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Q Solve the Schrodinger wave equation when a particle is in three dimensional box.

→ By a three dimensional box we mean the potential at the boundaries are infinite.

$$V(x,y,z) = \begin{cases} 0 & \text{for } 0<x<L,\ 0<y<L,\ 0<z<L \\ \infty & \text{for elsewhere} \end{cases}$$

We have assumed an infinity deep potential well inside a cube of side L.

The three dimensional Schrodinger's equ^n is,

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{(1)}$$

$$\Rightarrow \nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$$

$$\because V = \begin{cases} 0 < x < L \\ 0 < y < L \\ 0 < z < L \end{cases}$$

Writing ∇^2 in cartesian components

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2 z}{\partial z^2} + \frac{2mE}{\hbar^2}\psi = 0$$

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

$$\frac{d^2X}{X dx^2} + \frac{d^2Y}{Y dy^2} + \frac{d^2Z}{Z dz^2} + \frac{2mE}{\hbar^2}\psi = 0$$

We may put

$$\left.\begin{aligned} \frac{d^2X}{X dx^2} &= -K_x^2 \\ \frac{d^2Y}{Y dy^2} &= -K_y^2 \\ \frac{d^2Z}{Z dz^2} &= -K_z^2 \end{aligned}\right\} \quad \text{(2)}$$

because each is a function only of x, y & z respective

So, $K_x^2 + K_y^2 + K_z^2 = \frac{2mE}{\hbar^2}$

The solutions of X, Y and Z are respectively

$$\left.\begin{aligned} X(x) &= A_1 \sin K_x x + B_1 \cos K_x x \\ Y(y) &= A_2 \sin K_y y + B_2 \cos K_y y \\ \& \quad Z(z) &= A_3 \sin K_z z + B_3 \cos K_z z \end{aligned}\right\} \quad \text{(3)}$$