Application of Schrödinger Equation - 1
Steady state Schrödinger Equation & Particle in a box

Steady state form of Schrödinger Equation

$$\hat{E} = \frac{\hat{P}^2}{2m}$$

We can obtain Schrödinger Equation by substituting $\hat{P}$ and $\hat{E}$.

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

$$\hat{P} = -i\hbar\frac{\partial}{\partial x}$$

The corresponding wave function is $\Psi = A\, e^{-i/\hbar(Et-Px)}$--------- (1)

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

Equ (1) is splitting to time and space parts.

(1) $\Longrightarrow \Psi = A\, e^{-\frac{i}{\hbar}Et} \times e^{\frac{i}{\hbar}Px}$

Put $\Psi_0 = A\, e^{\frac{i}{\hbar}Px}$

$$\Psi = \Psi_0 e^{-\frac{i}{\hbar}Et}$$

Substituting in Schrodinger Equation.

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

$$\frac{\partial\Psi}{\partial t} = \Psi_0 \times \frac{\partial}{\partial t}\left(e^{-\frac{i}{\hbar}Et}\right)$$

$$= \Psi_0 \times \frac{-iE}{\hbar} \times e^{-\frac{i}{\hbar}Et} \text{ ---------- (2)}$$

$$\frac{\partial\Psi}{\partial x} = e^{-\frac{i}{\hbar}Et} \times \frac{\partial\Psi_0}{\partial x}$$

$$\frac{\partial\Psi^2}{\partial x^2} = e^{-\frac{i}{\hbar}Et} \times \frac{\partial\Psi_0{}^2}{\partial x^2} \text{ ----------- (3)}$$

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

Substituting (2) and (3) in above equation. We get

$$E\,\Psi_0 = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + V\Psi_0$$

$$E\,\Psi_0 - V\Psi_0 + \frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} = 0$$

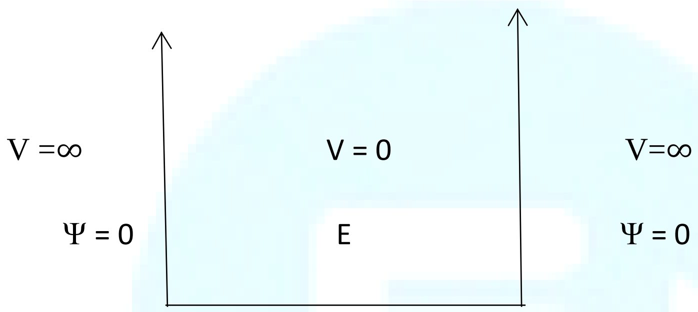
$$\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + (E - V)\,\Psi_0 = 0$$

Multiplying by $\frac{2m}{\hbar^2}$

$$\frac{\partial^2\Psi_0}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\,\Psi_0 = 0$$

Particle in a box

Consider a particle of mass m and energy E is trapped in a box of infinite height



E < V

Here $\Psi = 0 \begin{cases} for\ x < 0 \\ for\ x > l \end{cases}$

We have Schrodinger Equation

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\,\Psi = 0 \text{ ------ (1)}$$

Inside the box V = 0

$$(1) \Longrightarrow \frac{\partial^2\Psi}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi = 0$$

Put $K^2 = \frac{2mE}{\hbar^2}$

$$\frac{\partial^2\Psi}{\partial x^2} + K^2\Psi = 0$$

To solve this put $\frac{d}{dx} = D$

$D^2\Psi + K^2\Psi = 0$

$(D^2 + K^2)\Psi = 0$

$\Psi \neq 0$

$D^2 + K^2 = 0$

$D^2 = -K^2$

$D = 0 \pm iK$

If the solution is in the form $\alpha \pm i\beta$, in general Ψ can be written as

$\Psi = e^{\alpha x}$ [A cos βx + B sin βx]

Ψ = A cos kx + B sin kx -------- (2)

To find A and B apply the boundary condition

Boundary conditions

At x = 0 , Ψ = 0

(2) $\Longrightarrow$ 0 = A cos 0 + B sin 0

A = 0

When A = 0 equ (2) becomes

Ψ = B sin kx

At x = L , Ψ = 0

(2) $\Longrightarrow$ 0 = B sin KL

Sin KL = 0

KL = nπ

$K = \frac{n\pi}{L}$

$\Psi = B \sin \frac{n\pi x}{L}$

Normalization

$\int_{-\infty}^{\infty} |\Psi|^2 = 1$

$\Psi = B \sin \frac{n\pi x}{L}$

$\Psi^* = B \sin \frac{n\pi x}{L}$

$\int_0^L |\Psi|^2 \, dx = 1$

$\int_{-\infty}^{\infty} \Psi\Psi^* \, dx = 1$

$\int_0^L B^2 sin^2 \frac{n\pi x}{L} \, dx = 1$

On solving this we get B = $\sqrt{\frac{2}{L}}$

$\Psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

Here n = 1 corresponds to ground state and n = 2 corresponds to first excited state.

Total energy E = K + V

V = 0 $\Longrightarrow$ E = K

Also E = $\frac{P^2}{2m}$ but P = ħk

P = $\frac{h}{2\pi} \times \frac{2\pi}{\lambda}$

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

E = $\frac{\hbar^2 k^2}{2m}$

k = $\frac{n\pi}{L}$

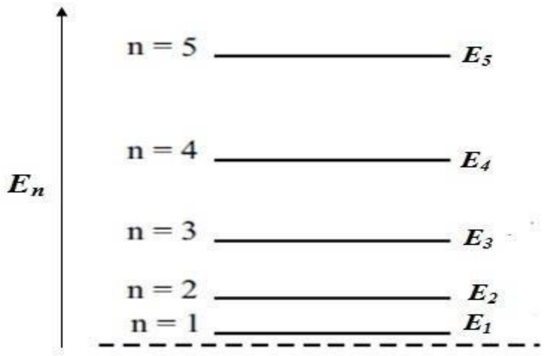
E = $\frac{n^2\pi^2\hbar^2}{2mL^2}$

For n = 1 ; $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$

For n = 2 ; $E_2 = 4 E_1$

For n = 3 ; $E_3 = 9 E_2$

Energy level diagram


n = 5
E_5
n = 4
E_4
E_n
n = 3
E_3
n = 2
E_2
n = 1
E_1