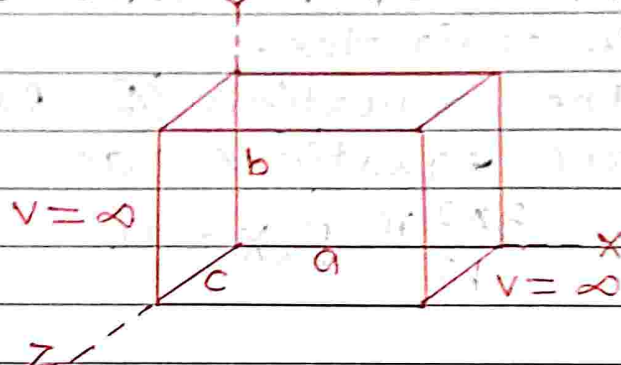


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PARTICLE IN A THREE-DIMENSIONAL BOX

Let us consider the motion of a particle of mass m confined to a three-dimensional box with dimensions a, b, c along x, y and z -axes. The potential energy of the particle is assumed to be zero within the box and is infinite (∞) outside the box and its boundaries.



Now, the Schrödinger's equation for the particle can be written as -

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - 0) \psi = 0 \quad (\because V = 0 \text{ within the box})$$

$$\text{or, } \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} E \psi = 0 \quad \text{--- (1)}$$

Let $\psi(x, y, z)$ be the product of three functions x, y and z which are functions of x, y and z .

(i.e.,

$$\psi(x, y, z) = X(x) \cdot Y(y) \cdot Z(z) \quad \text{--- (2)}$$

from eqn. (1) and (2) we get

$$YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} + \frac{8\pi^2 m E}{h^2} XYZ = 0 \quad \text{--- (3)}$$

Dividing eqn. (3) by XYZ , we get

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} + \frac{8\pi^2 m E}{h^2} = 0 \quad \text{--- (4)}$$

from eqn. (4) the first term is the function of x

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only and is independent of y and z . The second term is function of y only and is independent of x and z and the third term is function of z only and is independent of x and y . The fourth term is constant.

If energy E is written as the sum of three contributions associated with the three co-ordinates.

Then equation (4) can be separated into three equations as

$$\frac{\partial^2 X}{\partial x^2} + \frac{8\pi^2 m}{h^2} E_x X = 0 \quad \text{--- (5)}$$

$$\frac{\partial^2 Y}{\partial y^2} + \frac{8\pi^2 m}{h^2} E_y Y = 0 \quad \text{--- (6)}$$

$$\frac{\partial^2 Z}{\partial z^2} + \frac{8\pi^2 m}{h^2} E_z Z = 0 \quad \text{--- (7)}$$

Where $E = E_x + E_y + E_z$

The solutions of eqn (5), (6) and (7) are given as

$$X(x) = \sqrt{\frac{2}{a}} \sin \frac{n_x \pi x}{a} \quad \text{--- (8)}$$

Where $n_x = 1, 2, 3, \dots$

$$Y(y) = \sqrt{\frac{2}{b}} \sin \frac{n_y \pi y}{b} \quad \text{--- (9)}$$

Where $n_y = 1, 2, 3, \dots$

$$Z(z) = \sqrt{\frac{2}{c}} \sin \frac{n_z \pi z}{c} \quad \text{--- (10)}$$

Where $n_z = 1, 2, 3, \dots$

Now,

$$\psi(x,y,z) = XYZ = \sqrt{\frac{8}{abc}} \cdot \frac{\sin n_x \pi x}{a} \cdot \frac{\sin n_y \pi y}{b} \cdot \frac{\sin n_z \pi z}{c} \quad (11)$$

for a cubical box,

where $a = b = c$

We can write

$$\psi(x,y,z) = \sqrt{\frac{8}{a^3}} \frac{\sin n_x \pi x}{a} \cdot \frac{\sin n_y \pi y}{a} \cdot \frac{\sin n_z \pi z}{a} \quad (12)$$

Energy of a particle in a three-dimensional box $\Rightarrow$

Solutions of equation (5), (6) and (7) gives

$$E_x = \frac{n_x^2 h^2}{8ma^2}$$

$$E_y = \frac{n_y^2 h^2}{8mb^2} \quad \text{and}$$

$$E_z = \frac{n_z^2 h^2}{8mc^2}$$

So,

$$E = E_x + E_y + E_z = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$

Or,

$$E = \frac{h^2}{8m} \left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right] \quad (13)$$

for a cubical box,

where $a = b = c$ Then

$$E = \frac{h^2}{8ma^2} [n_x^2 + n_y^2 + n_z^2]$$