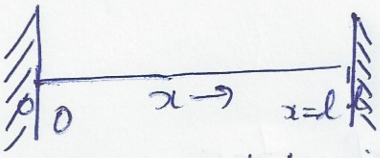
Particle in a 1D-box:

Objective: To describe the motion of a particle along a certain interval (in one-dimension). say, l.



Constraints: (i) The particle is allowed to move only within this interval

(ii) No external force acts on the particle (so its potential energy remains constant).

We started with this equation:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \qquad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

$m \Rightarrow$ mass of particle , E = energy (may be assumed to be purely kinetic energy)

$\hbar = \frac{h}{2\pi} \longrightarrow$ Plank's constant (6.62×10^{-34} Js)

$\psi(x) \Rightarrow$ Wave function of the particle or Probability Amplitude.

$\psi(x)\,\psi^*(x) \Rightarrow$ Probability density.

$$|\psi(x)|^2 \neq \psi(x)\,\psi(x)$$

How do we get to this equation?

$\Rightarrow$ Mainly inspired by de Broglie's idea (Matter has wave like properties)

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

$p \rightarrow$ momentum (particle aspect)

$\lambda \rightarrow$ wavelength (wave aspect)

$\Rightarrow$ Schrödinger started with the 1D-wave equation

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 u(x,t)}{\partial t^2}$$

$u(x,t) \Rightarrow$ Amplitude of the wave

$v \Rightarrow$ velocity of its propagation

(we can replace $u(x,t)$ with $\psi(x,t)$)

Schrödinger made one interesting assumption

$$\psi(x,t) = \psi(x) . \cos\omega t$$ (Product of two functions).

x, t are independent variables

x → displacement, t → time

$\psi(x,t)$ is a dependent function.

Questions to be asked ?

1. Was this done for simplification ?
2. Was this done to show some interference effects. ?
3. was it accidental ?

By the way, $\psi(x,t) = \psi(x)\cos\omega t$ represents a standing wave.

Standing wave = superposition of travelling waves.

Let us now start the derivation.

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \psi(x,t)}{\partial t^2} \quad \text{— (1)}$$

Partial differential equation.

If $\psi(x,t) = \psi(x)\cos\omega t$

$$\frac{\partial}{\partial x}\psi(x,t) = \frac{\partial \psi(x)}{\partial x}\cos\omega t$$

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\psi(x,t)\right) = \frac{\partial^2}{\partial x^2}\psi(x)\cos\omega t = \frac{d^2\psi(x)}{dx^2}\cos\omega t \quad \text{— (2)}$$

Likewise $\frac{\partial}{\partial t}\psi(x,t) = \psi(x)(-\sin\omega t).\omega$

$$\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t}\psi(x,t)\right) = \psi(x)(\cos\omega t)(-\omega^2)$$

$$\frac{\partial^2 \psi(x,t)}{\partial t^2} = \psi(x)\cos\omega t\,(-\omega^2) \quad \text{— (3)}$$

Using the expressions (Eqns (2) & (3)) in Eq.(1)

$$\frac{d^2\psi(x)}{dx^2}\cancel{\cos\omega t} = -\frac{\omega^2}{v^2}\cancel{\cos\omega t}\,\psi(x)$$

Using the following relations

$\omega = 2\pi\nu \rightarrow$ frequency

Angular frequency

$v = \nu\lambda$ $\quad$ $\lambda = \frac{h}{p}$

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

$$\frac{\omega^2}{v^2} = \frac{4\pi^2\cancel{\nu^2}}{\cancel{\nu^2}\lambda^2} = \frac{4\pi^2}{\lambda^2}$$

or $\quad p^2 = 2m(E - V(x))$

or $\quad$ if $V(x) = 0 \Rightarrow p^2 = 2mE$

So $\quad \frac{\omega^2}{v^2} = \frac{4\pi^2}{h^2}\cdot p^2 = \frac{4\pi^2}{h^2}\cdot 2m(E - V(x))$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{4\pi^2}{h^2}\cdot 2mE\;\psi(x)$$

or

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \underbrace{\frac{2mE}{\hbar^2}}_{\rightarrow k^2}\cdot\psi(x) = 0}$$

This is nothing but the equation that we started with

$$\boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0} \quad \text{—— (4)}$$

Let us try to reexpress this equation.

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}\cdot(E - V(x))\,\psi(x)$$

or

$$\boxed{-\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2}\cdot\psi(x) + V(x)\,\psi(x) = E\,\psi(x)} \quad \text{—— (5)}$$

When $V(x) = 0$, Eq. (5) reduces to a much simpler form

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x). \quad \text{—— (6)}$$

⇓ This is nothing but an eigen value equation.

$$\hat{A}\,\psi = a\,\psi.$$

$\hat{A}$ → Operator

ψ → function → (This function is often known as 'Eigen function')

a → constant (This constant is often known as 'Eigen value')

'ψ' is the eigen function of the operator, $\hat{A}$.
'a' is the eigenvalue associated with ψ.

In its more general formulation, Eq (7) may be expressed as follows.

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

or

$$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]}_{\hat{A}\ \text{(operator)}}\psi(x) = \underbrace{E}_{\text{Energy eigenvalue}}\,\psi(x). \quad \text{— (7)}$$

This special operator is called the 'Hamiltonian' operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

The energy, E comprises the kinetic and potential energy.