Schrodinger's Wave Equation

Dr. Prasanta Ghosh

School of Physics, MIT-WPU Pune

WAVE FUNCTION AND PROBABILITV INTERPRETATION

Waves represent the Propagation of a Disturbance in a medium.

We are familiar with light waves, sound waves, and water waves, These waves are characterized by some quantity that varies with position and time.

We can’t specify in similar way what is actually varying in De Broglie waves, since microparticles exhibit wave properties.

It’s assumed that a quantity Ψ represents a De Broglie Wave, This quantity Ψ is called a wavefunction. Ψ describes the wave as a function of position and time. Ψ is a complex-valued function.

According to Heisenberg uncertainty principle, we can only know the probable value in a measurement. The probability cannot be negative.

Hence Ψ cannot be a measure of the presence of the particle at the location (x,y,z). But it is certain that it is in someway an index of the presence of the particle at around **(x,y,z,t).**

Probability Interpretation of Wave Function given by Max Born

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.* In other words,

Probability, P, of finding the particle in an infinitesimal volume dV (= $dx\ dy\ dz$) is proportional to $|\psi(x, y, z)|^2\ dx\ dy\ dz$ at time t.

or
$$P \propto |\psi(x,y,z)|^2\ dV$$

$|\psi|^2$ is called the **probability density** and ψ is the **probability amplitude**.

Now, as De Broglie waves are probability waves, and as $|\psi|^2$ represents the probability density, we have

$|\psi|^2$ = Probability of finding the particle per unit length (for 1D De Broglie wave) or per unit volume (for 3D De Broglie wave)

Thus,

$|\psi|^2 dx$ = Probability of finding the particle in a region having length dx

$\int_{-x_1}^{+x_2} |\psi|^2 dx$ = Probability of finding the particle in a region in the De Broglie wave between x_1 and x_2

$\int_{-\infty}^{+\infty} |\psi|^2 dx$ =Total probability of finding the particle in the entire space =1

(This is because, a real particle must exist somewhere in the entire space). Also as $|\psi|^2$ signifies probability density, we expect

$$\int_{-\infty}^{+\infty} |\psi|^2 dx \neq 0 \quad \text{and} \quad \int_{-\infty}^{+\infty} |\psi|^2 dx \neq \infty$$

Since the particle is certainly to be found somewhere in space, we must have,

$$\iiint |\psi|^2 \, dx \, dy \, dz = 1 \qquad \dots (1)$$

the triple integral extending over all possible values of x, y, z.

A function ψ satisfying this relation is called a '***normalised wave function***' and equation (1) is known as the '***normalisation condition***'. Thus, ψ has to be a normalisable function.

Besides being normalisable, ψ must also satisfy the following conditions:

- ψ must be a single valued function, because ψ is related to the probability of finding the particle at a given place and time, and the probability can have only one value at a given point and time.

- ψ must be finite, because the particle exists somewhere in space, and so integral over all space must be finite.

- ψ and its derivatives $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ must be continuous everywhere in the region where ψ is defined.

Schroedinger started with De Broglie's idea of matter waves and developed it into a mathematical theory known as ***'wave mechanics'***. Schroedinger's wave equation is the mathematical representation of matter waves associated with a moving particle. There are two types of Schroedinger's wave equations:

- Schroedinger's time independent wave equation
- Schroedinger's time dependent wave equation.

Schrodinger's Time Independent (steady state) Equation

- According to the De Broglie's theory a particle of **mass m** moving with **velocity v** has a wave system of **wavelength $\lambda = h/mv$.**
- **Ψ is the quantity** which vibrates to produce the matter wave.

- **Consider a system of stationary waves associated with a particle. X, Y, Z are the coordinates of the particle and Ψ denote the wave displacement of matter waves at time t.**
- By using the wave equation for the three dimensional wave with the wave velocity we can form the Schrodinger's Time Independent Equation

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

Kinetic Energy **Potential Energy** **Total Energy**

Schrodinger's Time Dependent (steady state) Equation

- **Consider a system of stationary waves associated with a particle. X, Y, Z are the coordinates of the particle and Ψ denote the wave displacement of matter waves at time t.**
- By eliminating E from Schrodinger's Time Independent Equation we can get the Schrodinger's Time Dependent Equation
- By using the wave equation for the three dimensional wave with the wave velocity we can form the Schrodinger's Time Dependent Equation

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

Applications of Schrodinger's Time Independent Wave Equation

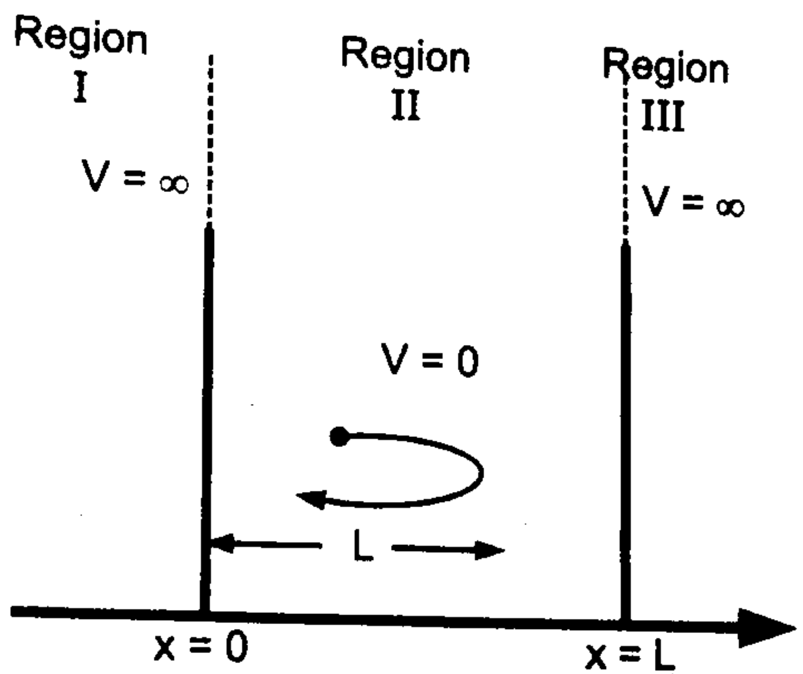
- **PARTICLE IN A RIGID BOX (INFINITE POTENTIAL WELL)**
- **PARTICLE IN A NON-RIGID BOX (FINITE POTENTIAL WELL)**
- **TUNNEL EFFECT**

Applications of Schrodinger’s Time Independent Wave Equation : PARTICLE IN A RIGID BOX

- Considering just a one-dimensional box of length L. In this case particle confined between infinitely high walls and particle cannot have infinitely high potential energy behind the walls.

- The potential energy V

$$
\boxed{V = \begin{cases} \infty & x < 0 \\ 0 & 0 \le x \le L \\ \infty & x > L \end{cases}}
$$



PARTICLE IN A RIGID BOX

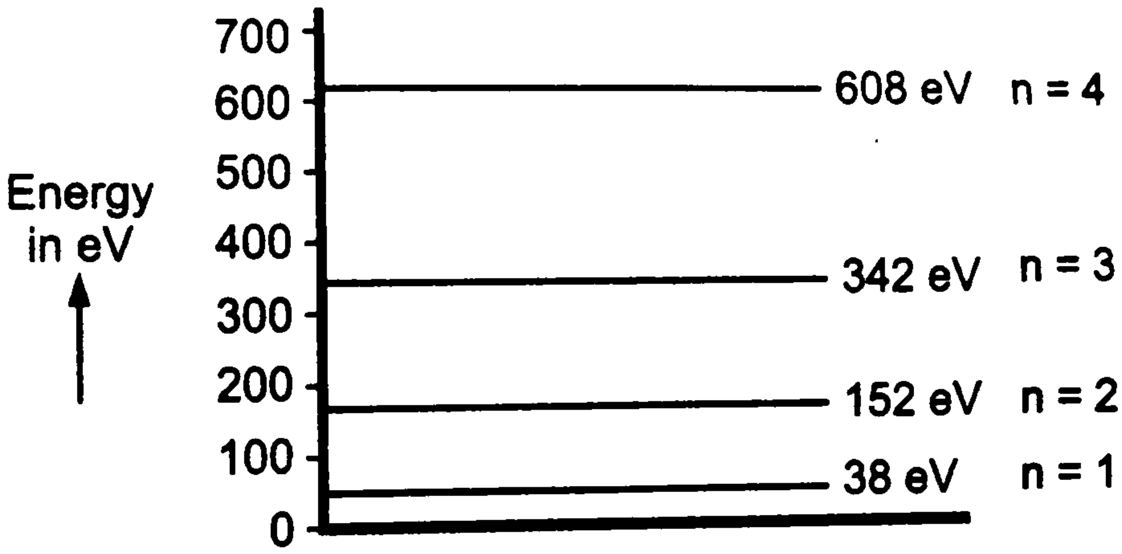
- We will use the Schrodinger's time independent wave equation to solve the case.

- There are many (discrete) values of Energy which will satisfy the boundary conditions. Quantization of energy has therefore arisen in a natural way

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

PARTICLE IN A RIGID BOX

- Energy level of an electron trapped in a potential well of width 1 A°



$$E_n = 6 \times 10^{-18}\, n^2 \text{ joules}$$

$$= \frac{6 \times 10^{-18}}{1.6 \times 10^{-19}}\, n^2 \text{ eV}$$

$$\cong 38\, n^2 \text{ eV}$$

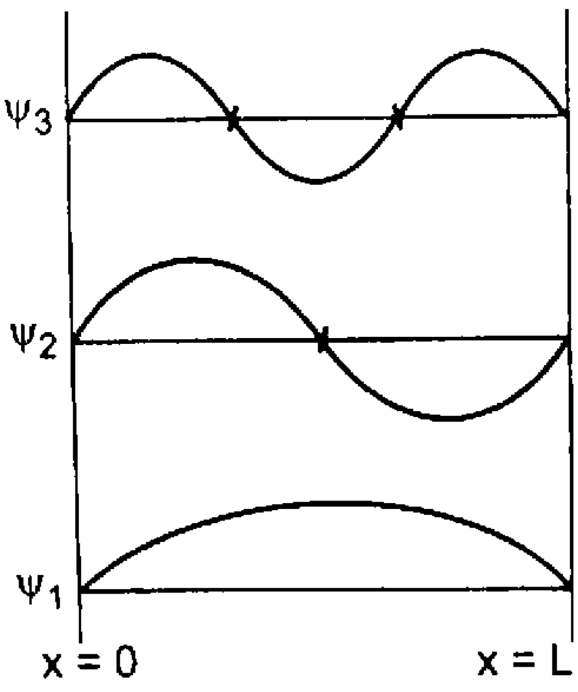
Wave Function of PARTICLE IN A RIGID BOX

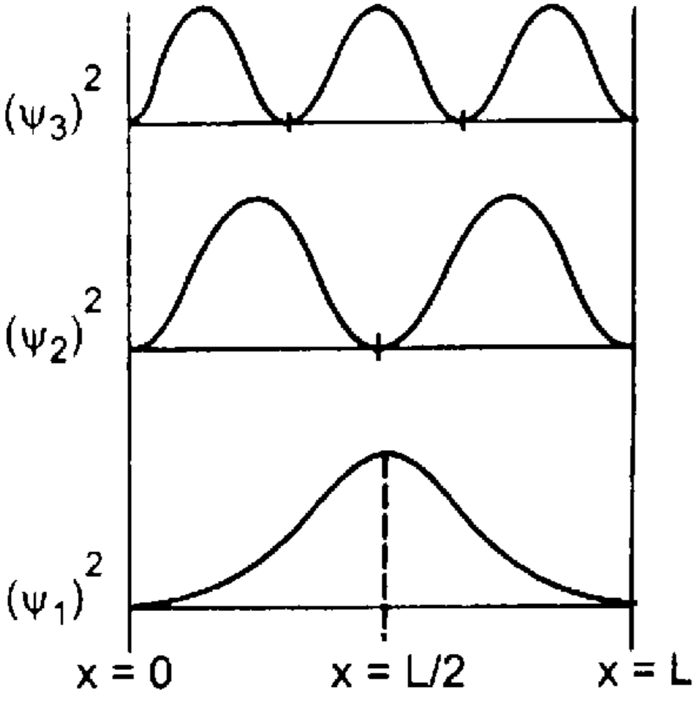
- The normalized wave functions for the particle in a one-dimensional box of length L

$$\boxed{\psi_n = \frac{2i}{\sqrt{2L}} \sin \frac{n\pi}{L} x = i\sqrt{\frac{2}{L}} \cdot \sin \cdot \frac{n\pi}{L} x}$$

Wave Function of PARTICLE IN A RIGID BOX

- Three wave functions and the correspond probability densities for a quantum particle in a box.



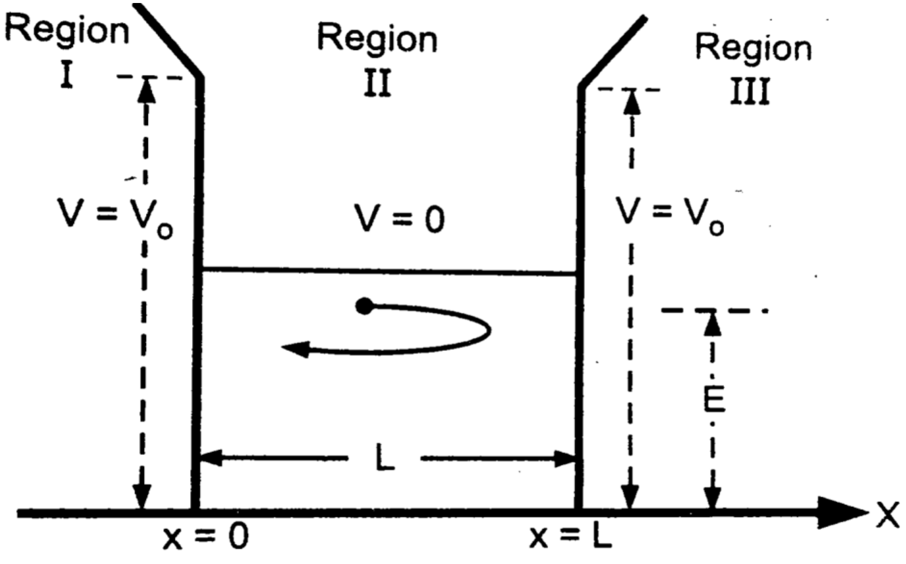


PARTICLE IN A NON-RIGID BOX

- Considering just a non-rigid box of length L. In this case the walls of the square well are infinitely thick, but of finite height.

- The potential energy V

$$= \begin{cases} V & x < 0 & \text{region I} \\ 0 & 0 \leq x \leq L & \text{region II} \\ V & x > L & \text{region III} \end{cases}$$



PARTICLE IN A NON-RIGID BOX

- We will use the Schrodinger's time independent wave equation to find wave function of the particle inside and on the two side of the box .

$$\psi_{I}(0) = \psi_{II}(0)$$

$$A = P + Q$$

$$\psi_{II}(L) = \psi_{III}(L)$$

$$P e^{ikL} + Q e^{-ikL} = D e^{-k'L}$$

$$\left|\frac{\partial \psi_{I}}{\partial x}\right|_{x=0} = \left|\frac{\partial \psi_{II}}{\partial x}\right|_{x=0}$$

$$Ak' = iPk - iQk$$

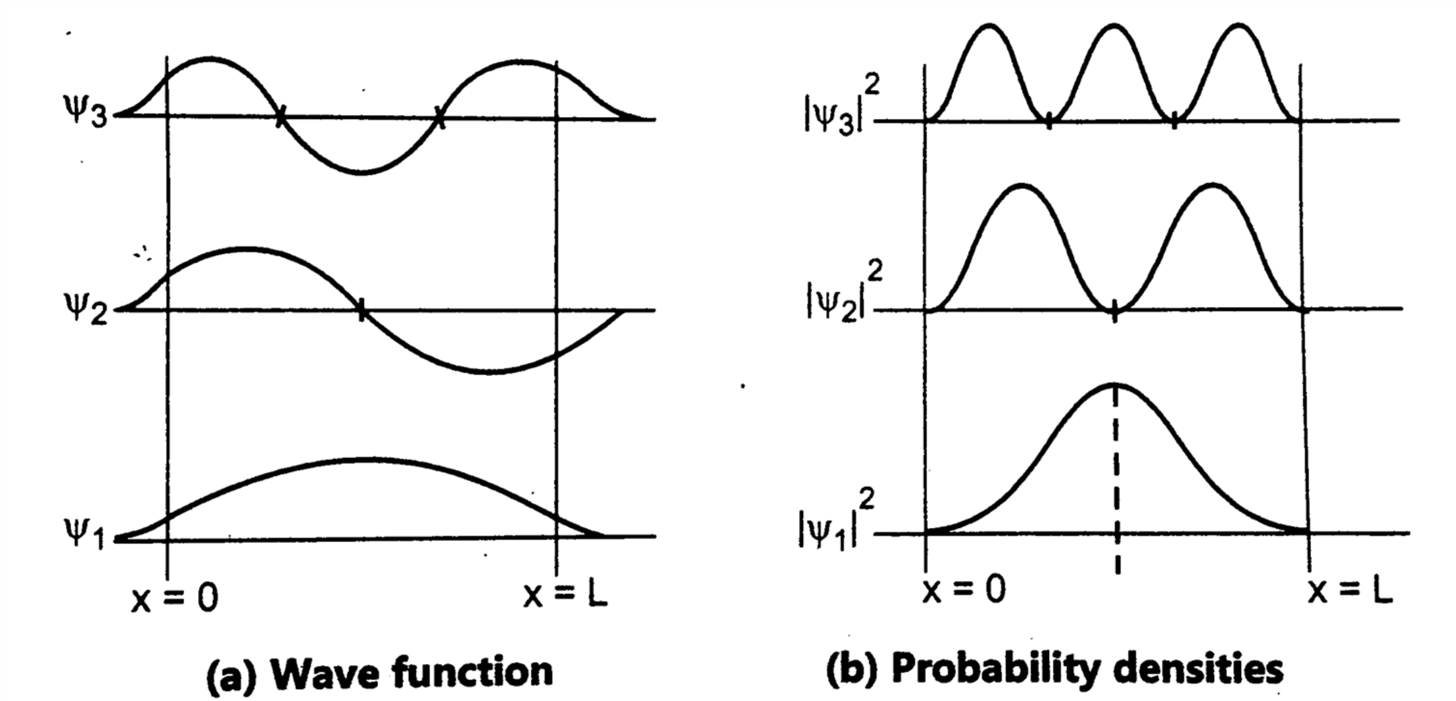
$$\left|\frac{\partial \psi_{II}}{\partial x}\right|_{x=L} = \left|\frac{\partial \psi_{III}}{\partial x}\right|_{x=L}$$

$$Pike^{ikL} - Qike^{-ikL} = -Dk'e^{-k'L}$$

obtained by using the property of the wave function that ψ and $\frac{\partial \psi}{\partial x}$ must be continuous everywhere in the region where ψ is defined.

PARTICLE IN A NON-RIGID BOX

- wave function and corresponding probability density.



PARTICLE IN A NON-RIGID BOX

- Energy level of a particle in a rigid box and non-rigid box.