



Engineering Physics (303192102)

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CHAPTER 1

MODERN PHYSICS

Introduction

- A new branch of study in Physics which is indispensable in **understanding the mechanics of particles in the atomic and sub-atomic scale**
- In Classical Mechanics it is unconditionally accepted that position, mass, velocity, acceleration etc. of a particle can be measured accurately, which, of course, true in day to day observations (Macro scale)
- In Quantum Mechanics the Foundation of principles are purely probabilistic in nature as it is impossible to measure simultaneously the position and momentum of a particle at microscale

Some basic insights to Quantum Mechanics

- Max Planck proposed the Quantum theory to explain Blackbody radiation
- Einstein applied it to explain the Photo Electric Effect
- In the meantime, Einstein's mass – energy relationship ($E = mc^2$) had been verified in which the radiation and mass were mutually convertible
- Louis de-Broglie extended the idea of dual nature of radiation to matter, when he proposed that matter possesses wave as well as particle characteristics

Failure of Classical Physics

- Classical Mechanics describes the motion of macroscopic objects. It provides extremely accurate results as long as the domain of the study is restricted to large objects and the speed involved does not approach the speed of light.
- This unexplainable behavior at microscopic level gave birth to Quantum Mechanics or it was called as **Failure of Classical Physics** which could not explain the behavior of element / matter at microscopic level.
- There are three failures of Classical Physics

1. Black Body Radiation

2. Structure of an Atom

3. Photoelectric effect

Black Body Radiation

- In 1897, Lummer and Pringshem measured the intensities of different wavelength of Blackbody or Cavity radiations.
- An ideal body that absorbs all radiation incident upon it regardless of frequency of radiation a body is called a **Black body**.
- The ability of the body to radiate is closely related to ability to absorb the radiation. Since a body at constant temperature is in thermal equilibrium with its surrounding it must absorb energy from them at the same rate as it emits energy.
- **Light entering the cavity is trapped inside by the multiple reflection from the walls. When heated, the black body would emit more from a unit area than any other body at a given temperature.**

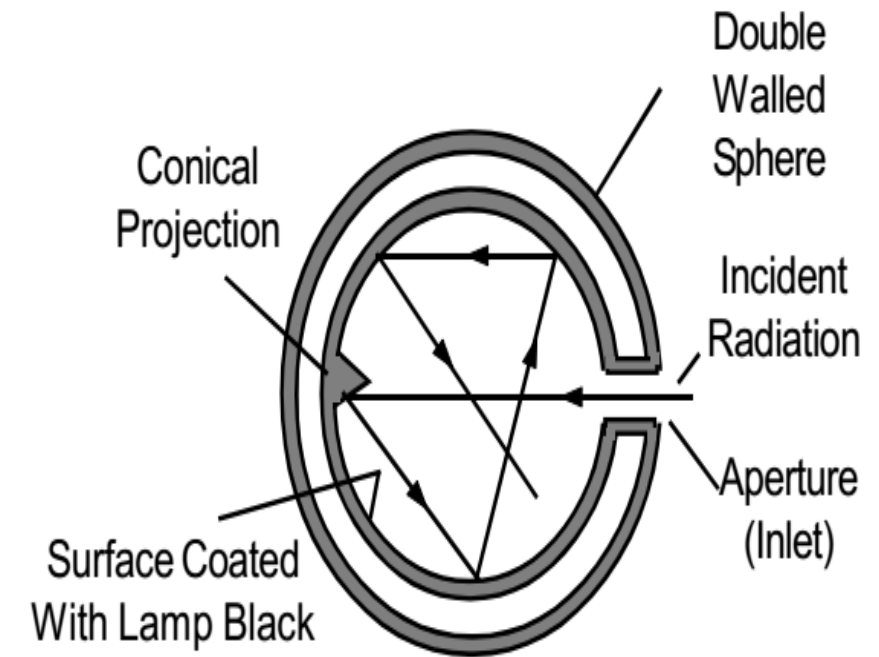


Fig.1: A spherical cavity blackened inside and completely closed except a narrow aperture serves as an ideal black body

https://thefactfactor.com/facts/pure_science/physics/perfectly-black-body/8243/

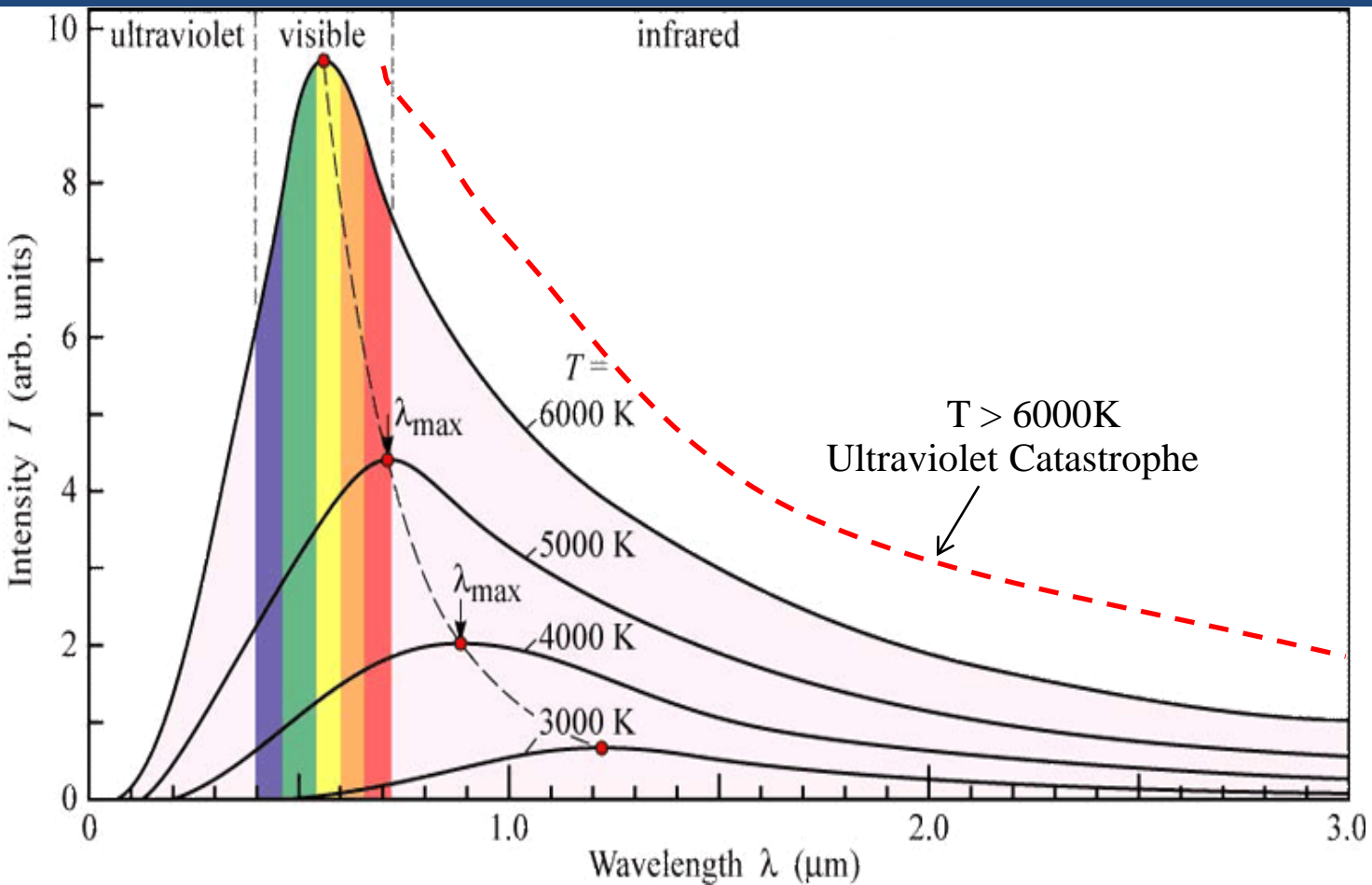


Fig.2: The energy distributed in the different wavelength in the spectrum of a black body radiation can be shown as the figure

The energy of radiation emitted from a black body at a temperature T given by,

$$E \propto T^4$$

$$E = \sigma T^4$$

σ = Stefan's Constant = $5.6704 \times 10^{-8} \text{ watt/m}^2 \text{ K}^4$

From the spectral distribution following results are considered:

1. At given temperature T , energy is not distributed uniformly throughout the spectrum.
2. At given temperature T , intensity of the radiation increases with increase in wavelength till it reaches its maximum, then intensity reduces with increase in wavelength λ .
3. With increase in temperature, the wavelength $\lambda_m (m = 1, 2, 3, \dots)$ decreases.
Wien's displacement law states that the peak of wavelength, λ_{max} at which the maximum emission occurs for any given temperature, is inversely proportional to the absolute temperature of body.

$$\lambda_m = \frac{2.8978 \times 10^{-3}}{T} \text{ mK}$$
$$\lambda_m \cdot T = \text{constant} = 0.28978 \text{ cmK}$$

The above equation is called as the **Wien's Displacement Law**

4. The area under the curve gives the total energy emitted at given temperature.

Rayleigh-Jeans explanation and Planck's proposition:

According to the distribution of energy in spectrum was given by

$$E_{\lambda}d\lambda = \frac{8\pi KT}{\lambda^4} d\lambda \quad - (1)$$

$$E_{\nu}d\nu = \frac{8\pi\nu^3 KT}{c^3} d\nu \quad - (2)$$

Where $KT = \text{Thermal Energy}$

Equation (1) is called as **Rayleigh-Jeans law**

- The radiation emitted by the atoms is reflected back and forth in cavity to form a system of standing waves for each frequency and when thermal equality is attained the average rate of emission of radiant energy atomic oscillation is equal to the rate of absorption of radiant energy by walls.
- This energy was calculated for a long wavelength. In the energy spectrum graph, the formula agreed for long wavelength and but goes towards Infinity at the shorter wavelength end. This contradiction came to the note as **Ultraviolet Catastrophe**.

The failure of Rayleigh-Jeans formula gave the first indication of inadequacy of classical physics

Planck's radiation law or Planck's proposition

- Planck recognized the reason for ultraviolet catastrophe was that Rayleigh assumed the standing waves in cavity of body consist of fundamental modes of vibration. Each having energy KT , thus making the total energy of the cavity Infinity.
- Planck suggested that an oscillating atom can only absorb or remit energy only in quantities that are integral multiple of $h\nu$

This discrete energy $h\nu$ is called Energy Quantum,

In general,

$$E = nh\nu \quad ; (n = 1, 2, 3, \dots)$$

Where $n = \text{Quantum number of Oscillation}$

$$h = \text{Planck's Constant} = 6.626 \times 10^{-34} \text{ J.s}$$

- Using a Maxwell Boltzmann distribution law, Planck obtained the energy density in black body radiation as

$$E(\nu) = \frac{8\pi h\nu^3}{c^3} \left(\frac{1}{e^{\frac{h\nu}{KT}} - 1} \right)$$

This Equation is Planck's radiation law.

Wave Particle Duality

According to the de-Broglie the photons of light having frequency f and has a momentum as p
Therefore its wavelength can be given as,

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

Now the momentum of photon is given by,

$$p = \frac{E}{c} \quad - (1)$$

We know that, in a vacuum the frequency is given by,

$$f = \frac{c}{\lambda}$$
$$\therefore c = \lambda \cdot f \quad - (2)$$

Substituting equation (2) in equation (1)

$$p = \frac{E}{\lambda \cdot f}$$

Also, for a photon, we know that $E = h \cdot f$ - (3)

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

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

$$\therefore \lambda = \frac{h}{p} \quad - (4)$$

$$\therefore \lambda = \frac{h}{mv} \quad - (5)$$

Equation (4) and (5) represents general de-Broglie equation that can be applied for particles and waves.

In some cases, momentum is given as $p = \gamma mv$ where $\gamma = \text{Relativistic Factor}$ which is given by

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

Compton Effect

- Compton Effect gives direct and conclusive evidence in support of the particle nature of electromagnetic radiation.
- *When a monochromatic beam of X-rays (or the electromagnetic radiation of short wavelengths) of wavelength λ is allowed to incident on scattering materials, the beam scattered contains the radiation of longer wavelength λ' . The difference between λ and λ' i.e., $\lambda' - \lambda$ is known as **Compton shift** and the effect is called as a **Compton Effect**.*
- The Compton shift does not depend on the wavelength of incident radiation and nature of scattering materials. **It depends on the scattering angle** only.

$$\therefore \lambda' - \lambda = \frac{h}{mc} (1 - \cos \theta) \quad - (6)$$

The above equation is called as the **Compton Shift in Electron's wavelength**.

Compton Shift

The below figure represents the scenario for before and after collision of an electromagnetic radiation of low wavelength with electron.

- **Before Collision:** The Energy of incident radiation be given as, $E = \frac{hc}{\lambda}$. As the wave is in motion, the momentum be $p = \frac{h\nu}{c}$ or $p = \frac{h}{\lambda}$. As the electron, initially is at rest, its energy be E_0 and its momentum be 0 (zero).
- **After Collision:** The electron is recoiled at an angle ϕ and the energy and momentum changes to E_e and p_e . The radiation is scattered at an angle θ with the energy $E' = \frac{hc}{\lambda'}$ and momentum p' .
- **Note: The scattered wave will have longer wavelength.**

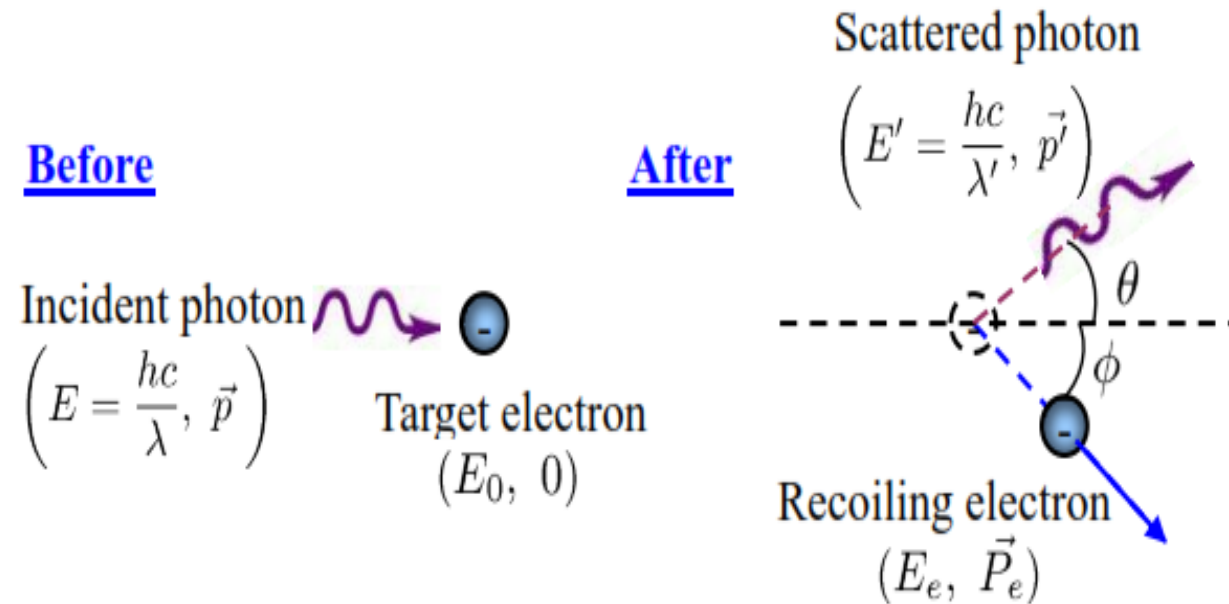


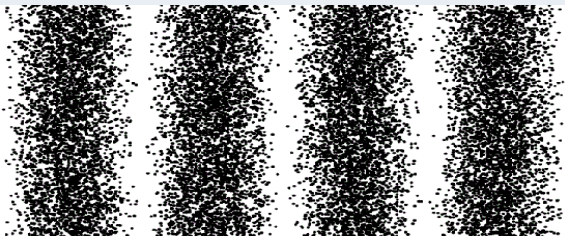
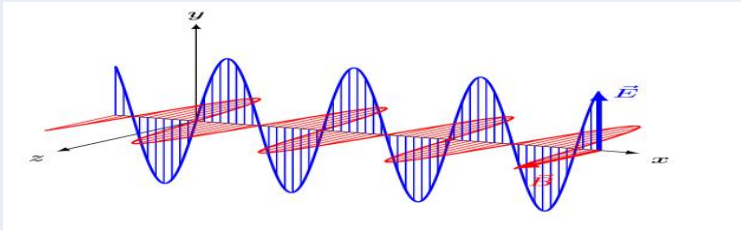

Fig.3: Compton Scattering

Importance of Compton Effect

Compton Effect is an important milestone in development of Modern Physics.

Compton Effect proves the following:

1. It proves the particle nature of the Electromagnetic radiation
2. This verifies the Planck's Quantum hypothesis
3. It provides indirect verification of the relation, $m = \frac{m_0}{\sqrt{1-v^2/c^2}}$ and $E = mc^2$ as these relations can be used in delivering the expression for Compton Effect.

	Matter Waves	Electromagnetic Waves	Mechanical Waves
DEFINITION	Matter waves are the waves that consist of particles	An electromagnetic wave is a type of wave that travels through space, carrying electromagnetic radiant energy	A mechanical wave is a wave that is an oscillation of matter and is responsible for the transfer of energy through a medium
COMPOSITION	Particles (which have mass and volume)	Photons	Caused by a disturbance or vibration in matter
ELECTRIC AND MAGNETIC FIELDS	Not associated with Electric and Magnetic Field	Associated with Electric and Magnetic Field	Shows minor influence under high Electric and Magnetic Fields
WAVELENGTH	$\lambda = \frac{hc}{E}$	$\lambda = \frac{h}{p}$	$\lambda = \frac{1}{f}$
EXAMPLES	A Beam of Electrons	Radio waves, IR Radiation, UV Radiation, Visible Light etc.	Water waves, sound waves, seismic waves.
REPRESENTATION			 ©L.Perera

Heisenberg Uncertainty Principle

Due to the dual nature of matter, it is a very difficult to locate the exact position and momentum of the particle simultaneously.

The Heisenberg uncertainty principle states **the product of uncertainty is the measurement of the position Δx and uncertainty in measurement of momentum Δp is always constant and it is at least equal to Planck's constant.**

$$\Delta x \cdot \Delta p = \hbar$$

But experimentally it is being proved that,

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

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi^2}$$

Also, we can write,

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2\pi} ; \Delta J \cdot \Delta \theta \geq \frac{\hbar}{2\pi}$$

Where ΔE & Δt determine energy & time respectively and ΔJ & $\Delta \theta$ are uncertainties in measurement of angular momentum and angle respectively.

Schrödinger Wave Equation

- The de-Broglie hypothesis states that a wave is associated with material during its motion.
- It should be very clear that what type of wave is associated with the motion of the particle and what type of mechanics is required for the formulation for such waves.
- Erwin Schrödinger worked extensively on wave mechanics, which used to deal with **the matter wave**.

He gave two very important **equations for motion of matter waves**.

1. **Time Independent Schrödinger Equation**
2. **Time Dependent Schrödinger Equation**

Schrödinger Wave Equation

Wave Function

From the analysis of electromagnetic waves, sound waves and other such waves, it has been observed that the waves are characterized by certain definite properties.

- In case of electromagnetic waves, electric and magnetic field vary periodically. In a similar way, the matter wave varies in a quantity called wave function denoted by Ψ .
- Schrödinger distributed amplitude of matter waves in terms of wave function Ψ . **This wave function $\Psi(x, y, z)$ is a quantity which gives the idea of probability of finding the particle in a particular region of space.**
- The wave function $\Psi(r, t)$ gives the complete knowledge of behaviour of particle and $\Psi(r)$ gives the stationary state which is independent of time.

Well behaved functions

Wave functions with all these properties can yield physically meaningful results when used in calculations, so only such well-behaved wave functions are admissible as the mathematical representation of real bodies. To summarise,

1. Ψ must be continuous and single valued everywhere.
2. $\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}$ must be continuous and single valued everywhere.
3. Ψ must be normalised which means that Ψ must go to 0 as $x \rightarrow \pm\infty, y \rightarrow \pm\infty, z \rightarrow \pm\infty$ in order that $\int |\Psi|^2 dV$ overall space be a finite constant.

Physical Significance of Wave Function

Normalisation

It is usually convenient to have $|\Psi|^2$ be equal to the Probability Density P of finding the particle described by Ψ rather than merely be proportional to P

If,

$$|\Psi|^2 = P$$

Then,

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

A wave function which obeys equation (1) is said to be normalised.

Where $|\Psi|^2 = P = \text{Probability Density}$

This is given as

$$|\Psi|^2 = \Psi^* \Psi \cdot dV$$

The equation becomes

$$\int_{-\infty}^{+\infty} \Psi^* \Psi \cdot dV = 1$$

Where Ψ is the wave function and Ψ^* is the complex conjugate of that wave function.

Note: The Probability that the electron or a particle located somewhere must be unity.

$$P = \int_{x_1}^{x_2} |\Psi_n|^2 dx \quad - (2)$$

Equation shows the probability of finding any particle between x_1 and x_2 in nth state.

Eigen values and Eigen functions

The Schrödinger equations may have many solutions out of these solutions; some are imaginary, which have no significance.

The solutions which have significance for certain value are called the Eigen values. In an atom, Eigen values correspond to the energy values that are associated with different orbitals of atom.

The solution of the wave equation for this definite value of E gives the corresponding value of wave function Ψ known as Eigen functions.

Only these Eigen functions have a physical significance which satisfies following conditions

1. They must be single valued function
2. They should be finite
3. They should be continuous throughout the entire space under consideration.

Time Independent Schrödinger Equation

We know from matter waves that a material particle is equal to or equivalent to a wave packet.

Now, Ψ be the wave displacement for the matter wave at any time t . Ψ is the wave function, which is the finite, single valued and periodic function

This wave function $\Psi(x)$ is represented as,

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

Also, we know the total energy of system

$$E = \text{Kinetic Energy} + \text{Potential Energy}$$

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

$$= \frac{1}{2}mv^2 + U$$

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

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

– (1)

Now in our wave function

$$\Psi(x) = e^{i(kx-\omega t)} \quad - (2)$$

k = wave vector = $\frac{2\pi}{\lambda}$ and ω = angular velocity

Differentiating equation (2) with respect to x

$$\begin{aligned} \frac{d\Psi(x)}{dx} &= ike^{i(kx-\omega t)} \\ \frac{d\Psi(x)}{dx} &= ik\Psi \end{aligned}$$

Again differentiating above equation with respect to x

$$\begin{aligned} \frac{d^2\Psi(x)}{dx^2} &= ike^{i(kx-\omega t)} \cdot ik \\ \frac{d^2\Psi(x)}{dx^2} &= i^2 k^2 e^{i(kx-\omega t)} \\ \frac{d^2\Psi(x)}{dx^2} &= -k^2\Psi \end{aligned} \quad - (3)$$

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

$$\therefore k = \frac{2\pi}{h} \times p$$
$$k = \frac{p}{\hbar}$$

Substituting above value of k in equation (3)

$$\therefore \frac{d^2\Psi(x)}{dx^2} = -\left(\frac{p}{\hbar}\right)^2 \Psi(x)$$
$$\therefore -\hbar^2 \frac{d^2\Psi(x)}{dx^2} = p^2 \Psi(x) \quad - (4)$$

Now from equation (1) is $E = \frac{p^2}{2m} + U,$

Operating both side with $\Psi(x)$

$$\therefore E\Psi(x) = \frac{p^2}{2m}\Psi(x) + U\Psi(x)$$

Substituting equation (4) in above equation

$$\therefore E\Psi(x) = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + U\Psi(x)$$

$$\therefore E\Psi(x) - U\Psi(x) = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2}$$

$$\therefore \frac{2m}{\hbar^2} (E - U)\Psi(x) = -\frac{d^2\Psi(x)}{dx^2}$$

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - U)\Psi(x) = 0$$

This above equation is called **Time Independent Schrödinger Equation** for one dimension

For 3D, Time Independent Schrödinger Equation is given as,

$$\nabla^2 \Psi(\mathbf{r}) + \frac{2m}{\hbar^2} (E - U) \Psi(\mathbf{r}) = 0$$

Where, $\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$ is called as **Laplacian operator**

Time Dependent Schrödinger Equation

The Time Dependent Schrödinger Equation can be obtained by eliminating E from Time Independent Schrödinger Equation

The wave function for particle is given as,

$$\Psi(x, t) = e^{i(kx - \omega t)} \quad - (1)$$

Now, $E = hf$ for particle

$$\begin{aligned} \therefore E &= \frac{h}{2\pi} \times 2\pi f \\ E &= \hbar\omega \end{aligned} \quad - (2)$$

The Energy of a wave particle is given as $\hbar\omega$ while the momentum of the particle is given as $\hbar k$. These are the desired relation.

Differentiating equation (1) with respect to t ,

$$\therefore \frac{d\Psi(x, t)}{dt} = e^{i(kx - \omega t)} \cdot (-i\omega)$$

$$\therefore \frac{d\Psi(x, t)}{dt} = -i\omega\Psi(x, t)$$

Also from equation (2) $E = \hbar\omega$, operating Ψ on both sides

$$\begin{aligned}
 E\Psi(x, t) &= \hbar\omega\Psi(x, t) \\
 -\frac{i}{\hbar}E\Psi(x) &= -i\omega\Psi(x) \\
 \therefore \frac{d\Psi(x, t)}{dt} &= -\frac{i}{\hbar}E\Psi(x, t) \\
 \therefore E\Psi(x, t) &= -\frac{\hbar}{i} \frac{d\Psi(x, t)}{dt} \\
 E\Psi(x, t) &= i\hbar \frac{d\Psi(x, t)}{dt}
 \end{aligned}
 \qquad
 \left[\because \frac{d\Psi(x, t)}{dt} = -i\omega\Psi(x, t) \right]
 \qquad
 - (3)$$

Schrödinger's equation is given as

$$E\Psi(x, t) = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x, t)}{dx^2} + U\Psi(x, t)$$

Substituting equation (3) in above equation

$$i\hbar \frac{d\Psi(x, t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x, t)}{dx^2} + U\Psi(x, t)$$

$$\left[-\frac{\hbar^2}{2m} \frac{d^2\Psi(x, t)}{dx^2} + U \right] \Psi(x, t) = i\hbar \frac{d\Psi(x, t)}{dt} \quad - (4)$$

This equation (4) is called **Time Dependent Schrödinger Equation** for one dimension

For 3D,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U \right] \Psi(r, t) = i\hbar \frac{d\Psi(r, t)}{dt}$$

In above equation is $\left[-\frac{\hbar^2}{2m} \nabla^2 + U \right]$ called **Hamiltonian Operator (H)** denoted by H whereas $E\Psi(x, t) = i\hbar \frac{d\Psi(x, t)}{dt}$ Which operates on $\Psi(x, t)$ is called **Energy Operator (E)**

Thus we can write equation (4) as,

$$H\Psi(x, t) = E\Psi(x, t)$$

Momentum operator

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

$$\therefore \frac{d\Psi(x)}{dx} = ik\Psi(x)$$

We know, $p = \hbar k$, $k = \frac{p}{\hbar}$

$$\frac{d\Psi(x)}{dx} = i \frac{p}{\hbar} \Psi(x)$$

$$\frac{\hbar}{i} \frac{d\Psi(x)}{dx} = p\Psi(x)$$

$$p\Psi(x) = -i\hbar \frac{d\Psi(x)}{dx}$$

The above equation represents momentum operator which operates $\Psi(x)$ on for 1D.

For 3D, momentum operator is given by $\hat{p} = -i\hbar \nabla$

Particle in One Dimensional Potential Box

Consider a free particle of mass ' m ' placed inside a one-dimensional box of infinite height and width a .

The motion of the particle is restricted by the walls of the box. The particle is bouncing back and forth between the walls of the box at $x = 0$ and $x = a$.

Since the potential energy of particle at the bottom of the potential well is very low, moving particle energy is assumed to be zero between $x = 0$ and $x = a$.

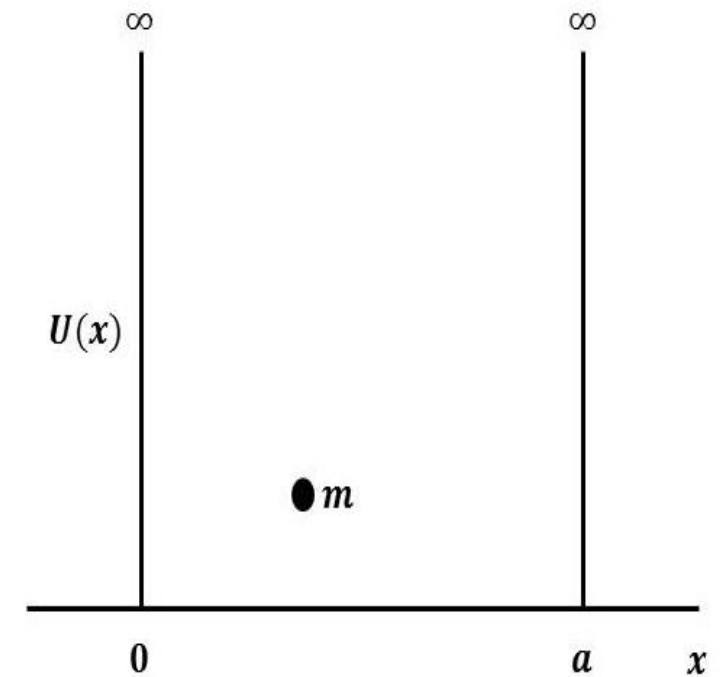


Fig.4: One-dimensional box
(Infinite Potential Well)

The P.E. of the particle outside the walls is infinite.

The particle cannot escape from the box when,

1. $U = 0$ for $0 < x < a$
2. $U = \infty$ for $0 \geq x \geq a$

Since the particle cannot be present outside the box, its wave function is zero.

i.e., $|\Psi|^2 = 0$ for $0 > x > a$
 $|\Psi|^2 = 0$ for $x = 0$ and $x = a$

The Schrödinger one – dimensional time independent equation is

$$\nabla^2 \Psi(x) + \frac{2m}{\hbar^2} (E - U(x)) \Psi(x) = 0 \quad - (1)$$

For freely moving particle $U(x) = 0$

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

Taking,

$$\frac{2mE}{\hbar^2} = k^2 \quad - (3)$$

Equation (1) becomes

$$\frac{d^2 \Psi(x)}{dx^2} + k^2 \Psi(x) = 0 \quad - (4)$$

Equation (1) is similar to eq. of harmonic motion and the solution of above Equation is written as

$$\Psi(x) = A \sin kx + B \cos kx \quad - (5)$$

where A, B and k are unknown quantities and to calculate them it is necessary to construct boundary conditions.

Hence boundary conditions are

When $x = 0$, $\Psi = 0$. Hence, from equation (5),

$$\begin{aligned} 0 &= 0 + B \\ \Rightarrow B &= 0 \end{aligned} \quad - (6)$$

When $x = a$, $\Psi = 0$. Hence, from equation (5),

$$A \sin ka + B \cos ka = 0 \quad - (7)$$

But from equation (6), $B = 0$ therefore equation (7) may turn as

$$A \sin ka = 0$$

Since the electron is present in the box, $A \neq 0$

$$\therefore \sin ka = 0$$

$$\begin{aligned} \therefore ka &= n\pi \\ \therefore k &= \frac{n\pi}{a} \end{aligned}$$

Substituting the value of k in Equation (3)

$$\begin{aligned}\frac{2mE}{\hbar^2} &= \left(\frac{n\pi}{a}\right)^2 \\ E &= \left(\frac{n\pi}{a}\right)^2 \cdot \frac{\hbar^2}{2m} \\ &= \left(\frac{n\pi}{a}\right)^2 \cdot \frac{h^2}{8m\pi^2} \\ \therefore E &= \frac{n^2 h^2}{8ma^2}\end{aligned}$$

Thus, In general the above equation is given as,

$$\therefore E_n = \frac{n^2 h^2}{8ma^2} \tag{9}$$

Eq. (9) represents an energy level for each value of n .

The Wave Equation can be written as

$$\Psi(x) = A \sin\left(\frac{n\pi x}{a}\right) \tag{10}$$

Let us find the value of A, if an electron is definitely present inside the box, then

$$\begin{aligned}P &= \int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = 1 \\ \int_0^a A^2 \sin^2 \left(\frac{n\pi x}{a} \right) dx &= 1 \\ \int_0^a \sin^2 \left(\frac{n\pi x}{a} \right) dx &= \frac{1}{A^2} \\ \int_0^a \frac{1 - \cos \left(\frac{2n\pi x}{a} \right)}{2} dx &= \frac{1}{A^2} \\ A &= \sqrt{\frac{2}{a}}\end{aligned}\tag{11}$$

From equation (10) & (11)

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad - (12)$$

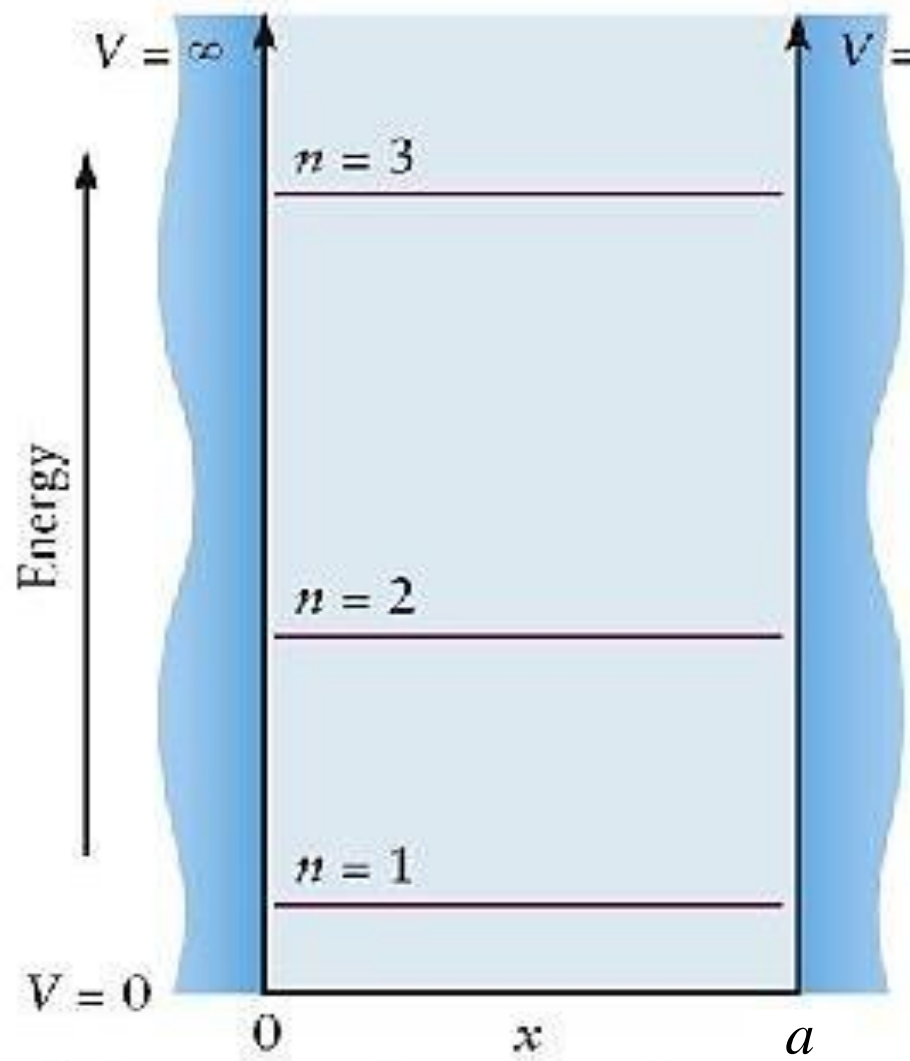
The wave function in n^{th} energy level is given in Equation (12).

Therefore the particle in the box can have discrete values of energies. These values are quantized. Not that the particle cannot have zero energy .

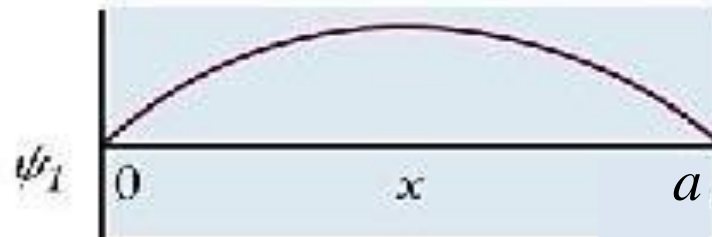
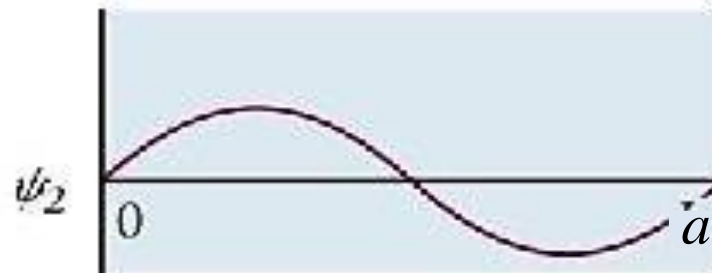
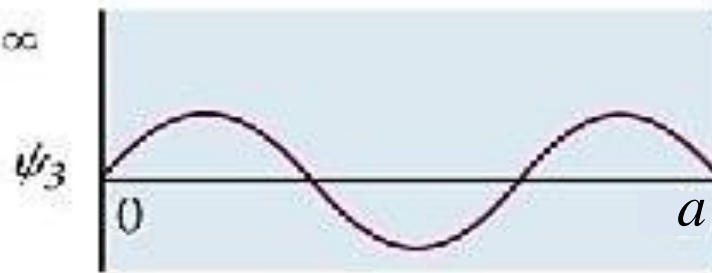
The normalized wave functions Ψ_1, Ψ_2, Ψ_3 given by equation (12).

The values corresponding to each E_n value is known as **Eigen value** and the corresponding wave function is known as **Eigen function**.

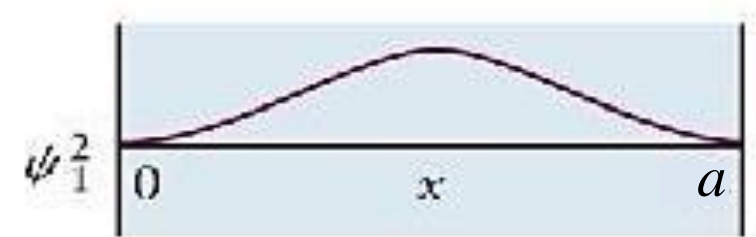
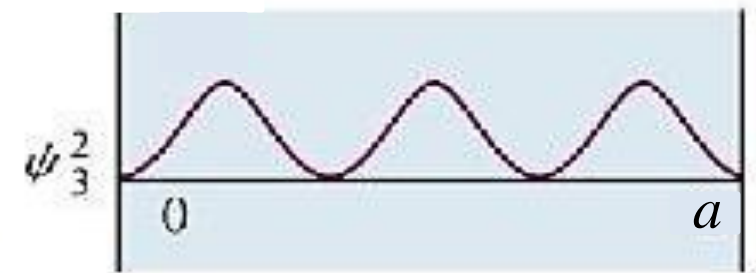
- The wave function Ψ_1 has two nodes at $x = 0$ and $x = a$
- The wave function Ψ_2 has three nodes at $x = 0, x = a/2$ and $x = a$
- The wave function Ψ_3 has four nodes at $x = 0, x = a/2, x = 2a/3$ and $x = a$
- **The wave function Ψ_n has $(n + 1)$ nodes with Boundary Conditions**
- **The wave function Ψ_n has $(n - 1)$ nodes without Boundary Conditions**



(a) Energy levels



(b) Wave functions



(c) Probabilities

Substituting the value of $E = \frac{p^2}{2m}$ in equation (3), we get

$$\left(\frac{2m}{\hbar^2}\right) \cdot \left(\frac{p^2}{2m}\right) = k^2$$

$$\left(\frac{p^2}{\hbar^2}\right) = k^2$$

$$k = \left(\frac{p}{\hbar}\right) = \frac{p}{\frac{h}{2\pi}} = \left(\frac{2p\pi}{h}\right)$$

$$k = \left(\frac{2\pi}{\lambda}\right)$$

where k is known as wave vector.

Tunneling Effects

Scattering from a Potential Barrier in One Dimension

Suppose that the height of the potential barrier is V_0 and the width is L and that scattering particles have energy $E < V_0$. Then the picture can be divided into three regions:

Region 1: $(-\infty < x < 0): E > V(x)$

Region 2: $(0 < x < L): E < V(x)$

Region 3: $(L < x < \infty): E > V(x)$

Where,

$$V(x) = 0; x < 0$$

$$V(x) = V_0; x = 0, 0 < x < L, x = L \text{ and}$$

$$V(x) = 0, x > L$$

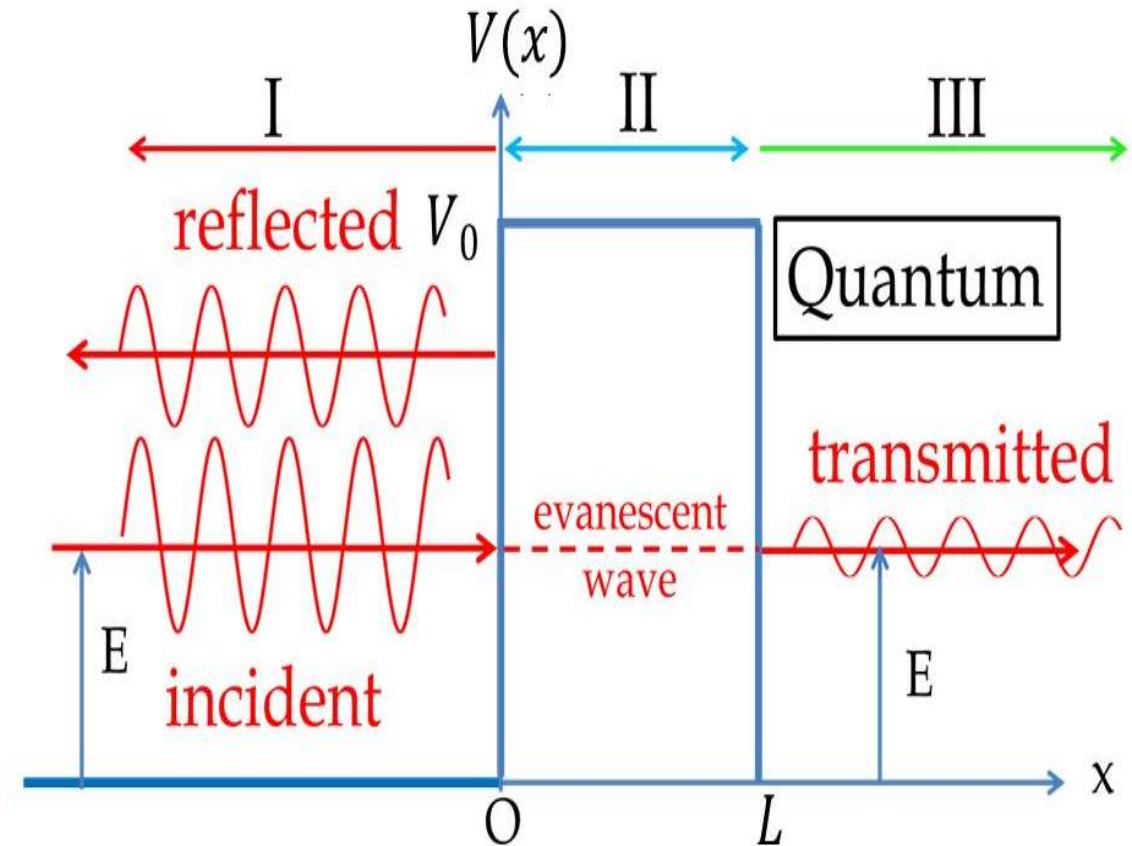
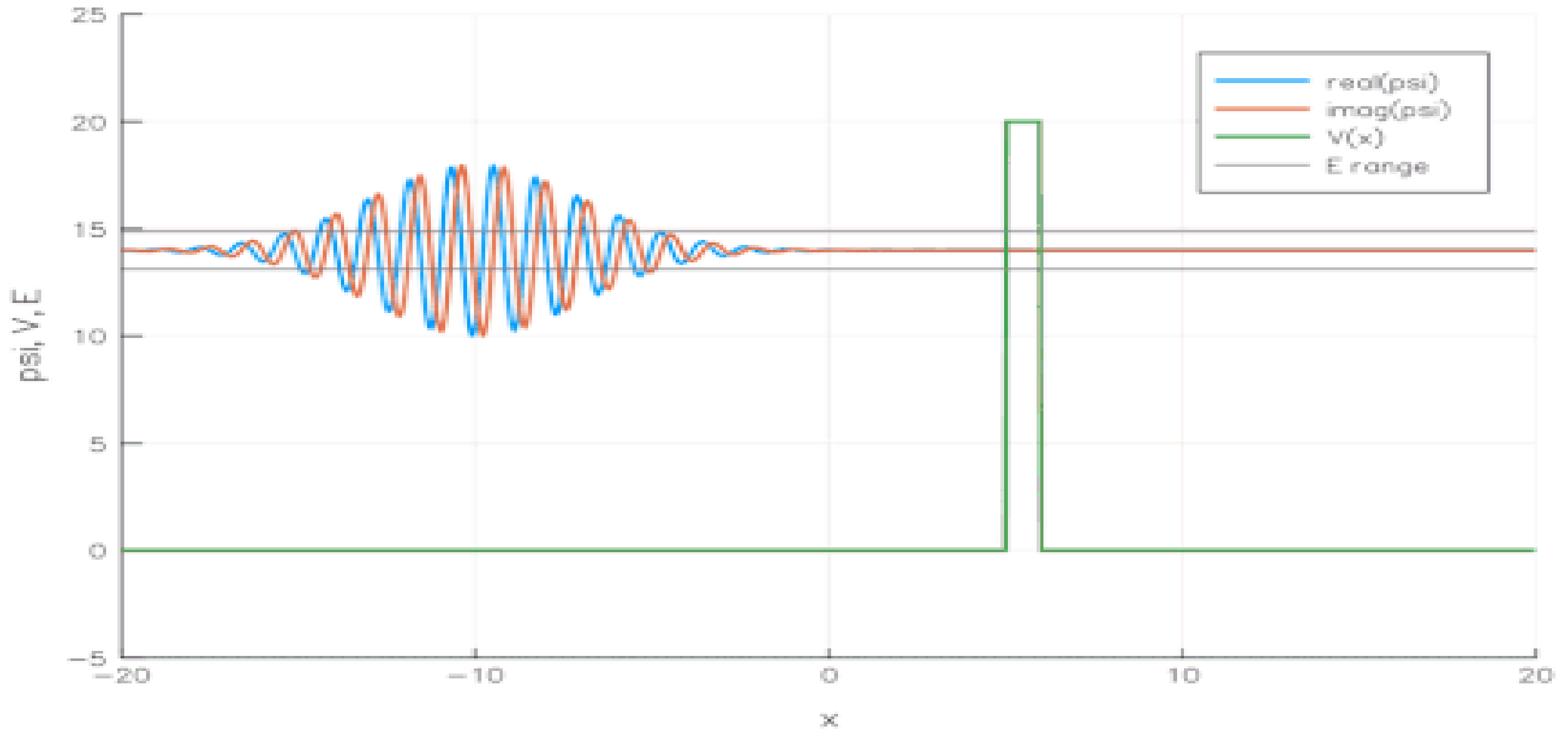


Fig.5: Quantum Tunneling

Tunneling



In *Region 1*, the potential is zero. A moving wave thus has energy greater than the potential. This is also true in *Region 3*. However, in *Region 2*, the energy of the wave is less than the potential.

Therefore, the Schrödinger equation yields two different differential equations depending on the region:

Region 1 and Region 3:

$$\frac{d^2\Psi}{dx^2} = \alpha^2\Psi, \quad \alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

Region 2:

$$\frac{d^2\Psi}{dx^2} = \beta^2\Psi, \quad \beta = \sqrt{\frac{2m(V - E)}{\hbar^2}}$$

The general solutions can be written as linear combinations of oscillatory terms in *Region 1 and Region 3*, and as linear combinations of growing and decaying exponentials in *Region 2*:

$$\Psi(x) = \begin{cases} Ae^{i\alpha x} + Be^{-i\alpha x} & : \text{Region 1} \\ Ce^{i\beta x} + De^{-i\beta x} & : \text{Region 2} \\ Fe^{i\alpha x} & : \text{Region 3} \end{cases}$$

The plane waves that travel to the right are of the form $e^{i\alpha x}$ and plane waves that travel to the left are of the form $e^{-i\alpha x}$. A particle (plane-wave) enters from the left and will partially transmit and partially reflect. However, no particle enters from the right heading towards the left; therefore, there is no $Ge^{-i\alpha x}$ term above in *Region 3*.

The coefficients above are fixed by the continuity of the wave function and its derivative at each point where the potential changes. One obtains two conditions from continuity at $x = 0$ and $x = L$

$$A + B = C + D \quad \text{--- (1)}$$

$$Ce^{\beta L} + De^{-\beta L} = Fe^{i\alpha L} \quad \text{--- (2)}$$

And two conditions from continuity of the derivative at $x = 0$ and $x = L$

$$Ai\alpha - Bi\alpha = C\beta - D\beta \quad - (3)$$

$$C\beta e^{\beta L} + D\beta e^{-\beta L} = Fi\alpha e^{i\alpha L} \quad - (4)$$

Dividing (3) by $i\alpha$ and adding to (1) obtains

$$2A = \left(1 + \frac{\beta}{i\alpha}\right)C + \left(1 - \frac{\beta}{i\alpha}\right)D \quad - (5)$$

Similarly, dividing (4) by β and adding or subtracting from (2) obtains

$$2Ce^{\beta L} = \left(1 + \frac{i\alpha}{\beta}\right)Fe^{i\alpha L} \quad - (6)$$

$$2De^{\beta L} = \left(1 - \frac{i\alpha}{\beta}\right)Fe^{i\alpha L} \quad - (7)$$

Combining (5), (6), and (7) yields an equation for A in terms of F :

$$2A = \left(1 + \frac{\beta}{i\alpha}\right) \left(1 + \frac{i\alpha}{\beta}\right) \frac{F e^{i\alpha L} e^{-\beta L}}{2} + \left(1 - \frac{\beta}{i\alpha}\right) \left(1 - \frac{i\alpha}{\beta}\right) \frac{F e^{i\alpha L} e^{\beta L}}{2}$$

Which can be rearranged to,

$$\frac{A e^{-i\alpha L}}{F} = \cosh(\beta L) + i \left(\frac{\beta^2 - \alpha^2}{2\alpha\beta} \right) \sinh(\beta L)$$

Now the probability of a wave to tunnel through the barrier is equal to the probability of the wave function in *Region 3* divided by the probability of the wave function in *Region 1*.

Multiplying the above equation by its conjugate and taking the inverse, the probability of transmission is therefore quantified by

$$T = \frac{|F|^2}{|A|^2} = \cosh^2(\beta L) + i \left(\frac{\beta^2 - \alpha^2}{2\alpha\beta} \right) \sinh^2(\beta L)$$

Since $\cosh^2(x) - \sinh^2(x) = 1$,

$$T = \left[1 + \left(\frac{\beta^2 + \alpha^2}{2\alpha\beta} \right) \sinh^2(\beta L) \right]^{-1}$$

Defining $\gamma = \left(\frac{\beta^2 - \alpha^2}{2\alpha\beta} \right)$ makes the solution more compact

$$T = \frac{1}{1 + \gamma^2 \sinh^2(\beta L)}$$

This can also be rewritten in terms of the energies:

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left(\frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \right]^{-1}$$

Naturally, the probability of reflection is $1 - T$; hence,

$$R = \frac{\gamma^2 \sinh^2(\beta L)}{1 + \gamma^2 \sinh^2(\beta L)}$$

Macroscopically, objects colliding against a wall will be deflected. This is analogous to the reflection probability being 100% and transmission probability being 0%. The above example shows that it is possible for matter waves to "go through walls" with some probability, given that a matter wave has sufficient energy or the barrier being sufficiently narrow (small L).

Note that, for a very wide or tall barrier (L very large) or $E \ll V_0$, the \sinh term in the expression for T goes to ∞ , yielding $T \approx 0$: for a very wide or tall barrier, there is almost no transmission.

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