretation, the square of its absolute magnitude i.e. $|\Psi|^2$ evaluated at a particular place at a particular time is proportional to the probability of finding the body there at that time.

The wave function carries information about the particle's wave-like behavior. It also provides information about the momentum and energy of the particle at any instant of time.

The physical significance of Ψ could be realized through its probabilistic nature.

Probability density (Born interpretation) :

A probability interpretation of the wave function was given by Max Born in 1926. He suggested that "*the square of the magnitude of the wave function $|\Psi|^2$ evaluated in a particular region represents the probability of finding the particle in that region*". The Probability density is the probability of finding the particle in a unit volume. The wave functions are usually complex with both real and imaginary parts. But the probability of occurrence of an event must be a positive real quantity. If Ψ is the wave function associated with a moving particle, then the probability in such a case is taken as $\Psi^* \Psi$, i.e. the product of the wave function with its complex conjugate.

i.e. **Probability density, $P = |\Psi|^2 = \Psi^* \Psi$**

Since the probability of finding the body somewhere is finite, we have the total probability over all space equal to certainty. Probability density can have values anywhere between 0 and 1.

For example: If $\Psi = A + iB$

Where, A & B are real.

Complex conjugate of Ψ is $\Psi^* = A - iB$

Therefore, $P = |\Psi|^2 = \Psi^* \Psi = A^2 - i^2 B^2 = A^2 + B^2$

Hence, $|\Psi|^2 = \Psi^* \Psi$ is always a positive real quantity.

Normalization:

If Ψ is the wave function associated with a particle, then $|\Psi|^2$ is proportional to the probability density P of finding the body described by ψ ; The integral of $|\Psi|^2$ over all space must be finite since the body is present somewhere.

If $\int_{-\infty}^{+\infty} |\Psi|^2 dV = 0$, then the particle does not exist. $|\Psi|^2$ cannot be negative or complex because of the way it is defined.

If $|\Psi|^2$ is equal to be P , then

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

This equation is called the **normalization condition** and a wave function that obeys this equation is said to be **normalized**.

Characteristics of a wave function:

Wave function ' Ψ ' must be single valued since the probability can have only one value at a particular place and time. Since the probability can have any value between zero and one, the wave function must be continuous. Momentum being related to the space derivatives of the wave function, the partial derivatives $\partial\Psi/\partial x$, $\partial\Psi/\partial y$ and $\partial\Psi/\partial z$ must also be continuous and single valued everywhere.

Thus, the important *characteristics of wave function* are as follows:

- (1) Ψ must be finite, continuous and single valued everywhere.
- (2) $\partial\Psi/\partial x$, $\partial\Psi/\partial y$ and $\partial\Psi/\partial z$ must be finite, continuous and single valued everywhere.
- (3) ψ must be normalizable. i.e. $\int_{-\infty}^{+\infty} |\Psi|^2 dv = 1$

Wave functions satisfying the above conditions are called **well-behaved wave functions**.

Schrodinger's wave equation:

Based on de Broglie's idea of matter waves, Schrodinger developed a mathematical theory which plays the same role as Newton's law in classical mechanics. Schrodinger's wave equation is the fundamental equation of wave mechanics. In quantum mechanics the wave function Ψ corresponds to the wave variable y of wave motion in general. However, Ψ unlike y is not itself a measurable quantity and is complex.

The motion of a free particle of mass m , moving in the $+x$ direction can be described by the wave function.

$$\Psi = Ae^{-i(\omega t - kx)} \text{ -----(1)}$$

But $\omega = 2\pi\nu = 2\pi (E/h) = (E / \hbar)$ where $\hbar = h/2\pi$

and $k = 2\pi/\lambda = 2\pi (p/h) = (p / \hbar)$

where E is the total energy and p is the momentum of the particle.

Substituting in the equation (1), we get,

$$\Psi = Ae^{-\frac{i}{\hbar}(Et - px)} \text{ ----- (2)}$$

Differentiating equation (2) with respect to x twice, we get,

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2 \Psi}{\hbar^2} \text{ or } p^2 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \text{ ----- (3)}$$

Differentiating equation (2) with respect to t , we get,

$$\frac{\partial \Psi}{\partial t} = \frac{-iE}{\hbar} \Psi \text{ or } E\Psi = -\frac{\hbar}{i} \frac{\partial \Psi}{\partial t} \text{ ----- (4)}$$

The total energy of the particle can be written as

$$E = \frac{p^2}{2m} + V \text{ ----- (5)}$$

where V is the potential energy of the particle and $\frac{p^2}{2m}$ is the kinetic energy of the particle.

Multiplying both sides of the equation by Ψ

$$E\Psi = \frac{p^2 \Psi}{2m} + V\Psi \text{ ----- (6)}$$

Substituting for $p^2 \Psi$ and $E\Psi$ from equation (3) and (4)

$$-\frac{\hbar}{i} \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \text{ ----- (7)}$$

This is known as **Schrodinger's time dependent equation in one dimension.**

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In many situations the potential energy of a particle does not depend on time, vary only with the position of the particle. Hence, Schrodinger wave equation may be simplified by removing all reference to 't'.

The wave function Ψ in equation (2) may also be written as

$$\Psi = A e^{-i/\hbar(Et-Px)} = A e^{-iEt/\hbar} \cdot e^{iPx/\hbar}$$

$$\text{Or, } \Psi = \psi e^{-\frac{iEt}{\hbar}} \text{ ----- (8)}$$

where, $\psi = A e^{iPx/\hbar}$ and ψ is a position dependent function.

Differentiating the above equation (8) with respect to 't' once,

$$\frac{\partial \Psi}{\partial t} = \frac{-iE}{\hbar} \cdot \psi e^{-\frac{iEt}{\hbar}} \text{ -----(9)}$$

And differentiating the above equation (8) twice with respect to 'x'

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} e^{-\frac{iEt}{\hbar}} \text{ -----(10)}$$

Substituting results from (8), (9) and (10) in equation (7) we get,

$$-\frac{\hbar}{i} \frac{-iE}{\hbar} \cdot \psi \cdot e^{-\frac{iEt}{\hbar}} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} e^{-\frac{iEt}{\hbar}} + V \psi e^{-\frac{iEt}{\hbar}}$$

Dividing through by the common exponential factor $e^{-\frac{iEt}{\hbar}}$ and simplifying we get

$$E\psi = \frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi$$

$$\text{Or, } \frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V)\psi = 0 \text{ ----- (11)}$$

This is the **Schrodinger's one-dimensional time independent wave equation** for a particle in one dimension.

In three dimensions, the above equation may be written as

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

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

This equation is known as the steady state or time independent Schrodinger wave equation in three dimensions.

Eigen values and Eigen functions:

The term Eigen come from the German words and mean proper or characteristic values or functions respectively. The values of energy E_n for which the Schrodinger's equation can be solved are called 'Eigen values' and the corresponding wave functions ψ_n are called 'Eigen functions'. The Eigen functions possess all the characteristics properties of wave functions in general.

Application of Schrodinger's Equation:**Particle in one dimensional potential well of infinite depth (Particle in a box):**

The simplest problem for which Schrodinger's time independent equation can be applied and solved is the case of a particle trapped in a box with impenetrable walls.

Consider a particle of mass m and energy E travelling along positive x -axis inside a box of width L . The particle is thus restricted to move inside the box by reflections at $x=0$ and $x=L$

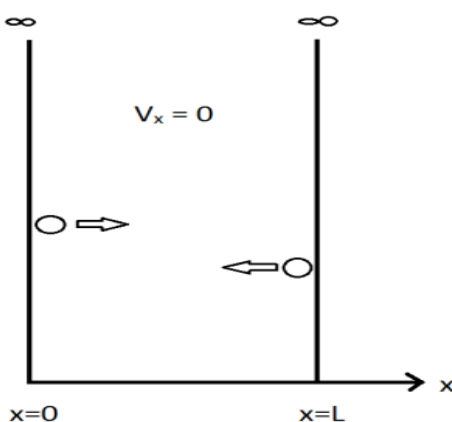


Figure: Schematic for a particle in a box. The height of the wall extends to infinity.

The height of the wall extends to infinity. The particle does not lose any energy when it collides with the walls and hence the total energy of the particle remains constant. The potential energy ' V ' of the particle is considered to be zero inside the box and infinite outside. Since the total energy of the particle cannot be infinite, it is restricted to move within the box. The example is an oversimplified case of an electron acted upon by the electrostatic potential of the ion cores in a crystal lattice.

Since the particle cannot exist outside the box,

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

We have to evaluate the wave function inside the box.

Schrodinger's wave equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V)\psi}{\hbar^2} = 0 \text{----- (1)}$$

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The potential energy 'V' of the particle is considered to be zero inside the box. Therefore, we can write

$$\frac{d^2\psi}{dx^2} + \frac{2m E \psi}{\hbar^2} = 0 \quad \text{for } 0 < x < L$$

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \text{----- (2)}$$

Here $k^2 = \frac{2m E}{\hbar^2} \text{----- (3)}$

The solution of the above equation (2) is of the form,

$$\psi = A \sin kx + B \cos kx \text{----- (4)}$$

where A and B are constants.

Applying the boundary condition, that is $\psi=0$ at $x = 0$, then above equation becomes

$$A \sin 0 + B \cos 0 = 0 \text{ or } B = 0.$$

Again, we have $\psi = 0$ at $x = L$.

$$\text{Then, } A \sin kL = 0$$

If $A = 0$, the wavefunction will become zero irrespective of the value of x . Hence, A cannot be zero.

Therefore, $\sin kL = 0$, only when, $kL = n\pi$,

Or $k = (n\pi/L) \text{----- (5), where } n=1,2,3 \dots$

Above equation (4) can be written as,

$$\psi = A \sin (n\pi x/L) \text{----- (6)}$$

The wave functions or the Eigen functions are given by

$$\psi_n = A \sin \left(\frac{n\pi x}{L} \right) \text{----- (7)}$$

To evaluate A in this function, one has to perform normalization of the wave function. Applying normalization condition,

$$\int_{-\infty}^{+\infty} |\psi_n|^2 dx = 1$$

$$i.e \int_0^L A^2 \sin^2 \left(\frac{n\pi x}{L} \right) dx = 1$$

Using $\sin^2 \theta = \frac{1}{2} (1 - \cos 2\theta)$ we will get,

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

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

$$\frac{A^2}{2} \left[L - \frac{L}{2n\pi} (\sin 2n\pi) \right] = 1 \quad (\text{Because, } \sin 2n\pi = 0)$$

$$\frac{A^2 L}{2} = 1 \Rightarrow A^2 = \frac{2}{L}$$

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

Thus the equation (7) becomes,

$$\psi_n = \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi}{L} \right) x \text{-----} (8)$$

This equation is called as Eigen wave function

Now substituting equation (5) in equation (3),

$$\left(\frac{n\pi}{L} \right)^2 = \frac{2mE}{\hbar^2}$$

From the above result, energy eigen values may be written as

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{where } n = 1, 2, 3, \dots$$

$$\text{Or } E_n = \frac{n^2 h^2}{8mL^2} \quad \text{Because, } \hbar^2 = \frac{h^2}{4\pi^2}$$

From this equation, we infer that the energy of the particle is discrete as n can have integer values. In other words, the energy is quantized. We also note that n cannot be zero because in that case, the wave function as well as the probability of finding the particle becomes zero for all values of x . Hence, $n = 0$ is forbidden. The lowest energy the particle can possess is corresponding to $n = 1$ and is equal to

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

This is called ‘ground state energy’ or ‘zero-point energy’.

The energy levels corresponding to $n > 1$ are called excited energy levels. The energies of higher excited levels are

$$n = 2, \quad E_2 = \frac{2^2 h^2}{8mL^2} = 4 E_1 - 1^{\text{st}} \text{ excited energy state}$$

$$n = 3, \quad E_3 = \frac{3^2 h^2}{8mL^2} = 9 E_1 - 2^{\text{nd}} \text{ excited energy state}$$

$$n = 4, \quad E_4 = \frac{4^2 h^2}{8mL^2} = 16 E_1 - 3^{\text{rd}} \text{ excited energy state}$$

and so on....

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The higher excited states will have energies like $4E_1$, $9E_1$, $16E_1$, etc. This indicates that the energy levels are not equally spaced.

Wave Functions, Probability densities and Energy levels a particle in a box in its ground state & excited states:

Case (i): For $n = 1$, i.e. ground state, the Eigen function is

$$\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \text{ ----- (8)}$$

Here, $\psi_1 = 0$, for both $x = 0$ & $x = L$ and $\psi_1 = \text{maximum}$ for $x = \frac{L}{2}$

$$\text{and } E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \Rightarrow E_1 = \frac{\hbar^2}{8mL^2} \text{ (Because, } \hbar = \frac{h}{2\pi} \text{)}$$

Case (ii): For $n = 2$, i.e. First excited state, the Eigen function is

$$\psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

Here, $\psi_2 = 0$, for $x = 0, \frac{L}{2}, L$ and $\psi_2 = \text{maximum}$ for $x = \frac{L}{4}, \frac{3L}{4}$

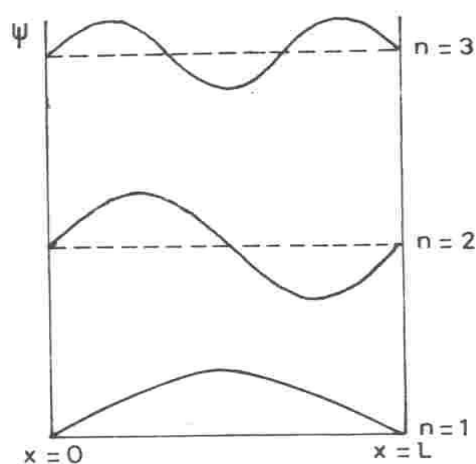
$$\text{and } E_2 = \frac{2^2 \pi^2 \hbar^2}{2mL^2} \Rightarrow E_2 = \frac{4\hbar^2}{8mL^2} = 4E_1 \text{ (Because, } \hbar = \frac{h}{2\pi} \text{)}$$

Case (iii): For $n = 3$, i.e. Second excited state, the Eigen function is

$$\psi_3 = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$$

Here, $\psi_3 = 0$, for $x = 0, \frac{L}{3}, \frac{2L}{3}, L$ and $\psi_3 = \text{maximum}$ for $x = \frac{L}{6}, \frac{L}{2}, \frac{5L}{6}$

$$\text{and } E_3 = \frac{3^2 \pi^2 \hbar^2}{2mL^2} \Rightarrow E_3 = \frac{9\hbar^2}{8mL^2} = 9E_1 \text{ (Because, } \hbar = \frac{h}{2\pi} \text{)}$$



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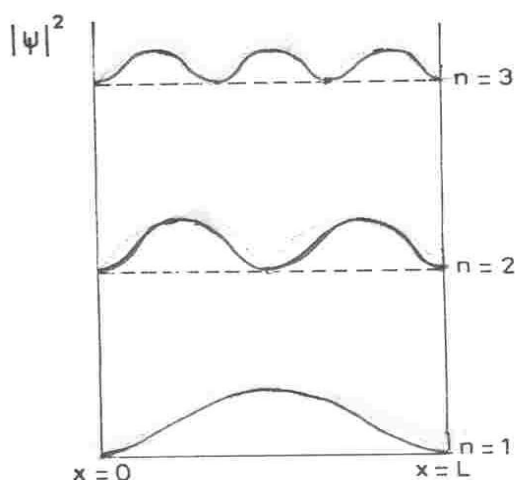


Figure a

Figure b

Figure (a) shows the variation of the wave function inside the box for different values of n and figure (b) shows the probability densities of finding the particle at different places inside the box for different values of n . Thus, the probability of finding the particle at the lowest energy level is maximum at the center of the box and for all value of n , the particle is not found at the walls of the box.

Other Applications:

- (1) Tunneling of alpha particle ($E = \text{few MeV}$) emitted by radio-active nuclei from nucleus of potential wall of 25 MeV high. The probability of escape is so small; it strikes the wall $\sim 10^{38}$ times or more before it emerges.
- (2) Tunneling also occurs in tunnel diodes – Tunneling of electron through potential barrier, even though its energy is less than barrier height.
- (3) The ability of electrons to tunnel through a potential barrier is used in the scanning tunneling microscope.

Problems:

1. In an electron diffraction apparatus, the electron beam is accelerated to a potential of 25 kV. Calculate the de Broglie wavelength associated with the electrons.

Given: $m = 9.1 \times 10^{-31} \text{ kg}$, $h = 6.626 \times 10^{-34} \text{ JS}$. ($e = 1.602 \times 10^{-19} \text{ C}$)

Solution: De Broglie wavelength $\lambda = \frac{h}{\sqrt{2meV}} =$

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-19} \times 25 \times 10^3}} = 0.076 \text{ \AA}$$

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2. Calculate the momentum of an electron and the de-Broglie wavelength associated with it if its kinetic energy is 1.5 keV.

Solution: deBroglie wavelength of an electron, $\lambda = \frac{h}{p}$

where, momentum, $P = \sqrt{2meV}$

Therefore, $P = \sqrt{2 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-19} \times 1.5 \times 10^3} = 2.09 \times 10^{-23} \text{ kgms}^{-1}$

$$\text{de Broglie wavelength } \lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-19} \times 1.5 \times 10^3}} = 3.17 \times 10^{-11} \text{ m}$$

$$= 0.317 \text{ \AA}$$

3. The position and momentum of an electron with energy 0.5 keV are determined. What is the minimum percentage of uncertainty in the momentum if the uncertainty in the measurement of its position is 0.5 angstroms unit

$$\Delta x \Delta p \geq h/4\pi$$

$$\Delta p_{\min} = \frac{h}{4\pi \Delta x}$$

$$\Delta x = 0.5 \text{ \AA} = 0.5 \times 10^{-10} \text{ m} = 5.0 \times 10^{-11} \text{ m}$$

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$\Delta p_{\min} = \frac{6.626 \times 10^{-34}}{4\pi \times 5.0 \times 10^{-11}} = 1.055 \times 10^{-24} \text{ kg m/s}$$

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

$$m = 9.109 \times 10^{-31} \text{ kg}, \quad E = 0.5 \text{ keV} = 500 \text{ eV} = 500 \times 1.602 \times 10^{-19} \text{ J}$$

$$p = \sqrt{2 \times (9.109 \times 10^{-31}) \times (500 \times 1.602 \times 10^{-19})} = 1.208 \times 10^{-23} \text{ kg m/s}$$

$$\frac{\Delta p_{\min}}{p} \times 100 = \frac{1.055 \times 10^{-24}}{1.208 \times 10^{-23}} \times 100 \approx 8.7\%$$

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

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$$v = 4.8 \times 10^5 \text{ m/s, accurate to } 0.012\%$$

$$\Delta v = 0.00012 \times v = 57.6 \text{ m/s}$$

$$\Delta p = m \Delta v = (9.109 \times 10^{-31} \text{ kg})(57.6 \text{ m/s})$$

$$= 5.2468 \times 10^{-29} \text{ kg m/s}$$

From Heisenberg uncertainty,

$$\Delta x \Delta p \geq h / 4\pi$$

$$\Delta x = h / (4\pi \Delta p) = (6.626 \times 10^{-34}) / (4\pi \times 5.2468 \times 10^{-29})$$

$$\approx 1.00 \times 10^{-6} \text{ m}$$

5. A microscope using photons is employed to locate an electron within 0.2 \AA . Find the minimum uncertainty in momentum and in velocity of the electron (take $h = 6.63 \times 10^{-34} \text{ J s}$, $m_e = 9.10 \times 10^{-31} \text{ kg}$).

$$\text{Given: } \Delta x = 0.2 \text{ \AA} = 0.2 \times 10^{-10} \text{ m, } h = 6.63 \times 10^{-34} \text{ J s, } m_e = 9.10 \times 10^{-31} \text{ kg.}$$

Using the uncertainty relation $\Delta x \Delta p = h / 4\pi$, the minimum uncertainty in momentum is:

$$\Delta p = h / (4\pi \Delta x)$$

$$= 6.63 \times 10^{-34} / (4\pi \times 0.2 \times 10^{-10}) \text{ kg m/s}$$

$$= 2.64 \times 10^{-24} \text{ kg m/s}$$

The corresponding uncertainty in velocity is:

$$\Delta v = \Delta p / m_e$$

$$= 2.64 \times 10^{-24} / 9.10 \times 10^{-31} \text{ m/s}$$

$$= 2.9 \times 10^6 \text{ m/s}$$

$$\text{Answer: } \Delta p \approx 2.64 \times 10^{-24} \text{ kg m/s, } \Delta v \approx 2.9 \times 10^6 \text{ m/s.}$$

6. An electron is bound in an one dimensional potential well of width 1 \AA , but of infinite wall height. Find its energy values in the ground state, and also in the first two excited states.

Solution: Width of the potential well = $L = 1 \text{ \AA}$.

Energy corresponds to the ground state is E_0 (when $n = 1$) and in the first two excited states E_1 and $E_2 = ?$

$$\text{We know that, } E_n = \frac{n^2 h^2}{8 m L^2}$$

$$E_0 = \frac{1^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (1 \times 10^{-10})^2} = 6.0314 \times 10^{-18} \text{ J}$$

Quantum Computing and Modern Physics (PHY102)

$$E_0 = \frac{6.0314 \times 10^{-18}}{1.602 \times 10^{-19}} = 37.64 \text{ eV}$$

$$E_1 = \frac{2^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (1 \times 10^{-10})^2} = 4 \times E_0 = 4 \times 37.64 \text{ eV} = 150.56 \text{ eV}$$

Or, $E_1 = 4 \times 37.64 \text{ eV} = 150.56 \text{ eV}$.

$$\text{And } E_2 = \frac{3^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (1 \times 10^{-10})^2} = 9 \times E_0 = 9 \times 37.64 \text{ eV} = 338.76 \text{ eV}$$

Or, $E_2 = 9 \times 37.64 \text{ eV} = 338.76 \text{ eV}$.

7. An electron is trapped in a one dimensional potential well of width $1 \times 10^{-10} \text{ m}$ and infinite height. Find the amount of energy required to excite the electron to its first excited state.

Solution: Energy of the electron in the n th excited state is given by,

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

Energy required to take the electron from ground state ($n = 1$) to the first excited state ($n = 2$) is given by,

$$E = E_2 - E_1 = \frac{2^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (1 \times 10^{-10})^2} - \frac{1^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.11 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$E = 1.81 \times 10^{-17} \text{ J} \quad \text{Or,} \quad E = 112.87 \text{ eV}.$$

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Question Bank

UNIT I: Wave Mechanics

1. What are matter waves? Mention their characteristics.
2. What is deBroglie concept of matter waves? Derive an expression for de Broglie wavelength.
3. What are matter waves? Write a note on de Broglie hypothesis of matter waves.
4. Discuss phase velocity and group velocity.
5. Explain phase velocity and group velocity and hence derive expression for phase velocity / group velocity.
6. Derive the relation between group velocity and phase velocity.

Quantum Computing and Modern Physics (PHY102)

7. Obtain the relation between group velocity and particle velocity
8. Show that group velocity is equal to particle velocity.
9. What is a wave function? Mention important characteristics of wave function.
10. Discuss matter waves and wave function.
11. Write a note on matter waves and wave function.
12. Explain Heisenberg's uncertainty principle. And show that an electron does not exist inside the nucleus.
13. What is a wave function? Give its physical significance. What is normalization of a wave function?
14. Define the terms a) Wave function, b) Eigen value and c) Eigen function.
15. What is a wave function? Discuss its physical significance.
16. Discuss probability density and normalization of a wave function.
17. Explain the following terms: (i) Probability density (ii) Normalization of a wave function (6 marks)
18. Derive Schrodinger's time-independent one dimensional wave equation for a particle of mass m with energy E . (8 marks)
19. Set up the time-dependent one dimensional Schrodinger's wave equation for a particle of mass m . (6 marks)
20. Solve the Schrodinger's wave equation for a particle in one dimension potential well of infinite height and discuss about energy Eigen values. (8 marks)
21. Solve Schrodinger's wave equation for a particle in an infinitely deep potential well of width L and show that the energy values are quantized. (8 marks)
22. Obtain the solution of Schrodinger's wave equation for a particle in one dimensional potential well of infinite height and finite width. (8 marks)
23. Obtain the expression for energy Eigen value and Eigen function for a particle in an one dimensional potential well of infinite height. (8 marks)
24. Assuming the solution of Schrodinger's wave equation for a particle in an infinitely deep potential well, plot the wave function and probability density as a function of position inside the well. What conclusions can we draw from them? (6/8 marks)
25. Discuss the wave function, probability density and energy Eigen values for a particle in a potential well by considering its ground state and the first two excited states. (6/8 marks)
26. Using Schrodinger's wave equation for a particle in one dimension potential well of infinite height discuss wave functions, energy levels and probability densities. (6/8 marks).

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Problems: (4 marks)

1. Find the de Broglie wavelength associated with an electron travelling with a velocity 10^6 m/s.
2. Calculate the de Broglie wavelength associated with an electron with a kinetic energy of 2 keV.
3. Calculate the de Broglie wavelength associated with an electron subjected to a potential difference of 1.25 kV.
4. An electron beam is subjected to a potential of 10^3 volts. Find the de Broglie wavelength associated with the electrons.
5. Compare the energy of a photon with that of a neutron when both are associated with a wave length of 1\AA , given that the mass of neutron is 1.68×10^{-27} Kg.
6. An electron is bound in a one dimensional potential well of width 1\AA , but of infinite wall height. Find its energy values in the ground state and also in the first two excited states.
7. An electron is bound in a one dimensional potential well of width 4\AA , but of infinite wall height. Find its first three energy values.
8. An electron is trapped in a one dimensional region of length 1.2\AA . How much energy must be supplied to excite the electron from the ground level to the first excited state?
9. An electron is confined to move between two rigid walls separated by 20\AA . Find the de Broglie wavelength representing the first three allowed energy states of the electron and the corresponding energies (assume the potential to be zero).
10. A particle is moving in a one-dimensional box (of infinite height) of width 10\AA . Calculate the probability of finding the particle within an interval of 1\AA around the centre of the box, when it is in its state of least energy.
11. An electron has a speed of 4.8×10^5 m/s accurate to 0.012 % . with what accuracy the position of electron can be located?
12. A proton is confined to a nucleus of radius 5×10^{-15} m. Calculate the minimum uncertainty in its momentum. Also calculate the minimum kinetic energy the proton should have. The proton mass is 1.67×10^{-27} kg.
13. Uncertainty in time of an excited atom is about 10^{-8} s. What are the uncertainties in energy and in frequency of the radiation?
14. An electron is confined to a potential well of width 10 nm. Calculate the minimum uncertainty in its velocity.

Quantum Computing and Modern Physics (PHY102)

15. If the kinetic energy of an electron known to be about 1 eV, must be measured to within 0.0001 eV, what accuracy can its position be measured simultaneously?
16. An electron and a 150 gmbase ballare traveling at a velocity of 220 m/s, measured to an accuracy of 0.005 %. Calculate and compare uncertainty in position of each.
17. The uncertainty in the measurement of time spent by Iridium -191 nuclei in the excited state is found to be 1.4×10^{-10} seconds. Estimate the uncertainty that results in its energy in the excited state.
18. If the position of an electron in an atom is measured to an accuracy of 0.01 nm. What is the uncertainty in the velocity of the electron. If electron has this velocity, what is its kinetic energy in eV.
