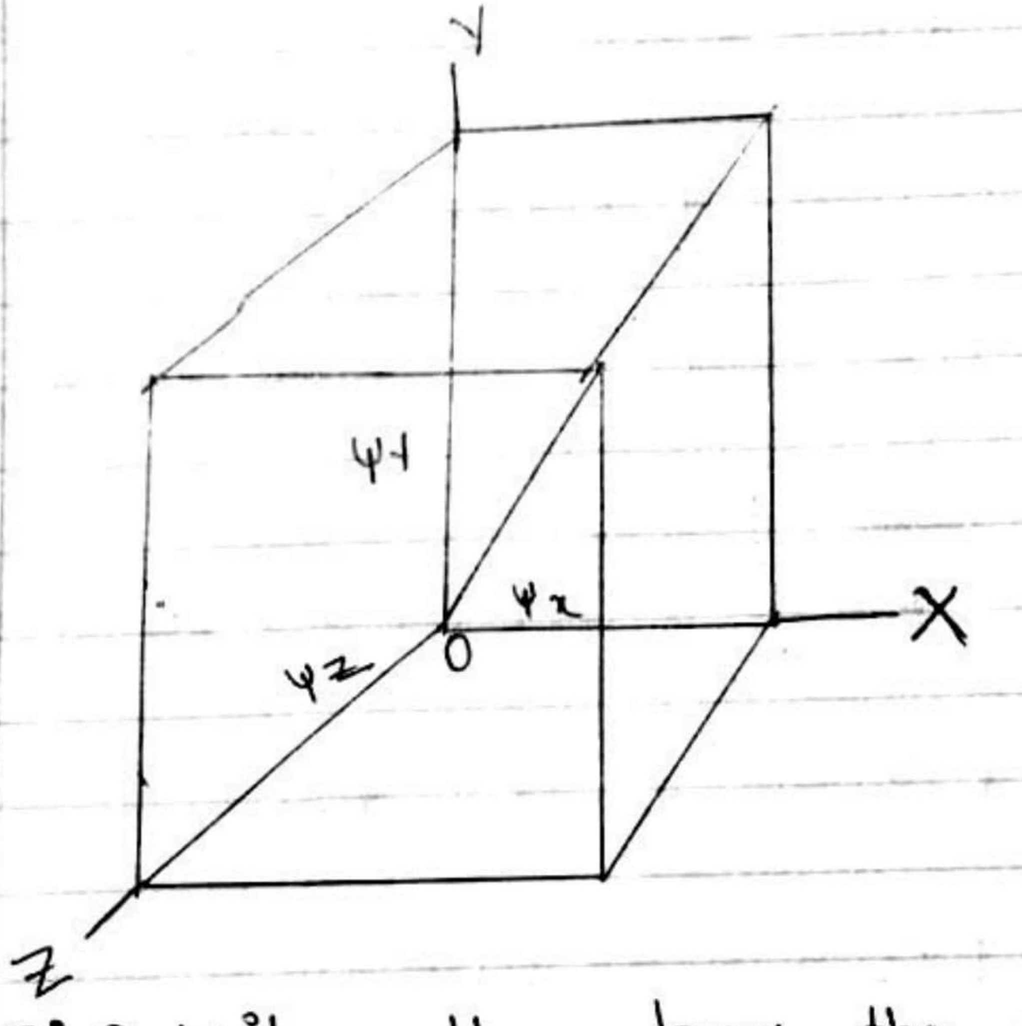
Solution of Schrodinger's Wave equation for Particle in Three dimensions:

Lets consider a particle moving in three dimension box.



a) Outside the box, the potential energy of the box is at the boundary of the box.

b) Inside the box, the potential energy will be equal to zero.

$$\nabla^{2\psi}_{xyz} + \frac{8\pi m^2}{h^2}(E.V)\psi xyz = 0 \quad \textbf{(i)}$$

Since $V = 0$, Inside the box

$$\Delta^2\psi xyz + \frac{8\pi^2 m}{h^2} E\psi xyz = 0 \quad \textbf{(ii)}$$

But, $\psi xyz\, \Delta^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

$$\psi xyz = \textbf{(iii)}$$

$$= \frac{\partial^2 \psi xyz}{\partial x^2} + \frac{\partial^2 \psi xyz}{\partial y^2} + \frac{\partial^2 \psi xyz}{\partial z^2}$$

$$+ \frac{8\pi^2 m}{h^2} \cdot E\psi xyz = \textbf{(iv)}$$

$$\psi xyz = \psi x \psi y \psi z.$$

$$\frac{\partial^2 \psi x\psi y\psi z}{\partial x^2} + \frac{\partial^2 \psi x\psi y\psi z}{\partial y^2} + \frac{\partial^2 \psi x\psi y\psi z}{\partial z^2}$$

$$+ \frac{8\pi^2 m}{h} E\psi x\psi y\psi z.$$

$$\psi y\psi z\frac{\partial^2 \psi x}{\partial x^2} + \psi x\psi z\frac{\partial^2 \psi y}{\psi y^2} + \cancel{\psi x}$$

$$+ \psi\psi z\frac{\partial^2 \psi z}{\partial z^2} + \frac{8\pi^2 m}{h^2} Exyz$$

$$\psi x \; \psi y \; \psi z = 0 \quad (v)$$

On dividing equation (5) by $\psi x \; \psi y \; \psi z$ we get

$$\frac{1}{\psi x}\frac{\partial^2 \psi x}{\partial x^2} + \frac{1}{\psi y}\frac{\partial^2 \psi y}{\partial y^2} + \frac{1}{\psi z}\frac{\partial^2 z}{\partial z^2}$$

$$+ \frac{8\pi^2 m}{h^2} E x y z = 0.$$

But $E x y z = E x + E y + E z$

$$\frac{1}{\psi x}\frac{\partial^2 \psi x}{\partial x^2} + \frac{1}{\psi y}\frac{\partial^2 \psi y}{\partial y^2} + \frac{1}{\psi z}$$

$$\frac{\partial^2 \psi z}{\partial z^2} + \frac{8\pi^2 m}{h^2} E x + E y + E z$$

$$\left(\frac{h^2}{8\pi^2 m}\right) \quad " \quad " \quad " \quad \frac{8\pi^2 m}{h^2} \times \frac{h^2}{8\pi^2 m}$$

$$E x + E y + E z = 0.$$

$$\frac{h^2}{8\pi^2 m}\left(\frac{1}{\psi x}\frac{\partial^2 \psi x}{\partial x^2}\right) + \frac{h^2}{8\pi^2 m}\left(\frac{1}{\psi y}\frac{\partial^2 \psi y}{\partial y^2}\right)$$

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

Equation (7) can be written as

$$-Ex = \frac{h^2}{8\pi^2 m}\left(\frac{1}{\psi x}\frac{\partial^2 \psi x}{\partial x^2}\right) \rightarrow 8A$$

$$-Ey = \frac{h^2}{8\pi^2 m}\left(\frac{1}{\psi y}\frac{\partial^2 \psi y}{\partial y^2}\right) \rightarrow 8B.$$

$$-Ez = \frac{h^2}{8\pi^2 m}\left(\frac{1}{\psi z}\frac{\partial^2 \psi z}{\partial yz^2}\right) \rightarrow 8C$$

Simplify the eq- 8A.

$$\frac{1}{\psi x}\frac{\partial^2 \psi x}{\partial x^2} = \frac{-8\pi^2 m}{h^2} Ex, \frac{\partial^2 \psi x}{\partial x^2} +$$

$$\frac{8\pi^2 m}{h^2} Ex\, \psi x = 0 \quad 9a$$

Equation(8b)

$$\frac{1}{\psi y}\frac{\partial^2 \psi y}{\partial y^2} = \frac{-8\pi^2 m}{h^2} Ey = \frac{\partial^2 \psi y}{\partial y^2}$$

$$+ \frac{8\pi^2 m}{h^2} Ey\, \psi y \quad 9b$$

(Equation 8C)

$$\frac{1}{\psi z}\frac{\partial^2 \psi z}{\psi z^2} = \frac{-8\pi^2 m}{h^2} Ez = \frac{\partial^2 \psi z}{\partial z^2} + \frac{8\pi^2 m}{h^2} Ez = 0 \quad 9c$$

Let $k^2 = \frac{8\pi^2 m E x}{h^2}$.

=> Solution of eq 9(a).

$$\frac{\partial^2 \psi x}{\partial x^2} + k^2 \psi x = 0.$$

The equation 9a has solution in the form of exponential like

$$\psi x = A e^{mx} \longrightarrow (10)$$

So, by inserting the value of "ψx" from eq (10) into eq (9a)

$$\frac{\partial^2}{\partial x^2} (A e^{mx}) + k^2 A e^{mx} = 0.$$

$$A . m^2 e^{mx} + A k^2 e^{mx} = 0.$$

$$(A e^{mx})(m^2 + k^2) = 0.$$

$A e^{mx} \neq 0$, So therefore $m^2 + k^2 = 0$.

For finding the value of m, we have

$$m^2 = -k^2$$
$$m^2 = i^2 k^2$$

$$m = \pm ik$$

By putting the value of i into equation 10

$$\psi x = Ae^{\pm ikx}$$
$$= Ae^{ikx} + Be^{-ikx}$$

By inserting the value

$$\psi x = A(\cos kx + i\sin kx)$$
$$+ B(\cos kx - i\sin x kx)$$

$$\psi x = A\cos kx + A\sin kx + B\cos kx - Bi\sin x\, kx.$$

$$\psi x = \cos(kx)(A+B) + i\sin(kx)(A-B).$$

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Let $A + B = D$.

$i(A - B) = C$.

$\psi x = D\cos(kx) + C\sin(kx)$ (11)

By applying boundary Condition.

$\psi x = 0$ at $x = 0$.

$\psi x = D\cos(kx) + C\sin(kx)$ 12

$0 = D\cos(k.0) + C\sin(k.0)$.

$0 = D\cos 0^\circ + C\sin 0^\circ$.

$D = 0$.

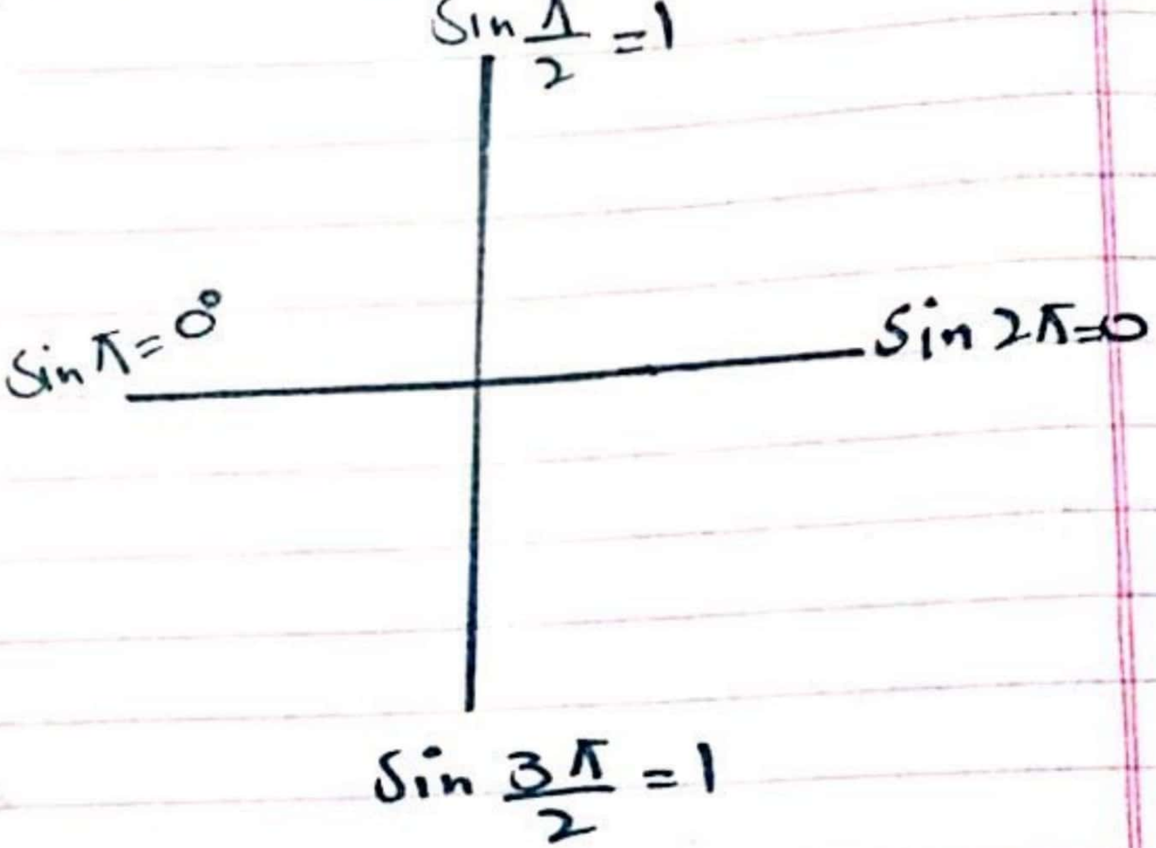
By inserting the value of $D = 0$ into eq 12.

By applying second boundary condition

$\psi x = 0, \; x = a$

$0 = C\sin ka$. $\quad ka = n\pi$.

After each π, sin will be zero.



$$\psi x = c\sin kx = 12$$

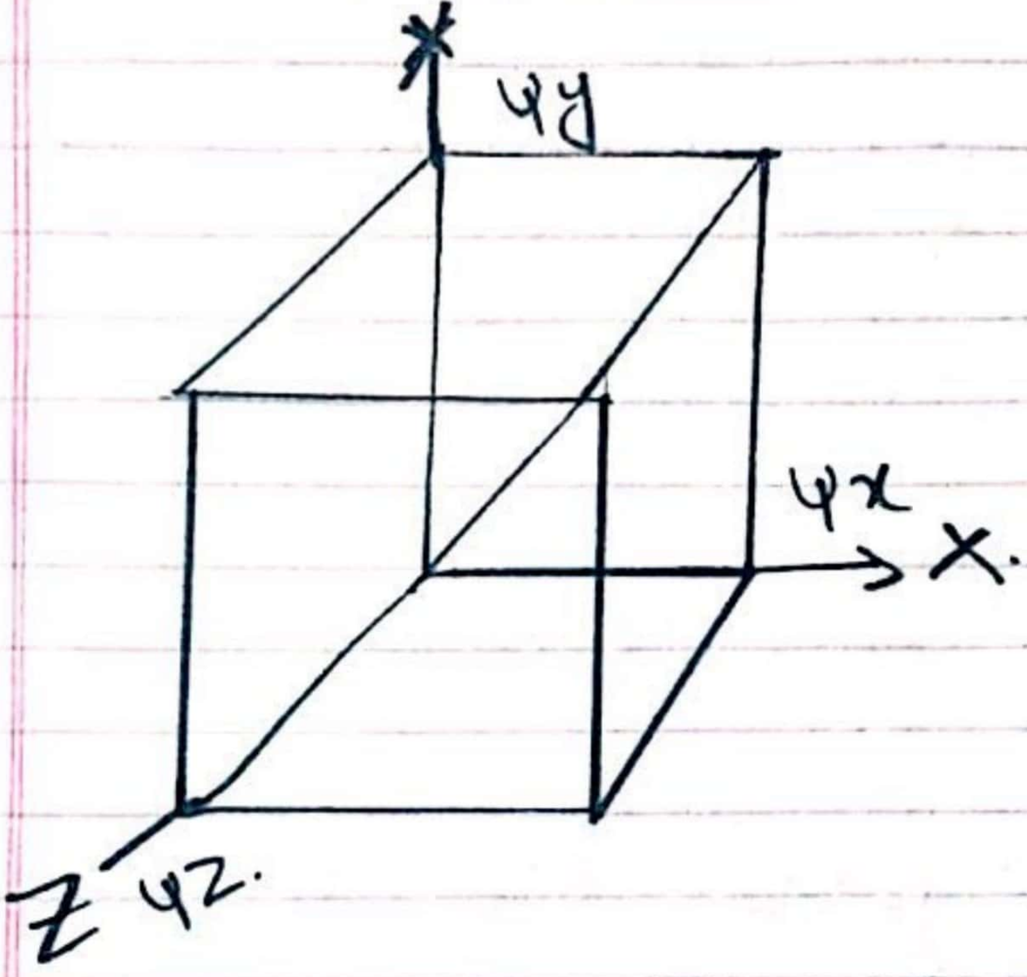
By putting the value of k into eq (12).

$$\psi x = c\sin\frac{n\pi x}{a} \rightarrow 13a$$

$$\psi y = c\sin\frac{n\pi y}{a} \rightarrow 13b$$

$$\psi z = c\sin\frac{n\pi z}{a} \rightarrow (13c).$$

Solution of Schrodinger's Wave equation for particle in 3D box.



Determination of Value of "C".

C = Constant and known as Constant of Normalization.

By applying conditions of Normalization.

$$\int_{-\infty}^{+\infty} \psi \; \psi^* \, d\psi = 1 \quad 14a$$

By subsituting the value of "ψx" from eq (13 a) to eq (14 a)

$$\Rightarrow \int_0^a C \sin\left(\frac{n\pi x}{a}\right) \cdot C \sin\frac{n\pi x}{a} dx = 1$$

$$\Rightarrow \int_0^a c^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1.$$

$$\Rightarrow c^2 \int_0^a \frac{1 - \cos 2\left(\frac{n\pi x}{a}\right)}{2} dx = 1.$$

$$\Rightarrow \frac{c^2}{2} \int_0^a \left(1 - \cos 2\left(\frac{n\pi x}{a}\right)\right) dx = 1$$

$$\Rightarrow \frac{c^2}{2} \left[\int_0^a dx - \int_0^a \cos 2\left(\frac{n\pi x}{2}\right) dx\right] = 1.$$

$$\frac{c^2}{2} \left[\Big| _0^a x \Big| - \int_0^a \frac{\sin\left(\frac{2n\pi x}{a}\right) dx}{2n\pi} \right]$$

$$\frac{c^2}{2}\left\{(a-0)-\frac{a}{2n\pi}\left[\frac{\sin 2n\pi a}{a}\right.\right.$$

$$\left.-\frac{\sin 2n.\pi.0}{a}\right]=1.$$

$$\frac{c^2}{a}(a)-\frac{a}{2n\pi}(\sin 2n\pi-\sin 0)=1.$$

$$\frac{c^2}{a}(a)-0=1.$$

$$\frac{c^2}{a}(a)-0=1$$

$$\frac{c^2}{a}(a)=1.$$

$$\boxed{c^2=\frac{2}{a}.}$$

By putting the value of c

$$\psi x = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \rightarrow 15a$$

$$\psi y = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi y}{a}\right) \quad 15b$$

$$\psi z = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi z}{a}\right) \quad 15c.$$

By subsituting the value of 15 a, b, c into eqn 5c

$$\psi xyz = \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \cdot \frac{\sin n\pi y}{a} \cdot \frac{\sin n\pi z}{a}$$

Result

$$\psi xyz = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi y}{a}\right) \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi z}{a}\right) \Rightarrow 16.$$

We can found the total wave function of a particle

Total energy:-

$$k^2 = \frac{8\pi^2 m}{h^2} Ex \rightarrow (1)$$

$$K = \frac{n\pi}{a} \rightarrow (ii)$$

$$K = \frac{n\pi^2}{a^2} \rightarrow (iii)$$

By comparing eq (i) & (iii)

$$\frac{8\pi^2 m E_x}{h^2} = \frac{n^2\pi^2}{a^2}$$

$$\Rightarrow E_x = \frac{n^2\pi^2}{a^2} \times \frac{h^2}{8\pi^2 m}$$

Etotal = Ex + Ey + Ez

By subsituting the value of Ex, Ey and Ez.

$$E_{total} = \frac{n^2{}_x h^2}{8ma^2} + \frac{n^2{}_y h^2}{8ma^2}$$

$$+ \frac{n^2{}_z h^2}{8ma^2}.$$

$$E_{total} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

If we have the value of $n^2x + ny^2 + nz^2$ than we can find the value of E total.

We can also find the ground state energy

$nx = ny = nz = 1.$

$$E\ total = \frac{h^2}{8m^2a}\left((1)^2 + (1)^2 + (1)^2\right)$$

$$E\ total = \frac{3h^2}{8ma^2} \rightarrow \text{Ground State energy}$$

If $nx = 1,\ ny = 1,\ nz = 2.$

$$E\ total = \frac{h^2}{8ma^2}(1^2 + 1^2 + 1^2).$$

$$= \frac{6h^2}{8ma^2}$$

If $nx = 1,\ ny = 2,\ nz = 1.$

$$E\ total = \frac{6h^2}{8ma^2}.$$

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If $n_x = 2.$

$n_y = 1$

$n_z = 1.$

then E_{total} would be

$$\boxed{E_{total} = \frac{6h^2}{8ma^2}.}$$