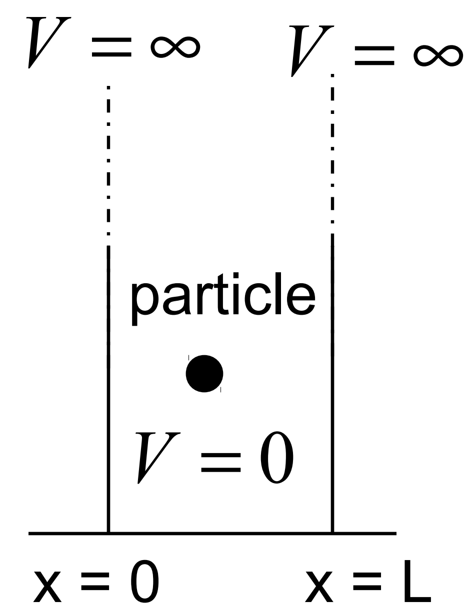
Particle in a Box

Consider a particle of rest mass m_o enclosed in a one-dimensional box (infinite potential well).



Boundary conditions for Potential

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } 0 > x > L \end{cases}$$

Boundary conditions for ψ

$$\psi = \begin{cases} 0 & \text{for } x = 0 \\ 0 & \text{for } x = L \end{cases}$$

Thus for a particle inside the box Schrodinger equation is

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m_o}{\hbar^2} E\psi = 0 \qquad \text{(i)} \qquad \therefore V = 0 \text{ inside}$$

$$\lambda = \frac{h}{p} = \frac{2\pi}{k}$$ (k is the propagation constant)

$$\Rightarrow k = \frac{p}{\hbar} = \frac{\sqrt{2m_o E}}{\hbar}$$

$$\Rightarrow k^2 = \frac{2m_o E}{\hbar^2} \qquad \text{(ii)}$$

Equation (i) becomes

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \qquad \text{(iii)}$$

General solution of equation (iii) is

$$\psi(x) = A \sin kx + B \cos kx \qquad \text{(iv)}$$

Boundary condition says ψ = 0 when x = 0

$$\psi(0) = A\sin k.0 + B\cos k.0$$

$$0 = 0 + B.1 \qquad \Rightarrow B = 0$$

Equation (iv) reduces to

$$\psi(x) = A\sin kx \qquad \text{(v)}$$

Boundary condition says ψ = 0 when x = L

$$\psi(L) = A\sin k.L$$

$$0 = A\sin k.L$$

$$A \neq 0 \quad \Rightarrow \sin k.L = 0$$

$$\Rightarrow \sin k.L = \sin n\pi$$

$$kL = n\pi$$

$$k = \frac{n\pi}{L} \qquad \text{(vi)}$$

Put this in Equation (v)

$$\psi(x) = A\sin\frac{n\pi x}{L}$$

When n # 0 i.e. n = 1, 2, 3…., this gives ψ = 0 everywhere.

Put value of k from (vi) in (ii)

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

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2m_o E}{\hbar^2}$$

$$\Rightarrow E = \frac{\hbar^2 k^2}{2m_o} \quad = \frac{n^2 h^2}{8m_o L^2} \qquad \text{(vii)}$$

Where n = 1, 2, 3….

Equation (vii) concludes

1. Energy of the particle inside the box can't be equal to zero. The minimum energy of the particle is obtained for n = 1

$$E_1 = \frac{h^2}{8m_o L^2} \qquad \textbf{(Zero Point Energy)}$$

If $E_1 \rightarrow 0$ momentum $\rightarrow 0$ i.e. $\Delta p \rightarrow 0$

$$\Rightarrow \Delta x \rightarrow \infty$$

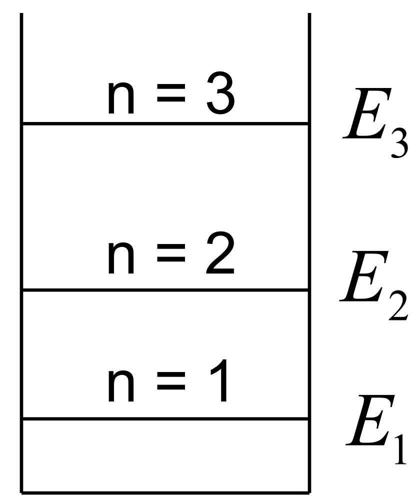
But $\Delta x_{\max} = L$ since the particle is confined in the box of dimension L.

Thus zero value of zero point energy violates the Heisenberg's uncertainty principle and hence zero value is not acceptable.

2. All the energy values are not possible for a particle in potential well.

   Energy is Quantized

3. E_n are the eigen values and 'n' is the quantum number.
4. Energy levels (E_n) are not equally spaced.



$$\psi_n(x) = A\sin\frac{n\pi x}{L}$$

Using Normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1$$

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

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

The normalized eigen function of the particle are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L}$$

Probability density figure suggest that:

1. There are some positions (nodes) in the box that will never be occupied by the particle.
2. For different energy levels the points of maximum probability are found at different positions in the box.

$|\psi_1|^2$ is maximum at L/2 (middle of the box)

$|\psi_2|^2$ is zero L/2.