

SUBJECT - CHEMISTRY

CLASS - B.Sc (Hons) PART-III

PAPER - V

TOPIC - Degree of degeneracy

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Q Determine the degree of degeneracy of the energy level $\frac{17h^2}{8ma^2}$ for a particle in a cubical box.

The energy of a particle in a cubical box is given by -

$$E = \frac{h^2}{8ml^2} (n_x^2 + n_y^2 + n_z^2)$$

from question

$$\frac{h^2}{8ml^2} (n_x^2 + n_y^2 + n_z^2) = 17 \cdot \frac{h^2}{8ml^2}$$

$$\text{or } n_x^2 + n_y^2 + n_z^2 = 17$$

possible arrangements for the sum of squared terms will be 17, are given as -

n_x	n_y	n_z
3	2	2
2	3	2
2	2	3

As three sets of quantum numbers give the same energy hence the degree of degeneracy is three.

Q List the restrictions on a wave function and explain how these lead to quantisation.

Ans A wave function describing a free particle inside a one dimensional box is given by -

$$\psi = A \sin \sqrt{\frac{2mE}{\hbar}} \cdot x + B \cos \sqrt{\frac{2mE}{\hbar}} \cdot x$$

This wave function does not tell us much information because it offers no restriction on the energy E of the particle.

Actually a free particle moving along the x -axis can have energy i.e a free particle has a continuous set of energy levels.

Quantisation, however, can take place when -

- 1 The particle is not entirely free
- 2 The particle be constrained to remain in a box.
- 3 The particle be influenced by the walls.
- 4 Since the potential is very high at the walls of the box, the probability of finding the particle at the walls is zero i.e $|\psi|^2 = 0$ at the walls. The Schrodinger equation is given by -

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad \dots (1)$$

$$\therefore \psi = A \sin kx + B \cos kx \quad \dots (2)$$

Conditions are (i) $\psi(0) = 0$ (ii) $\psi(a) = 0$

putting the first condition in equation (2) we get -

$$0 = B$$

putting the second condition in equation (2) we get -

$$0 = A \sin ka$$

$$A \neq 0$$

$$\text{So } \cancel{\sin ka} = \cancel{\sin \pi x}$$

$$\text{So } \sin ka = \sin n\pi$$

$$\text{or } ka = n\pi$$