# Unit 3
# Quantum Mechanics

Quantum mechanics is the fundamental branch of physics that deals with nature at the smallest scales, such as molecules, atoms, and subatomic particles. Unlike classical mechanics, which is deterministic and deals with macroscopic objects, quantum mechanics introduces the idea that particles can exhibit both wave-like and particle-like behaviour. This duality of matter and energy, and the probabilistic interpretation of physical quantities, are core to quantum theory.

Quantum mechanics evolved during the early 20th century when classical theories failed to explain several phenomena like black body radiation, the photoelectric effect, and atomic spectra. These anomalies prompted scientists to develop a new framework to accurately describe physical systems at microscopic scales. Quantum mechanics not only resolved these inconsistencies but also revolutionized our understanding of the universe, leading to the development of various technologies like lasers, semiconductors, and quantum computers.

## EXPERIMENTS LEADING TO QUANTUM NATURE OF MATTER

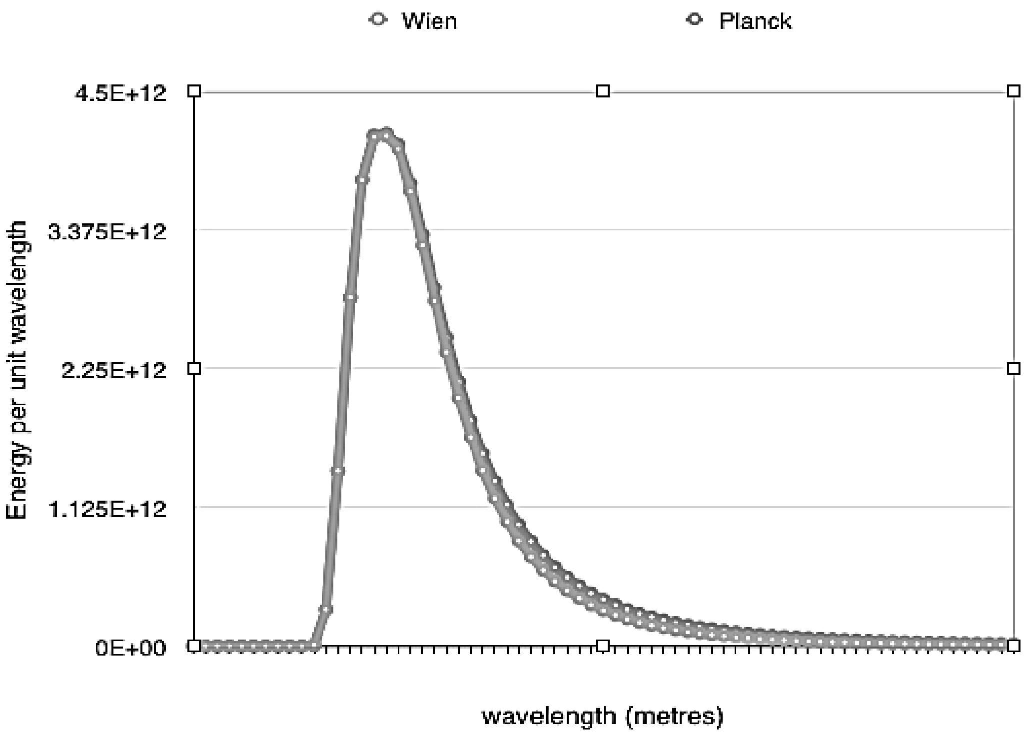
### 1. Black Body Radiation

Black body radiation refers to the electromagnetic radiation emitted by a perfect black body when heated. Classical physics, using the Rayleigh-Jeans law, predicted that the energy emitted should become infinite at short wavelengths, leading to what was called the ultraviolet catastrophe.

To solve this, Max Planck proposed that energy is not emitted continuously, but in discrete packets or quanta. He introduced a constant, now known as Planck's constant (h), and proposed that the energy of radiation is proportional to its frequency:

$$E = nh\nu \qquad where\ n = 1,2,3,\ldots$$

This marked the beginning of quantum theory, highlighting that energy is quantized.

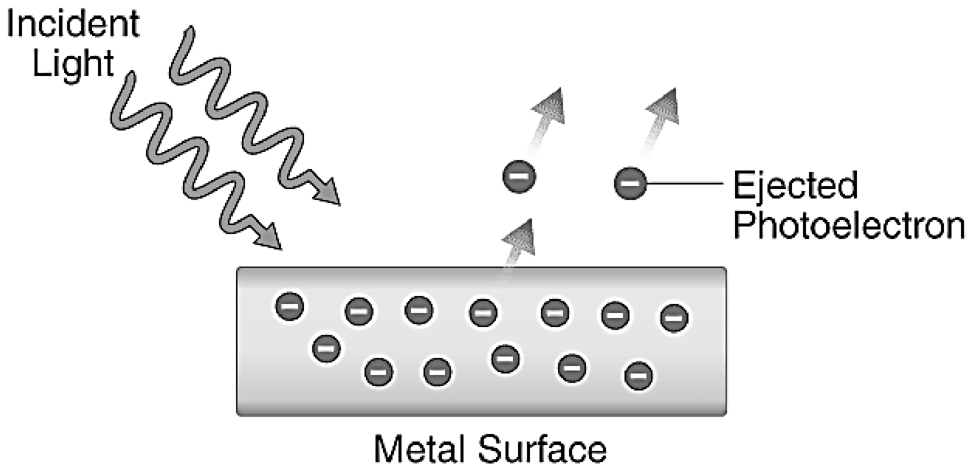


**2. Photoelectric Effect**

The photoelectric effect refers to the emission of electrons from a metal surface when light is shined upon it. Classical wave theory could not explain why electrons were emitted only when light of a certain minimum frequency was used, regardless of its intensity.
Albert Einstein explained this phenomenon by suggesting that light consists of particles called photons, each with energy $E = h\nu$. If this energy exceeds the work function (ϕ) of the metal, an electron is ejected. The kinetic energy (KE) of the emitted electron is given by:

$$KE = h\nu - \phi$$

This experiment confirmed the particle nature of light.

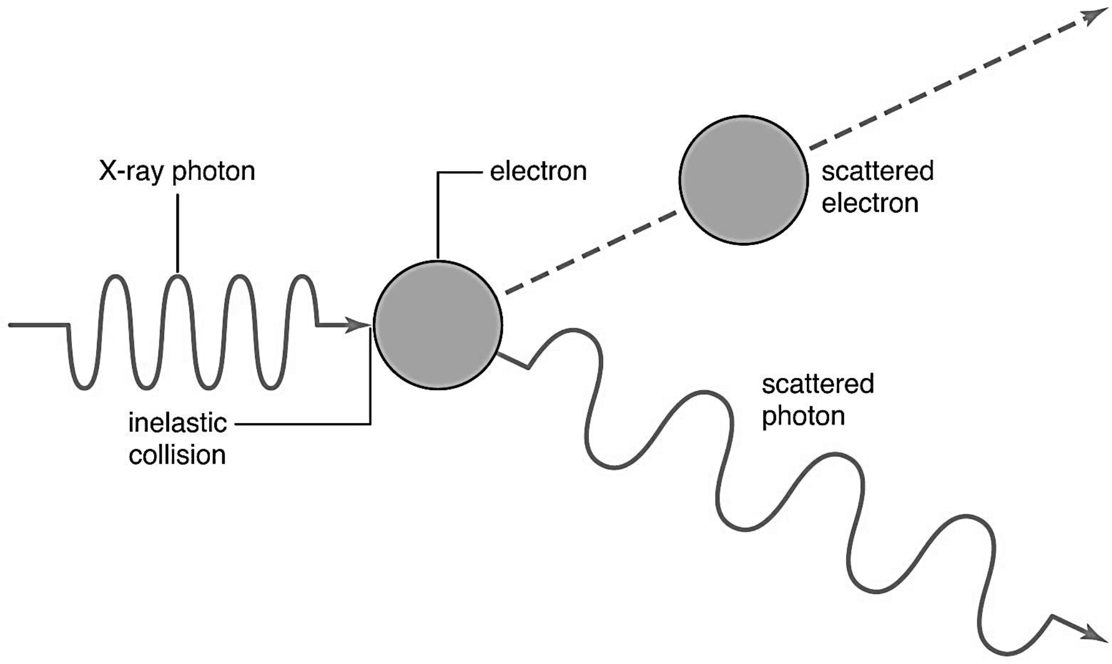



**3. Compton Effect**

Arthur Compton observed that when X-rays are scattered by electrons, the scattered rays have a longer wavelength than the incident rays. This phenomenon could not be explained using classical wave theory. Compton explained the effect using photon theory, treating X-rays as particles with momentum. The shift in wavelength, called the Compton shift, depends on the angle of scattering and is given by:

$$\lambda' - \lambda = \frac{\mathrm{h}}{\mathrm{m_e c}}(1 - cos\theta)$$

This provided strong evidence that photons carry both energy and momentum.

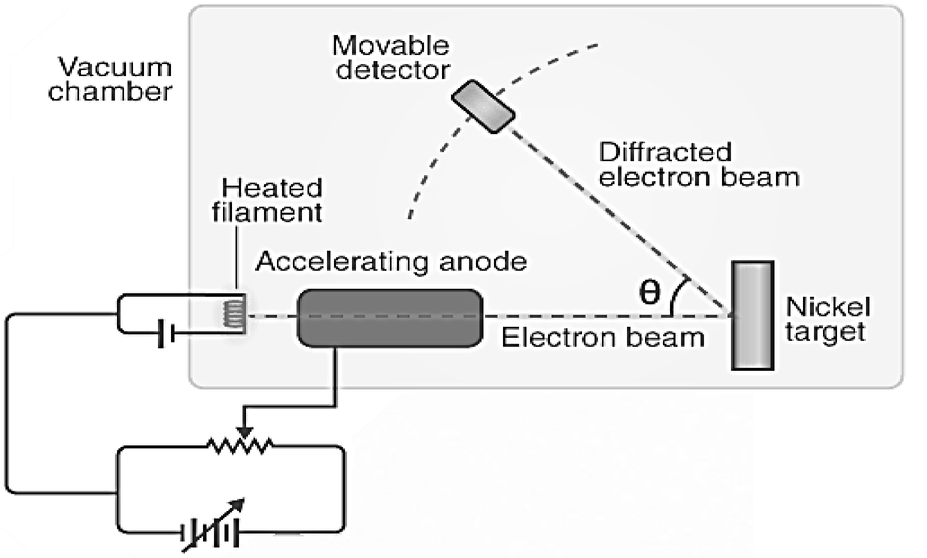


**4. Davisson-Germer Experiment**

This experiment provided direct evidence for the wave nature of electrons. When a beam of electrons was directed at a nickel crystal, the scattered electrons exhibited a diffraction pattern similar to that of X-rays. This supported de Broglie's hypothesis that particles such as electrons have a wavelength:

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

It confirmed the wave-particle duality of matter, a cornerstone of quantum mechanics.




## HEISENBERG'S UNCERTAINTY PRINCIPLE

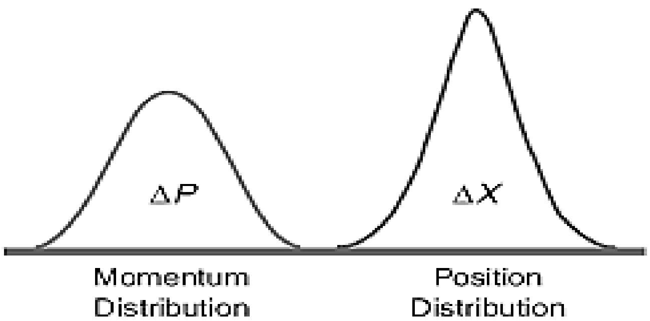
The Heisenberg Uncertainty Principle, formulated by Werner Heisenberg, states that it is fundamentally impossible to simultaneously measure the exact position and momentum of a particle. The more precisely one quantity is measured, the less precisely the other can be known.

**Mathematical Expression**

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

Where:

- $\Delta x$ is the uncertainty in position
- $\Delta p$ is the uncertainty in momentum
- $\hbar = \frac{h}{2\pi}$ is the reduced Planck's constant




**Significance**

- This principle introduces intrinsic limitations in measurement.
- It is not due to experimental imperfections but a fundamental property of nature.
- The principle explains the stability of atoms, as electrons cannot spiral into the nucleus due to the uncertainty in position and momentum.

**Applications**

- Explains why electrons cannot exist within the nucleus.
- Crucial in defining the behaviour of quantum systems like quantum wells and atoms.

## WAVE FUNCTION AND BASIC PROPERTIES

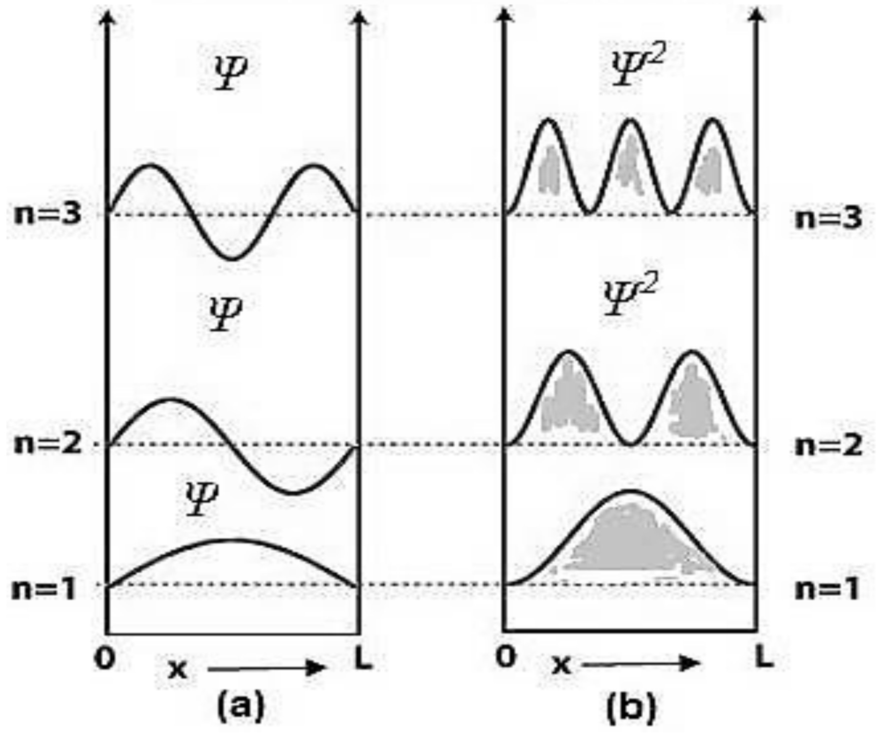
In quantum mechanics, the wave function $\Psi(x,t)$ describes the quantum state of a particle or system. It contains all the information about a system's behaviour. The square of the magnitude $|\ \Psi(x,t)\ |^2$ represents the probability density of finding the particle at position x and time t.

**Key Properties of Wave Function**

1. *Single-valued:* For a given point in space and time, Ψ must yield a single value.
2. *Continuous and Differentiable:* To satisfy the Schrödinger equation, Ψ must be smooth.
3. *Square-integrable:* The integral of $|\ \Psi(x,t)\ |^2$ over all space must be finite.
4. *Normalizable:* Wave function should be normalized such that:

$$\int_{-\infty}^{\infty} |\ \Psi(x,t)\ |^2\, dx = 1$$

The wave function is central to all of quantum mechanics, even though it does not have a direct physical meaning by itself. Only its square modulus is observable.




## SCHRÖDINGER EQUATION

The Schrödinger equation is the fundamental equation of quantum mechanics. It governs the time evolution and spatial distribution of wave functions.

**Time-Dependent Wave Equation (TDSE)**

Let

- The particle is non-relativistic.
- Energy is the sum of kinetic and potential energies.
- The wave nature of a particle is described by a wave function $\Psi(x,t)$.

According to De Broglie Hypothesis

A moving particle has an associated wave:

$$\lambda = \frac{h}{p}, \qquad E = h\nu$$

Also,

$$p = mv, \qquad E = \frac{p^2}{2m} + V(x)$$

Now, General Wave Equation for a Plane Wave is
Let the wave function for a free particle be:

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

Where:

- $k = \frac{2\pi}{\lambda}, \omega = 2\pi\nu$
- $p = \hbar k, E = \hbar\omega$

In quantum mechanics:

- Energy operator:

$$\hat{E} = i\hbar\frac{\partial}{\partial \mathrm{t}}$$

- Momentum operator:

$$\hat{p} = i\hbar\frac{\partial}{\partial \mathrm{x}}$$

Now, Total Energy:

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

So, applying operators:

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

This is the Time-Dependent Schrödinger Equation (TDSE):

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

**Time-Independent Wave Equation (TISE)**
Let

$$\Psi(x,t) = \psi(x)\cdot T(t)$$

Substitute in TDSE:

$$i\hbar\left(\psi(x)\cdot\frac{dT(t)}{dt}\right) = -\frac{\hbar^2}{2m}\left(T(t)\cdot\frac{\partial^2\psi(x)}{\partial x^2}\right) + V(x)\psi(x)T(t)$$

Divide both sides by $\psi(x)T(t)$:

$$i\hbar\frac{1}{\mathrm{T}}\frac{dT}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V(x)$$

Since LHS depends only on t and RHS only on xxx, both must be equal to a constant, say E (total energy).
Now, Time-Independent Equation is

$$\frac{dT}{dt} = -\frac{iE}{\hbar}T(t) \Rightarrow T(t) = e^{-iEt/\hbar}$$

Now the spatial part:

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

This is the Time-Independent Schrödinger Equation (TISE):

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

## PHYSICAL INTERPRETATION OF THE WAVE FUNCTION

The physical interpretation of the wave function was proposed by Max Born. According to his interpretation:
$|\ \Psi(x,t)\ |^2\ dx$ represents the probability of finding the particle between x and $x + dx$ at time t.

### Important Points

- $|\ \Psi\ |^2$ is a probability density, not the probability itself.
- The total probability over all space must be 1.
- The wave function must be normalized.
- Wave function is not directly observable; it is a mathematical tool used to calculate observable quantities.

## APPLICATIONS AND PROBLEMS IN QUANTUM MECHANICS

### Particle in a One-Dimensional Box

A particle confined in a box of length LL with infinitely high walls has zero potential energy inside and infinite outside.
**Potential:**

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & otherwise \end{cases}$$

**Boundary Conditions:**

$$\Psi(0) = \Psi(L) = 0$$

**Solutions:**

- Wave Function:

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

- Energy Levels:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \qquad n = 1,2,3, \ldots$$

The energy levels are quantized and increase with $n^2$.

### Particle in a Three-Dimensional Box

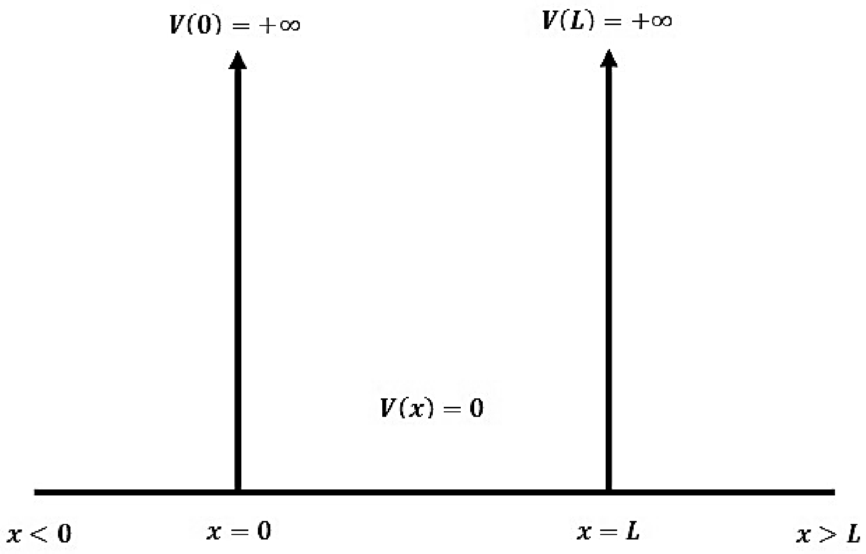
For a 3D box with sides $L_x, L_y, L_z$, the wave function is:

$$\Psi(x,y,z) = \frac{2}{\sqrt{L_x\ L_y\ L_z}} sin\left(\frac{n_x\pi x}{L_x}\right) sin\left(\frac{n_y\pi y}{L_y}\right) sin\left(\frac{n_z\pi z}{L_z}\right)$$

Energy levels are given by:

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

Each unique set of quantum numbers $(n_x, n_y, n_z)$ corresponds to a specific energy state.




*Particle in One-Dimensional Box(Infinite Potential Well)*

## QUANTUM MECHANICAL TUNNELLING

Quantum tunnelling is the phenomenon where a particle penetrates through a potential barrier even when its energy is less than the barrier height. This is strictly forbidden in classical mechanics but allowed in quantum theory.

### Mathematical Formulation

For a particle of energy EE approaching a barrier of height V0V_0 and width aa, the probability of tunnelling through the barrier is:

$$T \approx e^{-2\kappa a}$$

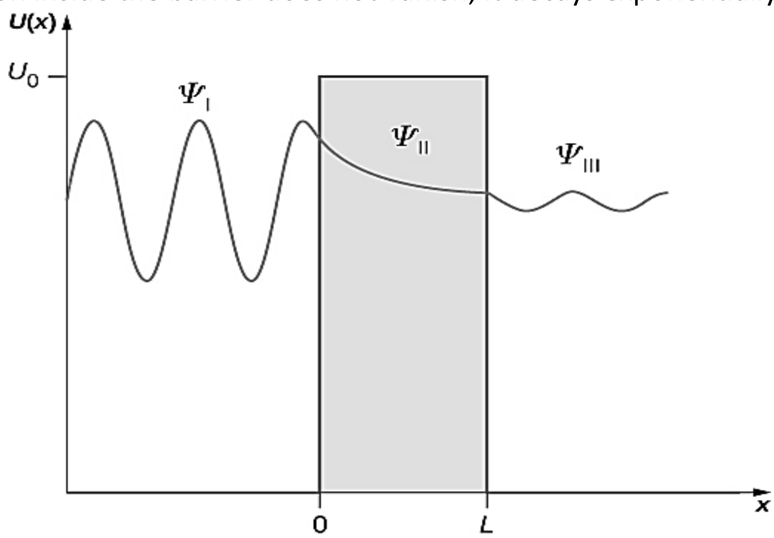
Where:

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar}}$$



### Physical Insight

- Even when classical physics predicts no transmission, quantum mechanics allows for a finite probability.
- The wave function inside the barrier does not vanish; it decays exponentially.



**Applications**

- *Tunnel Diodes:* Used in high-frequency electronics.
- *Scanning Tunnelling Microscope (STM):* Uses tunnelling to image surfaces at the atomic level.
- *Nuclear Fusion:* Tunnelling allows particles in stars to overcome repulsive forces.