

PARTICLE IN 3D CUBICAL BOX

Dr Rajeshkumar Mohanraman

Assistant Professor Grade 1
School of Advanced Sciences
VIT Vellore

Apply 1D box energy and wave function in 3D as

$$E_x = \frac{n_x^2 h^2}{8mL_1^2} \quad E_y = \frac{n_y^2 h^2}{8mL_2^2} \quad E_z = \frac{n_z^2 h^2}{8mL_3^2}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$$

Wave function

$$X(x) = \sqrt{\frac{2}{L_1}} \sin \left(\frac{n_x \pi x}{L_1} \right)$$

$$Y(y) = \sqrt{\frac{2}{L_2}} \sin \left(\frac{n_y \pi y}{L_2} \right)$$

$$Z(z) = \sqrt{\frac{2}{L_3}} \sin \left(\frac{n_z \pi z}{L_3} \right)$$

The wave function 3D as

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

$$\sqrt{\frac{2}{L_1}} \sin \left(\frac{n_x \pi x}{L_1} \right) \sqrt{\frac{2}{L_2}} \sin \left(\frac{n_y \pi y}{L_2} \right) \sqrt{\frac{2}{L_3}} \sin \left(\frac{n_z \pi z}{L_3} \right)$$

$$\psi(x, y, z) = \sqrt{\frac{8}{L_1 L_2 L_3}} \sin \left(\frac{n_x \pi x}{L_1} \right) \sin \left(\frac{n_y \pi y}{L_2} \right) \sin \left(\frac{n_z \pi z}{L_3} \right)$$

This is the total wave function of free particle in 3D box

The Energy of particle 3D as

$$E = E_x + E_y + E_z$$

$$E = \frac{n_x^2 h^2}{8mL_1^2} + \frac{n_y^2 h^2}{8mL_2^2} + \frac{n_z^2 h^2}{8mL_3^2}$$

$$E = \frac{h^2}{8m} \left[\frac{n_x^2}{L_1^2} + \frac{n_y^2}{L_2^2} + \frac{n_z^2}{L_3^2} \right]$$

This is the total energy of free particle in 3D box

Degeneracy of energy level of particle in 3D box

Distinct energy level posses same energy

$$E = \frac{h^2}{8m} \left[\frac{n_x^2}{L_1^2} + \frac{n_y^2}{L_2^2} + \frac{n_z^2}{L_3^2} \right]$$

total energy of free particle in 3D box

For cube $L_1=L_2=L_3$

$$E_{n_x, n_y, n_z} = \frac{h^2}{8mL^2} \left[n_x^2 + n_y^2 + n_z^2 \right]$$

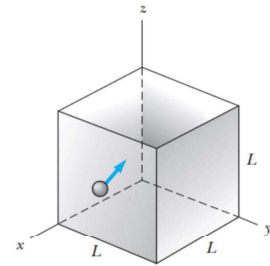


Figure 8.1 A particle confined to move in a cubic box of sides L . Inside the box $U = 0$. The potential energy is infinite at the walls and outside the box.