

$$\text{So that } N = (2\pi)^{-1/2} \quad \dots(17)$$

Hence, the normalized wave function become

$$\Phi_{\pm m}(\phi) = (2\pi)^{-1/2} \exp(\pm im\phi); m=0, 1, 2, 3, \dots \quad \dots(18)$$

We shall not attempt to give a complete solution of equation (9) but will merely state that if $\beta = \ell(\ell+1)$ where ℓ is the rotational quantum number, then this equation becomes a standard mathematical equation whose solutions are known to be associated legendre polynomials $P_{\ell}^{|m|}(\cos\theta)$ where, ℓ is either zero or a positive integer and $\ell \geq |m|$.

The normalized solutions are given by :

$$\Theta(\theta) = \Theta_{\ell, \pm m}(\theta) = \left[\frac{2\ell+1}{2} \frac{(\ell-|m|)!}{(\ell+|m|)!} \right]^{1/2} P_{\ell}^{|m|} \cos\theta \quad \dots(19)$$

The energy eigenvalues of the rigid rotor are obtained as follows :

$$\beta = 8\pi^2 IE / h^2 = \ell(\ell+1) \quad \dots(20)$$

$$\text{Thus, } E = \frac{\ell(\ell+1)h^2}{8\pi^2 I}; \ell = 0, 1, 2, 3 \quad \dots(21)$$

In spectroscopy it is customary to use the symbol J rather than l for the rotational quantum number so that the rotational energy levels are given by the expression.

$$E_J = \frac{J(J+1)}{8\pi^2 I}; J = 0, 1, 2, 3, \dots \quad \dots(22)$$

SOLVED PROBLEMS

1. The wave function (ψ) for hydrogen atom in terms of polar coordinates, is given by $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$. Which of the functions determines the shape of atomic orbitals ?
- (a) $R(r)$ (b) $\Theta(\theta)$ (c) $\Phi(\phi)$ (d) Both (b) & (c)

Soln. $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$

$R(r) \rightarrow$ Radial dependence of wavefunction (size of atomic orbital determined by radial part of wave function). $\Theta(\theta)\Phi(\phi) \rightarrow$ Angular dependence of wavefunction (shape of atomic orbital determined by angular part of wave function)

Correct option is (d)

2. Which of the following sets of quantum numbers is correct for an electron of $4f$ orbital ?

- (a) $n = 4, l = 3, m = +4, s = +\frac{1}{2}$ (b) $n = 4, l = 4, m = -4, s = -\frac{1}{2}$
- (c) $n = 4, l = 3, m = +1, s = +\frac{1}{2}$ (d) $n = 3, l = 2, m = -2, s = +\frac{1}{2}$

Soln. For $4f$ -orbital $n = 4, l = 3$

For $n = 4$, possible l -values are $l = 0, 1, \dots (n-1) = 0, 1, 2, 3$

For $l = 3$, possible m_l values are $m_l = -3, -2, -1, 0, 1, 2, 3$

Correct option is (c)