

Particle in a 3D Box (1)

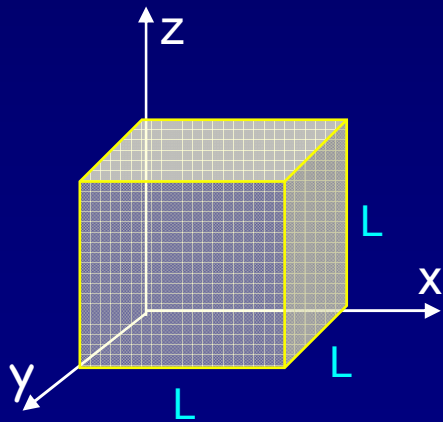
The extension of the Schrödinger Equation (SEQ) to 3D is straightforward in Cartesian (x,y,z) coordinates:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + U(x,y,z)\psi = E\psi$$

where $\psi \equiv \psi(x,y,z)$

Kinetic energy term: $\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$

Let's solve this SEQ for the particle in a 3D cubical box:



$$U(x,y,z) = \begin{cases} \infty & \text{outside box, } x \text{ or } y \text{ or } z < 0 \\ 0 & \text{inside box} \\ \infty & \text{outside box, } x \text{ or } y \text{ or } z > L \end{cases}$$

This $U(x,y,z)$ can be “separated”:
 $U(x,y,z) = U(x) + U(y) + U(z)$

$U = \infty$ if any of the three terms = ∞ .