❖ The Concept of Degeneracy Among Energy Levels for a Particle in Three Dimensional Box

The solution of Schrodinger wave equation for a particle of mass '*m*' trapped in three dimensional of sides *a*, *b* and *c* with zero potential inside and infinite potential outside provide the total wave function ψ as

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{abc}}\, Sin\frac{n_x\pi x}{a}\, Sin\frac{n_y\pi y}{b}\, Sin\frac{n_z\pi z}{c} \tag{27}$$

Where n_x, n_y, n_y are the discrete variable whose permitted values from boundary conditions can be 1, 2, 3, 4….∞. The variable *x*, *y* and *z* represent the position of the particle along the corresponding axis. Besides, the expression for total energy is

$$E_{n_x n_y n_z} = \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)\frac{h^2}{8m} \tag{28}$$

For a cubical box, all the sides become equal (*a* = *b* = *c*). Using this condition in equation (27), the total wave function representing different quantum mechanical states take the following form.

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{a^3}}\, Sin\frac{n_x\pi x}{a}\, Sin\frac{n_y\pi y}{a}\, Sin\frac{n_z\pi z}{a} \tag{29}$$

Similarly, the energy expression also changes to

$$E_{n_x n_y n_z} = \left(n_x^2 + n_y^2 + n_z^2\right)\frac{h^2}{8ma^2} \tag{30}$$

Now, in order to define various quantum mechanical states, we need to put valid set quantum numbers. The expression for first quantum mechanical and corresponding energy can be obtained by putting $n_x = n_y = n_z = 1$ in equations (29–30) i.e.

$$\psi_{111} = \sqrt{\frac{8}{a^3}}\, Sin\frac{\pi x}{a}\, Sin\frac{\pi y}{a}\, Sin\frac{\pi z}{a} \quad \text{and} \quad E_{111} = \frac{3h^2}{8ma^2} \tag{31}$$

Similarly, the next state with energy can be obtained by putting $n_x = n_y = 1$ and $n_z = 2$ in equations (29–30) i.e.

$$\psi_{112} = \sqrt{\frac{8}{a^3}}\, Sin\frac{\pi x}{a}\, Sin\frac{\pi y}{a}\, Sin\frac{2\pi z}{a} \quad \text{and} \quad E_{112} = \frac{6h^2}{8ma^2} \tag{32}$$

If $n_x = n_z = 1$ and $n_y = 2$; the wavefunction and energy become

$$\psi_{121} = \sqrt{\frac{8}{a^3}}\, Sin\frac{\pi x}{a}\, Sin\frac{2\pi y}{a}\, Sin\frac{\pi z}{a} \quad \text{and} \quad E_{121} = \frac{6h^2}{8ma^2} \tag{33}$$

If $n_y = n_z = 1$ and $n_x = 2$, the state with energy becomes

$$\psi_{211} = \sqrt{\frac{8}{a^3}}\, Sin\frac{2\pi x}{a}\, Sin\frac{\pi y}{a}\, Sin\frac{\pi z}{a} \quad \text{and} \quad E_{211} = \frac{6h^2}{8ma^2} \tag{34}$$

It can be clearly seen that three quantum mechanical states ψ_{112}, ψ_{121} and ψ_{211} possess the same amount of energy (i.e. $6h^2/8ma^2$); and therefore, are said to be degenerate. In other words, there are three different ways of existence of the particle inside the box so that the particle possesses $6h^2/8ma^2$ energy as total.

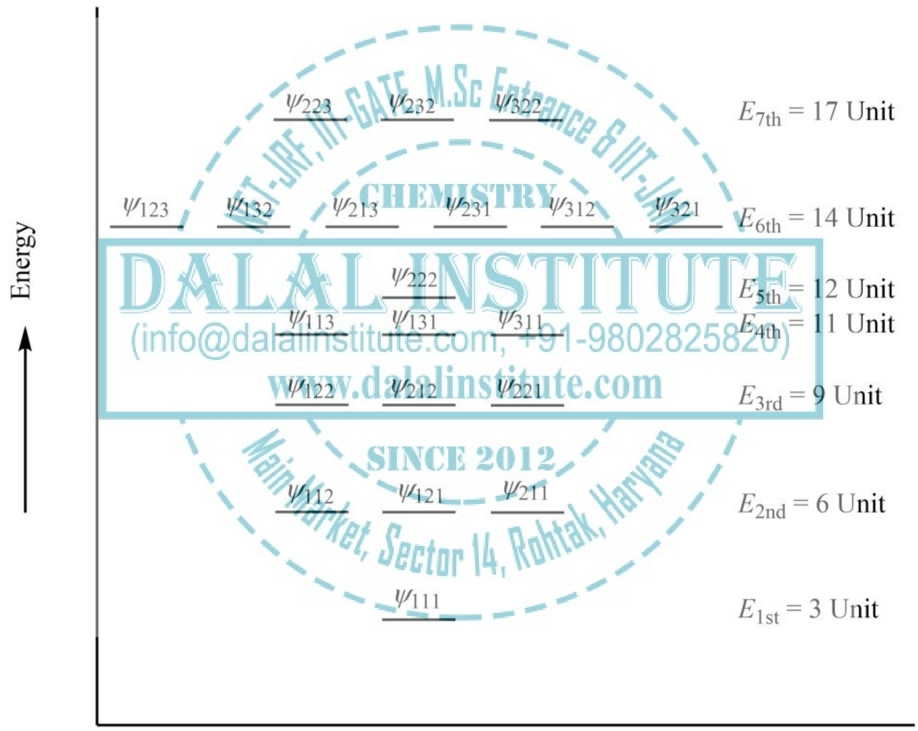

Figure 2. The energy level diagram representing different quantum mechanical states (in the units of $h^2/8ma^2$) for a particle trapped in a cubical box.

Hence, the degeneracy of the ground state is one i.e. there is only one way for the particle to exist in the box to create zero-point energy ($3h^2/8ma^2$). On the other hand, the degeneracy of first excited stated is 3 as ψ_{112}, ψ_{121} and ψ_{211}, all have 6 units of energy. Moreover, after careful examination of energy diagram, it can be concluded that degeneracy is 1 if $n_x = n_y = n_z$, 3 if $n_x = n_y$ or $n_y = n_z$ or $n_x = n_z$, and 6 if $n_x \neq n_y \neq n_z$.

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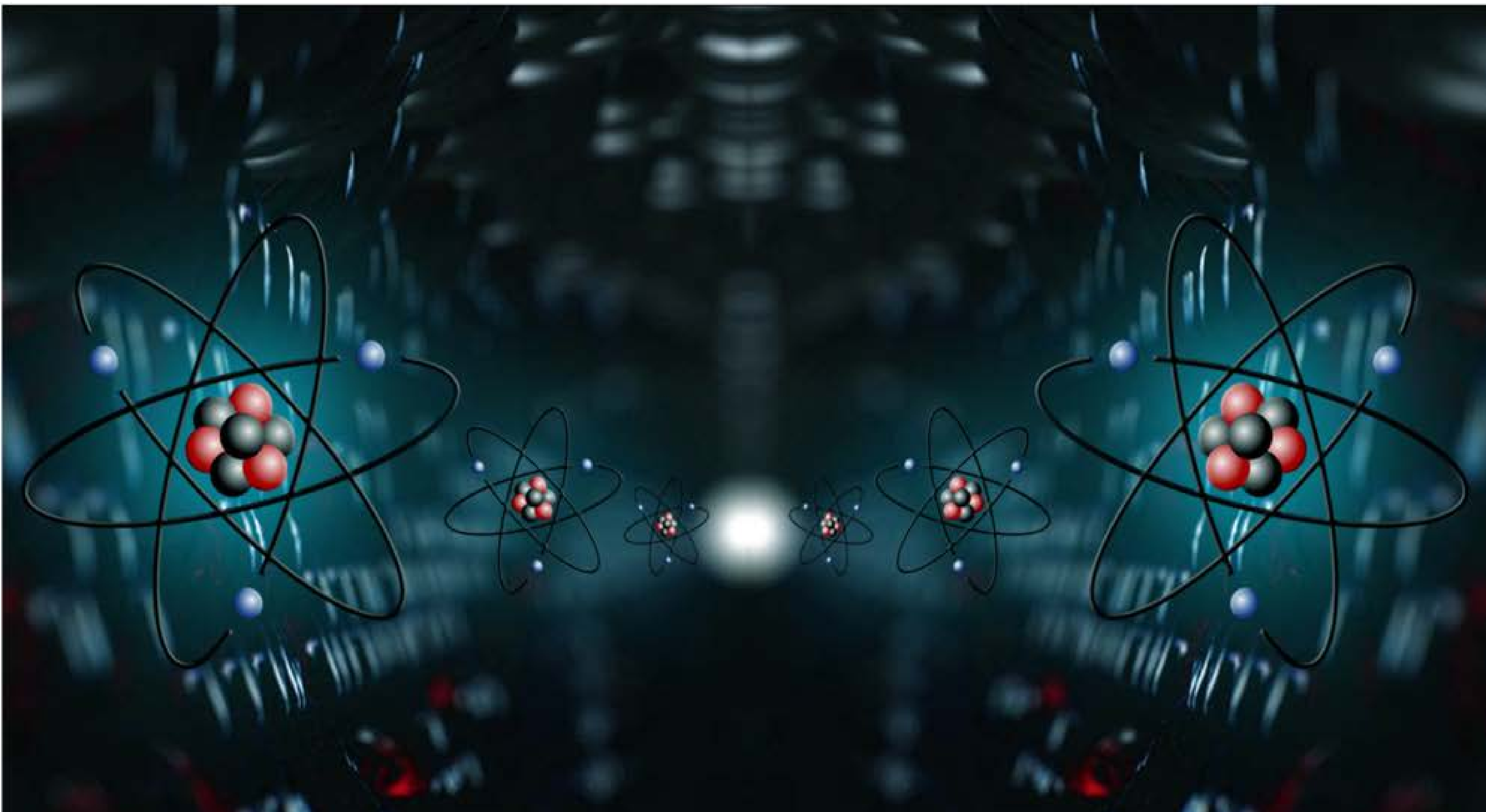

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