Note Title 19-10-2016

Particle in a box (3D)

$$E_{n_x, n_y, n_z} = E_{n_x} + E_{n_y} + E_{n_z} \quad \ldots (1)$$

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

Cube $\Rightarrow$ $$E = \frac{h^2}{8ma^2}\left[n_x^2 + n_y^2 + n_z^2\right] \quad \ldots (3)$$

For a cubic box, degeneracies are seen

Ground state: $n_x = 1 \quad n_y = 1 \quad n_z = 1 \qquad (1,1,1) \quad [1]$

$$\left.\begin{matrix} n_x = 2 & n_y = 1 & n_z = 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{matrix}\right\} \text{degenerate } [3]$$

$$\psi_{n_x, n_y, n_z}(x,y,z) = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right) \sin\left(\frac{n_z \pi}{c} z\right) \quad \ldots (4)$$

$$\psi(x,y,z) = \psi_{n_x}(x)\, \psi_{n_y}(y)\, \psi_{n_z}(z) \quad \ldots (5)$$

Particle in a 2-D box

$$\psi_{n_x, n_y}(x,y) = \sqrt{\frac{4}{ab}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right) \quad \ldots (6)$$

$$E_{n_x, n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2}\right) \quad \ldots (7)$$

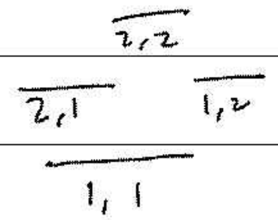
$$E_{n_x, n_y} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2) \quad \cdots \quad (8)$$

$\uparrow$

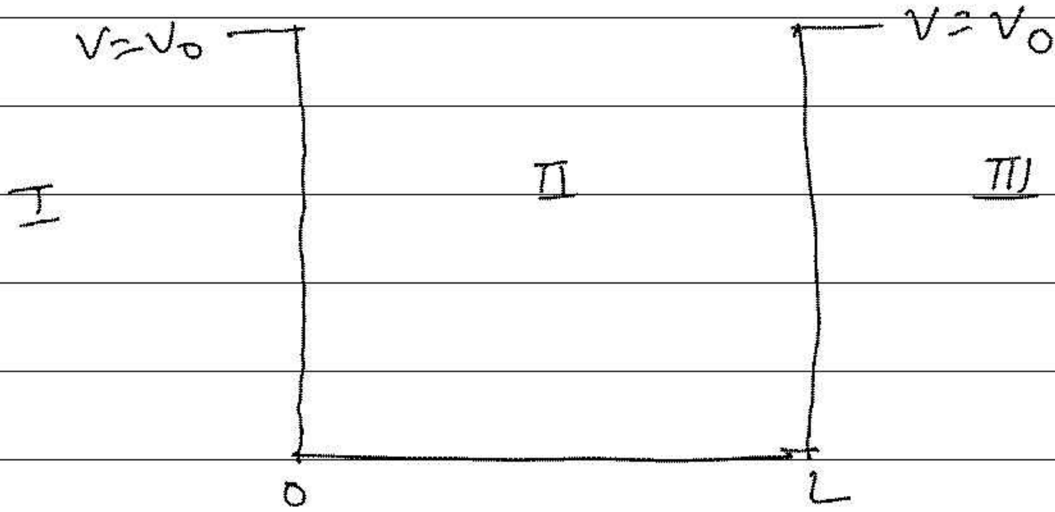
square box $[a = b]$

$n_x = 1, \ n_y = 1$ Degeneracy $= 1$

$\left.\begin{array}{l} n_x = 2, \ n_y = 1 \\ 1, \quad 2 \end{array}\right\}$ " $= 2$



Finite well System



Region I

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0 \psi = E\psi \quad \cdots \quad (1)$$

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} (V_0 - E)\psi \quad \cdots \quad (2)$$

$$k_1^2 = \frac{2m}{\hbar^2}(V_0 - E) \quad \ldots \quad (3)$$

I: $\psi_I = Ae^{-k_1 x} + Be^{k_1 x} \quad \ldots \quad (4)$

III: $\psi_{III} = Fe^{-k_1 x} + Ge^{k_1 x} \quad \ldots \quad (5)$

II: $\psi_{II} = C\sin k_2 x + D\cos k_2 x \quad \ldots \quad (6)$

$\psi_I = Ae^{-k_1 x} + Be^{k_1 x}$; $x < 0$

$\psi_I = Be^{k_1 x} \quad \ldots \quad (7)$

$\psi_{III} = Fe^{-k_1 x} + Ge^{k_1 x}$; $x > L$

$\psi_{III} = Fe^{-k_1 x} \quad \ldots \quad (8)$

Wavefunctions have to be continuous

$\psi_I(x=0) = \psi_{II}(x=0)$

$Be^{k_1 x} = C\sin k_2 x + D\cos k_2 x$

$x=0$ $\quad B = D \quad \ldots \quad (9)$

$$\psi_{II}(x=L) = \psi_{III}(x=L)$$

Slope of wavefunction has to be continuous

$$\frac{d\psi_I}{dx}(x=0) = \frac{d\psi_{II}}{dx}(x=0)$$

$$\frac{d}{dx} Be^{k_1 x} = \frac{d}{dx}\left[C\sin k_2 x + D\cos k_2 x\right]$$

$$k_1 Be^{k_1 x} = k_2 C\cos k_2 x - k_2 D\sin k_2 x$$

$x=0 \Rightarrow$ $k_1 B = k_2 C$ . . . (10)

Normalisation Condition

$$\int_{-\infty}^{0}\psi_I^2\,dx + \int_0^L \psi_{II}^2\,dx + \int_L^{\infty}\psi_{III}^2\,dx = 1$$

$$\psi_{III} = Fe^{-k_1 x} \qquad k_1 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$