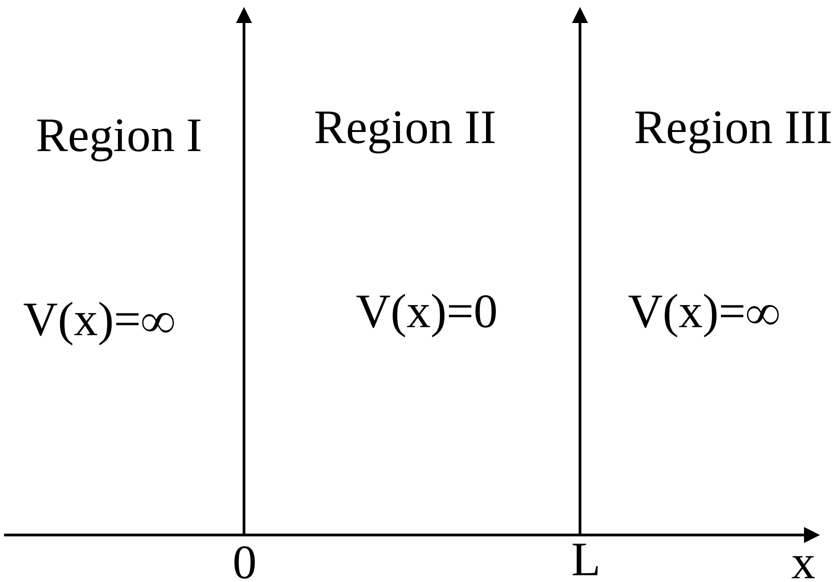
Particle in a 1-Dimensional Box



V(x)=0 for L>x>0
V(x)=∞ for x≥L, x≤0

Classical Physics: The particle can exist anywhere in the box and follow a path in accordance to Newton's Laws.

Quantum Physics: The particle is expressed by a wave function and there are certain areas more likely to contain the particle within the box.

Time Dependent Schrödinger Equation

$$\underbrace{\frac{-\hbar^2}{2m}\frac{d^2\Psi}{dx^2}}_{\text{KE}} + \underbrace{V(x)\Psi}_{\text{PE}} = \underbrace{E\Psi}_{\text{TE}}$$

Wave function is dependent on time and position function:

$$\Psi(x,t) = \overset{1}{\cancel{f}}(t)\psi(x)$$

Time Independent Schrödinger Equation

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

Applying boundary conditions:

Region I and III:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \infty * \psi = E\psi \longrightarrow |\psi|^2 = 0$$

Region II:

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

Finding the Wave Function

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

This is similar to the general differential equation:

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi \rightarrow \psi = A\sin kx + B\cos kx$$

So we can start applying boundary conditions:

x=0 ψ=0

$$0 = A\sin 0k + B\cos 0k \rightarrow 0 = 0 + B*1 \therefore B = 0$$

x=L ψ=0

$$0 = A\sin kL \quad A \neq 0 \rightarrow kL = n\pi$$ where n= $\mathbb{N}^*$

Calculating Energy Levels:

$$k^2 = \frac{2mE}{\hbar^2} \longrightarrow E = \frac{k^2\hbar^2}{2m} \longrightarrow E = \frac{k^2h^2}{2m4\pi^2}$$

$$\hbar = \frac{h}{2\pi}$$

$$E = \frac{n^2\pi^2}{L^2}\frac{h^2}{2m4\pi^2} \longrightarrow E = \frac{n^2h^2}{8mL^2}$$

Our new wave function:

$$\psi_{II} = A\sin\frac{n\pi x}{L}$$

But what is ‘A’?

Normalizing wave function:

$$\int_0^L (A\sin kx)^2\,dx = 1$$

$$|A|^2\left[\frac{x}{2} - \frac{\sin 2kx}{4k}\right]_0^L = 1$$

$$|A|^2\left[\frac{L}{2} - \cancel{\frac{\sin 2\frac{n\pi}{L}L}{4\frac{n\pi}{L}}}\right] = 1$$

Since n= $\mathbb{N}^*$

$$|A|^2\left(\frac{L}{2}\right) = 1 \rightarrow |A| = \sqrt{\frac{2}{L}}$$

Our normalized wave function is:

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