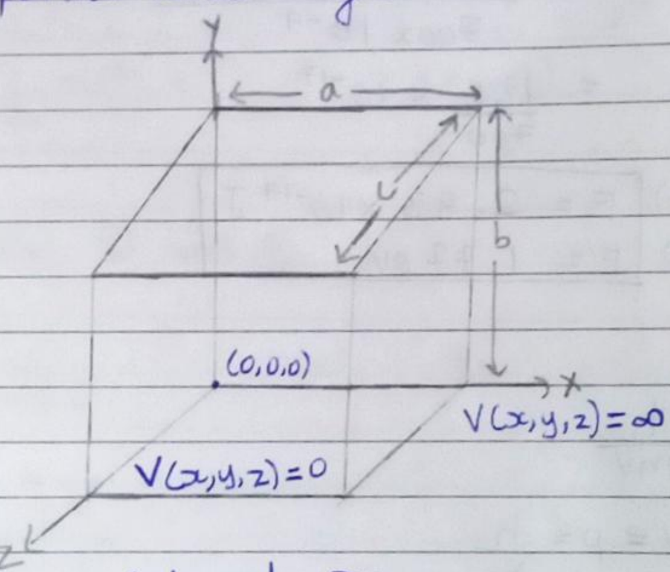
Vidhi Shah 21BCE1297 E2+TE2

BPHY101L DA2-A

⇒ PARTICLE IN A 3D BOX:

In quantum mechanics, the particle in a box model describes a particle free to move in a small space surrounded by impenetrable barriers.

The quantum particle in the 1D box can be expanded to consider a particle within higher dimensions such as a 3D box.



Schematic Diagram

→ Energy State:

Consider a particle which can move freely with in rectangular box of dimensions a×b×c with impenetrable walls.

- The potential can be written as:

$$V = \begin{cases} 0 & \text{Inside} \\ \infty & \text{At surfaces and outside} \end{cases}$$

- There is no force (i.e., no potential) acting on the particles inside the box ⇒ $V(\vec{r}) = 0$

- $\vec{r} = a\hat{x} + b\hat{y} + c\hat{z}$

- When the potential energy is infinite, then the wavefunction equals zero. When the potential energy is zero, then the wavefunction obeys the Time-Independent Schrödinger Equation :

$$-\frac{h^2}{2m} \nabla \psi(r) + V(r)\psi(r) = E\psi(r)$$

$$E\psi(x,y,z) = -\frac{h}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi(x,y,z)$$
$$+ V\psi(x,y,z) \quad - (1)$$

Using separation of variables to solve this partial differential equation

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

Solving,

$$\boxed{\begin{aligned} \psi(x,y,z) &= \sqrt{\frac{8}{abc}} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{n\pi}{b}y\right) \sin\left(\frac{n\pi}{c}z\right) \\ E_x + E_y + E_z = E &= \frac{h^2\pi^2}{2m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right] \end{aligned}}$$

Energy State in a 3D Box