MODULE 7: SOLUTION OF WAVE EQUATION

❖ Particle in one-dimension Box

To study the quantum mechanical behaviour of particle in one-dimension Box (Figure 1), we will use the time-independent Schrödinger equation. For this, we can write the potential of particle in one dimension Box as

\[ V(x) = 0 \quad \text{for} \quad 0 < x < a \]

and \[ V(x) = \infty, \quad \text{otherwise.} \]

Figure 1

Time independent Schrödinger equation is given as:

\[ H\psi = E\psi. \]

For region \( x < 0 \) and \( x > a \), the probability to find the particle in that region is zero, since the potential is infinity.

Therefore, we will consider the Schrödinger equation in the region \( 0 < x < a \)

\[ H\psi = E\psi \]

or \[ \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi \]

or \[ \frac{\partial^2 \psi}{\partial x^2} + \frac{2mE\psi}{\hbar^2} = 0 \]

or \[ \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{(where} \quad k = \frac{\sqrt{2mE}}{\hbar} \text{)} \]

(1).

The solution of equation (1) can be written as:

\[ \psi(x) = A \sin kx + B \cos kx \]

(2).

Now, from the property of wave-function, it must be continuous at the boundary. Therefore, from equation (2), \( \psi(0) = \psi(a) = 0 \). Substituting \( x = 0 \) in equation (2), we get \( \psi(0) = A \sin 0 + B \cos 0 = B \). So, it gives \( \psi(x) = A \sin kx \)

(3).

Similarly, substituting \( x = a \) in equation (3), we get:

\[ \psi(a) = A \sin kx = 0 \]

This gives

\[ ka = n\pi \quad \text{where} \quad n = 0,1,2,3,..... \]

(4).

But for \( n = 0 \), \( \psi(n) = 0 \) for any value of \( x \), so we will consider \( n = 1,2,3,..... \)

Therefore, substituting \( k = \frac{\sqrt{2mE}}{\hbar} \) in equation (4), we get

\[ \frac{\sqrt{2mE}}{\hbar} a = n\pi \]

or \( E = E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{where} \quad n = 1,2,3,..... \)

(5).
$E_n$ represents the discrete energy eigen value of the particle moving in one dimension Box.

Substituting $k = \frac{\sqrt{2mE}}{\hbar}$ in equation (3), we get $\psi(x) = \phi_n(x) = A \sin \frac{n\pi x}{a}$ \hspace{1cm} (6).

The value of `$a$' can be found by normalization condition, which is

\[
\int_0^a \left[\phi_n(x)\right]^2 dx = 1
\]

or

\[
A^2 \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1
\]

or

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

or

\[
\frac{A^2}{2} a = 1
\]

or

\[
A = \sqrt{\frac{2}{a}}.
\]

Hence, substituting `A` in equation (6), the wave-function of the particle is given by

\[
\phi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{where } n = 1, 2, 3, \ldots \hspace{1cm} (7).
\]

Figure 2 above represents the variation of wave-function with position $x$ for particle in the Box. Hence, from equation (5) and (7), we get the expression of energy and wave-function of the particle moving inside the one dimension Box.