

Chapter 3

Quantum Mechanics

Up to nineteenth century, classical mechanics proposed by Newton was enough to explain all types of motion. But to understand and deal the laws of particles or bodies on the atomic and subatomic scale, a new branch was introduced called quantum mechanics.

Classical Mechanics failed to explain photoelectric effect, atomic structure, optical spectra, black body radiation. But after the introduction of Planck's quantum theory, all these are successfully explained.

3.1 Quantum Theory

In 1900, Max Planck put forward a revolutionary theory called quantum theory. In that the molecules in a source emit energy not continuously but in small discrete packets called *quanta*.

Magnitude of energy of each packet is given by $E = h\nu$ where h is the Planck's constant. The value of $h = 6.626 \times 10^{-34} Js$

In 1905, Einstein used this theory to explain photoelectric effect. In 1913, Bohr made use of Planck's hypothesis to explain stability of atom.

3.2 De-Broglie Hypothesis

According to De-Broglie, any moving particle is associated with a wave. This wave associated with the moving particles are known as de-Broglie waves or matter waves.

De-Broglie wavelength is given by

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

where m is the mass of the particle and p is its momentum.

- If KE of moving particle is given by

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

That is

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

Then De Broglie wavelength

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \quad (3.1)$$

- If an electron is accelerated by a potential V , then $E = eV$.
Thus De-Broglie wavelength

$$\lambda = \frac{h}{\sqrt{2meV}} \quad (3.2)$$

Putting the values of $h = 6.626 \times 10^{-34} Js$, mass of electron $m = 9.1 \times 10^{-31} kg$, charge of electron $e = 1.6 \times 10^{-19} C$

We have

$$\lambda = \frac{12.3}{\sqrt{V}} A^\circ \quad (3.3)$$

$$\lambda = \sqrt{\frac{150}{V}} A^\circ \quad (3.4)$$

3.3 Concept of Uncertainty and Conjugate Observables

Uncertainty principle is a fundamental concept in quantum mechanics which states that it is impossible to simultaneously know with absolute precision the values of certain pairs of physical properties of a particle. This

means that the more accurately you measure one property, the less accurately you can measure the other.

Conjugate observables are pairs of physical properties that are linked by the uncertainty principle. Measuring one with high precision inherently limits the precision with which the other can be measured.

Common examples of conjugate observables include:

Position and momentum: The more precisely you know the position of a particle, the less precisely you can know its momentum, and vice versa.

Energy and time: The more precisely you know the energy of a system, the less precisely you can know the time at which it has that energy.

Angular momentum and angle: There's a similar uncertainty relation between angle and angular momentum.

3.4 Heisenberg's Uncertainty Principle

1. **Uncertainty in Position and Momentum:** According to Heisenberg's Uncertainty principle, it is impossible to measure both the position and momentum of an object precisely at same time.

It states that the product of the uncertainties in the position (δx) and momentum (δp) of a particle is greater than or equal to a constant value Planck's constant divided by 4π .

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

2. **Uncertainty in Energy and Time:** This principle relates the uncertainty in energy (δE) of a system to the uncertainty in the time (δt) over which it is measured.

$$\delta E \delta t \geq \frac{h}{4\pi}$$

This implies that systems with very short lifetimes have inherently uncertain energies, and vice versa.

3. **Uncertainty in Angular Momentum and Angle:** Similar to the position-momentum relationship, there's an uncertainty relation between angular momentum (J) and angle (θ).

This means that the more precisely you know the angular momentum of a system, the less precisely you can know its angular position.

$$\delta J \delta \theta \geq \frac{h}{4\pi}$$

3.4.1 Applications of Heisenberg's Uncertainty Principle

Some atomic phenomena can be explained using uncertainty principle.

Absence of Electron Inside the Nucleus

The diameter of the nucleus is in the order of 10^{-15}m . If an electron exists in the nucleus, it can be anywhere within the diameter of the nucleus. Then the uncertainty in position, $\delta x = 10^{-15}\text{m}$.

By Uncertainty Principle,

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

$$\delta p = \frac{h}{4\pi \delta x} = \frac{6.626 \times 10^{-34}}{4 \times 3.14 \times 10^{-15}} = 5.27 \times 10^{-20} \text{kgm/s}$$

The momentum of the electron p is of the order of $5.27 \times 10^{-20} \text{kgm/s}$

We have

$$E = pc = 5.27 \times 10^{-20} \times 3 \times 10^8 = 15.81 \times 10^{-12} \text{J}$$

$$E = \frac{15.81 \times 10^{-12}}{1.6 \times 10^{-19}} \text{eV} = 98.8 \text{MeV}$$

For an electron to exist in the nucleus, it must have an energy of this order. However, the energy of electron is of order of few MeV. So electrons do not exist within the nucleus.

Natural Line Broadening

Natural line broadening is an intrinsic property of spectral lines that arises from the finite lifetime of excited atomic or molecular states. It's a quantum mechanical effect rooted in the Heisenberg uncertainty principle.

If an atom is in the excited state, it undergoes a transition to the lower energy state. Such an atom remains in the excited state for about 10^{-8} second. i.e., $\delta t = 10^{-8} \text{s}$

We have

$$\delta E \delta t \geq \frac{h}{4\pi}$$

Since $E = h\nu$, we have

$$h\delta\nu = \frac{h}{4\pi\delta t} \text{ i.e., } \delta\nu = \frac{1}{4\pi \times 10^{-8}} = 0.7 \times 10^7 \text{ Hz} = 7 \text{ MHz}.$$

Here there is *an uncertainty in frequency of light emitted by an atom* and is of the order of MHz. So this width $\delta\nu$ of the emitted line is experimentally observed.

Spectral Line: A spectral line represents the energy difference between two quantum states. Due to the energy uncertainty of the excited state, the emitted photon's energy (and consequently, its frequency or wavelength) will have a spread, resulting in a broadened spectral line. That means *the emitted spectral line have a finite width*. This broadening of spectral line which cannot be reduced further is known as natural line broadening.

3.5 Wave Function

In quantum mechanics, a wave function (ψ) is a mathematical description of the quantum state of a particle. It is a function of position coordinates and time. Wave function (ψ) is a complex quantity. Wave function describes the behavior of a single particle.

3.5.1 Physical Significance of Wave Function

1. **Probability density:** The wave function ψ itself has no physical meaning, but the square of absolute magnitude $|\psi|^2$ gives the probability of finding the particle in unit volume (probability density), where ψ^* is the complex conjugate of ψ .

$$\text{i.e., } P(x) = \psi\psi^* = |\psi|^2$$

ψ , as such, is not an observable (physically measurable quantity). But $|\psi|^2$ is an observable. This is the statistical interpretation of ψ .

2. **Normalization:** A wave function that satisfies the condition

$$\int_{-\infty}^{\infty} \Psi\Psi^* dx dy dz = 1$$

is called normalized wave function. This condition means that *the probability to find the particle somewhere in the whole region where the particle trapped is unity*.

The solution of Schrodinger equation need not satisfy this above condition directly. But we can normalize it by multiplying the function by a suitable constant called normalization constant.

A *normalized wave function* has a clear physical interpretation. It represents a particle that definitely exists somewhere in space.

3.5.2 Properties of Wave Function

Essential requisites for a well behaved wave function (constraints on wave function) for a given system are

- Wave function ψ should be single valued.
- Wave function ψ should be finite.
- Wave function ψ and its first space derivatives $\frac{\partial \Psi}{\partial x}$, $\frac{\partial \Psi}{\partial y}$, $\frac{\partial \Psi}{\partial z}$ must be continuous across any boundary.
- Wave function ψ must be a normalized function.

3.6 Schrodinger Wave Equation

Schrodinger wave equations are the equation of motion which governs the propagation of matter waves. This equation defines the wave properties of particles and also predicts their particle- like behaviour.

3.6.1 Time Dependent Schrodinger Wave Equation

Consider a particle moving forward along the x-direction with momentum P. The differential equation of the wave associated with the particle is given as

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \times \frac{\partial^2 \psi}{\partial t^2} \quad (3.5)$$

The wave function of the particle is

$$\Psi_{(x,t)} = Ae^{i(kx - \omega t)} \quad (3.6)$$

Since we have

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

$$\text{Also, } \lambda = \frac{h}{p} \quad \text{i.e., } k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

Substituting for ω and k in equation (3.6), we get

$$\Psi_{(x,t)} = Ae^{\frac{i}{\hbar}(px-Et)} \quad (3.7)$$

Total energy of a particle is the sum of kinetic energy and potential energy. i.e., $E = \frac{1}{2}mv^2 + V$

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

Multiplying both sides by Ψ , we get

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi \quad (3.8)$$

Differentiating equation (3.7) w.r.t x , we have

$$\frac{\partial\Psi}{\partial x} = Ae^{\frac{i}{\hbar}(px-Et)} \times \frac{i}{\hbar}p$$

Again differentiating equation (3.7) w.r.t x , we have

$$\begin{aligned} \frac{\partial^2\Psi}{\partial x^2} &= Ae^{\frac{i}{\hbar}(px-Et)} \times \frac{i^2}{\hbar^2}p^2 \\ \frac{\partial^2\Psi}{\partial x^2} &= \frac{i^2}{\hbar^2}p^2 \times \Psi \end{aligned}$$

$$\text{i.e., } p^2\Psi = -\hbar^2 \frac{\partial^2\Psi}{\partial x^2} \quad (3.9)$$

Differentiating equation (3.7) w.r.t time,

$$\frac{\partial\Psi}{\partial t} = Ae^{\frac{i}{\hbar}(px-Et)} \times \frac{iE}{\hbar} = -\frac{iE}{\hbar}\Psi$$

$$\text{i.e., } E\Psi = i\hbar \frac{\partial\Psi}{\partial t} \quad (3.10)$$

Substituting, $p^2\Psi$ and $E\Psi$ in equation (3.8),

$$\text{We get } i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (3.11)$$

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

In three dimensions,

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \quad \text{where} \quad \nabla^2 \Psi = \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}$$

$$\text{Also, } i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad \text{where H is Hamiltonian operator.}$$

The value of

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V$$

For free particle, PE = V = 0, then

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi \quad (3.12)$$

3.6.2 Time Independent Schrodinger Wave Equation

In some cases, potential energy V of a particle does not depend on time, it varies with the position of the particle only and then the field is said to be stationary. In such stationary problems, Schrodinger equation can be simplified by separating out time- dependent and position – dependent parts.

Accordingly, we write the wave function as a product of a function of position $x(\psi_x)$ and a function of time $t(\phi_t)$

$$\text{Thus } \Psi_{(x,t)} = \psi_x \phi_t \quad (3.13)$$

Differentiating equation (3.13) w.r.t x twice,

$$\frac{\partial^2 \Psi}{\partial x^2} = \phi_t \frac{\partial^2 \psi}{\partial x^2} \quad (3.14)$$

Differentiating (3.13) w.r.t t once, we get

$$\frac{\partial \Psi}{\partial t} = \psi_x \frac{\partial \phi}{\partial t} \quad (3.15)$$

We have time dependent Schrodinger equation as

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (3.16)$$

Substituting equation (3.14) and equation (3.15) in equation (3.16),

$$i\hbar \psi_x \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \phi_t \frac{\partial^2 \psi}{\partial x^2} + V\psi_x \phi_t$$

Dividing throughout by $\psi_x \phi_t$, We get,

$$i\hbar \frac{1}{\phi_t} \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi_x} \frac{\partial^2 \psi}{\partial x^2} + V$$

The LHS is a function of t alone while the RHS is a function of x alone. For the equation to be consistent, each side must be equal to same constant K . Then

$$\begin{aligned} i\hbar \frac{1}{\phi_t} \frac{\partial \phi}{\partial t} &= K \\ \frac{\partial \phi}{\phi} &= -\frac{i}{\hbar} K dt \end{aligned} \quad (3.17)$$

Integrating equation (3.17), we get

$$\phi(t) = e^{-\frac{i}{\hbar} K t} \quad (3.18)$$

Substituting equation (3.18) in equation (3.13), we get

$$\Psi_{(x,t)} = \psi_x e^{-\frac{i}{\hbar} K t} \quad (3.19)$$

Again on differentiating equation (3.19) with respect to t , we get,

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} K \Psi$$

$$K\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (3.20)$$

Here we can see that K is identical with E , the total energy. Hence

$$E\Psi = K\Psi \quad (3.21)$$

Then we can write the Schrodinger's time dependent equation as

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

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

Rearranging,

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V)\Psi = 0 \quad (3.22)$$

This is *Schrodinger's time-independent equation in one dimension* or also called as steady state form of Schrodinger equation.

For free particle, potential energy, $V = 0$, then one dimensional time-independent Schrodinger equation becomes

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E\Psi = 0$$

In 3D form, $\nabla^2 \Psi + \frac{2m}{\hbar^2} (E - V)\Psi = 0$

3.7 Particle in 1-Dimensional box

Consider the motion of a particle of mass m confined to move between two walls of infinite height at $x = 0$ and $x = L$. The width of the box is L . Let this is moving along x - direction. It can move freely within the region $0 < x < L$, but can never cross to the right of the region $x > L$ or to the left of the region $x < 0$. It means $V = 0$ in the region $0 < x < L$ and rises to infinity at $V = \infty$ at $x = 0$ and $x = L$. This situation is called 1D potential box.

For a particle trapped in one dimensional box, $V = 0$.

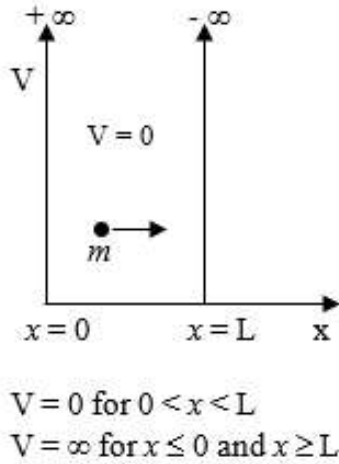


Figure 3.1: A particle in a 1D infinite potential well of dimension L .

For a particle trapped in one dimensional box, the 1-D Schrodinger equation is given as

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E \Psi = 0 \quad (3.23)$$

$$\text{Let } \frac{2m}{\hbar^2} E = k^2 \quad (3.24)$$

Putting equation (3.24) in equation(3.23), we get

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0 \quad (3.25)$$

The general solution of the equation (3.25) is

$$\Psi = A \sin(kx) + B \cos(kx) \quad (3.26)$$

Now we apply the continuity condition on Ψ . Since it is impossible to find the particle outside the box, Ψ must be zero for all points outside the box.

$$\Psi = 0 \quad \text{for } x \leq 0 \quad \text{and} \quad \Psi = 0 \quad \text{for } x \geq L \quad (3.27)$$

Applying first condition at $x = 0$ on equation (3.26),

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

Then $B = 0$. Then equation (3.26) becomes

$$\Psi = A \sin(kx) \quad (3.28)$$

Using the condition at $x = L$ on equation (3.26), we get

$$0 = A \sin kL \quad (3.29)$$

Since $A \neq 0$, $\sin kL$ must be equal to 0. Hence $\sin kL = 0$
That is, $kL = n\pi$ where n is the integer or

$$k = \frac{n\pi}{L} \quad (3.30)$$

Putting equation (3.30) in equation (3.28) we get

$$\Psi_n = A \sin\left(\frac{n\pi}{L}x\right) \quad (3.31)$$

To find A , apply the normalization condition,

$$\begin{aligned} & \int_0^L |\Psi|^2 dx = 1 \\ \text{i.e.,} & \int_0^L A \sin\left(\frac{n\pi}{L}x\right) \cdot A \sin\left(\frac{n\pi}{L}x\right) dx = 1 \\ \text{i.e.,} & A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \\ \text{i.e.,} & \frac{A^2}{2} \int_0^L \left[1 - \cos 2\left(\frac{n\pi x}{L}\right)\right] dx = 1 \\ \text{i.e.,} & \frac{A^2}{2} \left[x - \frac{\sin\left(\frac{2n\pi x}{L}\right)}{\left(\frac{2n\pi}{L}\right)} \right]_0^L = 1 \end{aligned}$$

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

Since $\sin 2n\pi = 0$

$$\frac{A^2}{2} \times L = 1 \quad (3.32)$$

$$A = \sqrt{\frac{2}{L}} \quad (3.33)$$

$$\text{Thus equation (3.31) becomes} \quad \Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x \quad (3.34)$$

This is the *normalized wave function of particle in a potential box of length L*.

The wave functions and probability densities for a particle in a one dimensional box is given in the Figure 3.2

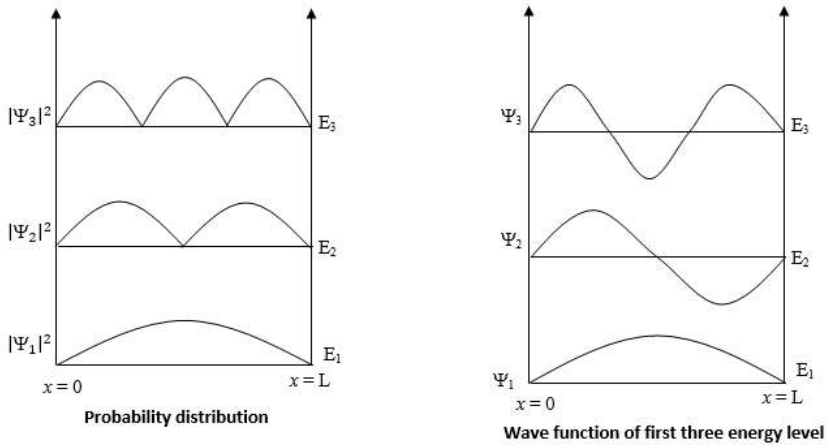


Figure 3.2: Energy eigen state of particle in a 1D box

3.8 Energy Eigen Values

In quantum mechanics, energy eigenvalues represent the specific, discrete energy values that a quantum system can possess.

According to quantum mechanics, a system can take only certain specific energies. Such discrete energies are the *energy eigen values* of the Schrodinger equation for the system.

Eigen functions: Associated with each energy eigenvalue is an eigen function, which represents the state of the system when it has that particular energy. We have

$$\frac{2m}{\hbar^2} E = k^2$$

$$\text{Then } E = \frac{k^2 \hbar^2}{2m} = \left(\frac{n\pi}{L} \right)^2 \left(\frac{\hbar^2}{2m} \right) = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

Therefore, the energy of the particle trapped inside the potential well is

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{where } n = 1, 2, 3, \dots \quad (3.35)$$

For ground state, $n = 1$,

$$E = \frac{(1)^2 \pi^2 \hbar^2}{2mL^2} = \frac{\pi^2 \hbar^2}{2mL^2} = E_1$$

For first excited state, $n = 2$

$$E = \frac{(2)^2 \pi^2 \hbar^2}{2mL^2} = \frac{4\pi^2 \hbar^2}{2mL^2} = 4E_1$$

For second excited state, $n = 3$

$$E = \frac{(3)^2 \pi^2 \hbar^2}{2mL^2} = \frac{9\pi^2 \hbar^2}{2mL^2} = 9E_1$$

Different values of energy for n are called energy eigen values and

$$\Psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right)x \quad \text{is the energy eigen function.}$$

3.9 Quantum Mechanical Tunneling

Consider a particle of mass m and energy $E < V_0$ incident on a potential barrier V_0 . Quantum mechanically, there will be a finite probability for the particle to penetrate through a barrier even if $E < V_0$. This phenomenon of tunneling through barriers higher than their own incident energy is known as *Quantum Mechanical Tunneling*.

Quantum mechanical tunneling is shown in Figure 3.3. The solution of the Schrödinger equation for the particle gives the wave function for the three regions.

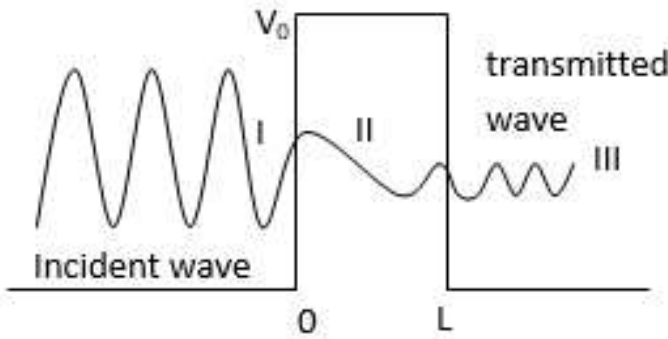


Figure 3.3: Quantum Mechanical Tunnelling

The concept of barrier penetration is used to explain a number of phenomenon in physics. Some of them are as follows.

- The emission of α -particles from radioactive nuclei.
- Barrier penetration in electronic devices such as tunnel diode and Josephson junction.
- Electron tunneling in scanning tunneling microscope.

3.10 Solved Numerical Problems

Example 3.10.1 Compute the de-Broglie wavelength of an electron whose kinetic energy is 10eV.

Solution:

We have

$$\begin{aligned}\lambda &= \frac{h}{\sqrt{2mE}} = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 10 \times 1.6 \times 10^{-19}}} \\ &= 3.88 \times 10^{-10} \text{m}\end{aligned}$$

Example 3.10.2 An electron and a proton have the same non-relativistic kinetic energy. Show that the proton has shorter de-Broglie wavelength.

Solution:

$$\begin{aligned}\text{We have } \lambda_P &= \frac{h}{\sqrt{2m_P E}} \quad \text{and} \quad \lambda_e = \frac{h}{\sqrt{2m_e E}} \\ \frac{\lambda_P}{\lambda_e} &= \sqrt{\frac{m_e}{m_P}}\end{aligned}$$

Since $m_P > m_e$, then $\lambda_P < \lambda_e$. Hence proton has shorter de-Broglie wavelength.

Example 3.10.3 An electron is confined to a box of length 10^{-9}m . Calculate its minimum uncertainty in its velocity.

Solution:

Given $\Delta x = 10^{-9}$

$$\begin{aligned}\Delta x \cdot m \Delta v &= \frac{\hbar}{2} \\ \Delta v &= \frac{\hbar}{2m\Delta x} = \frac{1.05 \times 10^{-34}}{2 \times 9.1 \times 10^{-31} \times 10^{-9}} = 5.7 \times 10^4 \text{m/s}\end{aligned}$$

Example 3.10.4 An electron moves with constant speed $v = 1.1 \times 10^6 \text{m/s}$. If the speed is measured to a precision of 0.1%, what is the maximum precision with which its position could be simultaneously measured.

Solution:

We have $p = mv$ where m is the mass of electron and v is its velocity.

We have $m = 9.11 \times 10^{-31} \text{ kg}$ and $v = 1.1 \times 10^6 \text{ m/s}$

$$\Delta P = \frac{0.1}{100} \times 10^{-24} = 10^{-27} \text{ Kgm/s.}$$

$$\begin{aligned} \Delta x &= \frac{\hbar}{2\Delta P} \times 10^{-24} \\ &= \frac{1.054 \times 10^{-34}}{2 \times 10^{-27}} \times 10^{-24} = 0.53 \times 10^{-7} \text{ Kgm/s.} \end{aligned}$$

Example 3.10.5 Find the energy of electron moving in 1-D in an infinitely high potential of width 1\AA .

Solution:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

Putting, $n=1$,

$$\begin{aligned} E_n &= \frac{(1)^2 \times (3.14)^2 (1.05 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2} \\ &= 5.972 \times 10^{-18} \text{ Joules} \end{aligned}$$

$$\text{For } n=2, \quad E_n = 5.972 \times 2 = 1.194 \times 10^{-17} \text{ J}$$

Example 3.10.6 An electron is confined to a 1-D box of width L is known to be in its first excited state. Determine probability density of electrons in central half.

Solution:

$$\begin{aligned} \Psi &= \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi}{L} \right) x \\ |\Psi|^2 &= \frac{2}{L} \sin^2 \left(\frac{n\pi}{L} \right) x \end{aligned}$$

To find the probability density of electron in central half, $x = \frac{L}{2}$

$$|\Psi|^2 = \frac{2}{L} \sin^2 \left(\frac{n\pi}{L} \right) \frac{L}{2} = 0$$

Example 3.10.7 Calculate the separation between the two lowest energy levels of an electron in a 1-D box of width 4\AA in joules. Given $m_e = 9.1 \times 10^{-31} \text{ kg}$ and $h = 6.625 \times 10^{-34} \text{ kg}$.

Solution:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$\begin{aligned} \text{Putting, } n=1, \quad E_1 &= \frac{(1)^2 \times (3.14)^2 \times (1.05 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times (4 \times 10^{-10})^2} \\ &= 3.7 \times 10^{-19} \text{ Joules} \end{aligned}$$

$$\text{For } n=2, \quad E_2 = 4 \times 3.7 \times 10^{-19} = 14.92 \times 10^{-19} \text{ J}$$

$$E_2 - E_1 = 14.92 \times 10^{-19} - 3.7 \times 10^{-19} = 11.9 \times 10^{-19} \text{ J}$$

3.11 Exercises

1. Compute the de-Broglie wavelength of an electron whose kinetic energy is 10KeV.

Hint: $1.2 \times 10^{-11} \text{ m}$

2. An electron remains in an excited state of an atom for 10^{-8} s . What is the minimum uncertainty in the energy of the state in eV.

Hint: $3.28 \times 10^{-8} \text{ eV}$

3. An electron is moving in a one dimensional box of infinite height and width 10\AA . Calculate the first three permitted energy levels.

Hint: $E_1 = 5.97 \times 10^{-20} \text{ J}$; $E_2 = 29.85 \times 10^{-20} \text{ J}$; $E_3 = 53.73 \times 10^{-20} \text{ J}$

4. For an electron in a 1-D box of width 1\AA , calculate the first three energy levels in eV.

Hint: $E_1 = 37.61\text{eV}$; $E_2 = 150.43\text{eV}$; $E_3 = 338.47\text{eV}$

5. Calculate the quantum number associated with a marble of mass 10g trapped to move with speed 1m/s in 1-D box of width 20cm .

Hint: $n \approx 6 \times 10^{13}$

6. If an electron's position can be measured to an accuracy of $2 \times 10^{-8}\text{m}$, how accurately can its velocity be known?

Hint: $\Delta v = 2894.28\text{m/s}$.