

Normalization condition of the function  $Y_\ell^{m_\ell}(\theta, \phi)$ :

$$\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_{l,m_l}^*(\theta, \phi) Y_{l,m_l}(\theta, \phi) \sin \theta \, d\theta \, d\phi = 1$$

**Solution of  $R(r)$  equation:** The radial part of the Schrodinger equation is,

$$-\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{2m}{\hbar^2} r^2 [E - V(r)] = C = -\ell(\ell+1) \quad [\because C = -\ell(\ell+1)]$$

$$\Rightarrow \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left\{ \frac{2m}{\hbar^2} [E - V(r)] - \frac{\ell(\ell+1)}{r^2} \right\} R = 0 \quad (18)$$

Now,  $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) = R(r)\Omega(\theta, \phi) = R(r)Y_\ell^{m_\ell}(\theta, \phi)$

This is the complete three-dimensional wave function of the Schrodinger wave equation for a particle moving in a spherically symmetric  $V(r)$ . For a bound system, the wave function must satisfy the condition that

$$R(r) \rightarrow 0, \text{ as } r \rightarrow \infty$$

If  $V(r)$  is known, then only an explicit solution of (18) can be found out. Since equation (18) depend on  $n$  and  $l$  can have a discrete set of values, the allowed energy values must be discrete say,  $E_1^\ell, E_2^\ell, \dots, E_n^\ell$ . The complete wave function of the particle corresponding to energy  $E_n$  can be written as

$$\psi_{n,\ell,m_\ell} = R_n^\ell(r) Y_{l,m_l}(\theta, \phi)$$

As  $m_\ell$  has  $(2\ell+1)$  values, ranging from  $-\ell$  to  $+\ell$  in integral steps, there will be  $(2\ell+1)$  wave function, each differing in  $m_\ell$ -values. Thus the energy state of the particle is  $(2\ell+1)$  fold degenerate. The quantities  $n, \ell$  and  $m_\ell$  are known as the principal quantum number, orbital quantum number and azimuthal quantum number respectively. These quantum numbers are needed to specify the different states.

### 5.5 Hydrogen atom :

The simplest of the atoms is the hydrogen atom, consisting of a single electron moving around the nucleus containing only one nucleon (the proton) under a central force arising out of the Coulombian electrostatic attractive force. It forms the basis for the theoretical formulation of more complex atomic systems containing more than one electron. The old quantum theory was first proposed by N. Bohr (in 1912) on the basis of hydrogen atom. Schrodinger gave the solution of the wave equation for hydrogen atom is 1926 formulating the wave mechanics. There was extensive development of quantum theory of the hydrogen atom by the subsequent workers, viz, W. Heisenberg, max Born and Jordon and Pauli.

The results of hydrogen atom was successfully extended to other hydrogenic atoms. The hydrogenic atoms are of two types:

- (i) Ionised atoms containing only one electron moving around the nucleus, which may consist of more than one proton and neutron. Singly ionised Helium ( $\text{He}^+$ ), doubly ionised Lithium ( $\text{Li}^{++}$ ), triply ionised Beryllium ( $\text{Be}^{+++}$ ) are some of the hydrogenic atoms.
- (ii) Atoms or, ions with closed shells and only one electron in the outermost shell form the second type of hydrogenic atoms. Atoms of alkali metal and alkaline earth ions are the examples.

#### The wave equation for the hydrogen atom:

The hydrogen or, hydrogenic atom is a two-particle system consisting of an electron of charge  $-e$  moving round the nucleus of charge  $+Ze$ . The electron in this system moves under the central force arising out of the Coulombic electrostatic attraction between the nucleus and the electron along the radius of the circular path of motion.

The potential energy of the system in absence of any external field is,

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{ze^2}{r}$$

The potential energy is independent of  $\theta$  and  $\phi$  and thus spherically symmetric. Reducing the two body problem into one body problem, the 3-D Schrodinger equation in spherical polar coordinates can be written as

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2) \frac{\partial \psi}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2\mu}{\hbar^2} [E - V(r)] \psi = 0$$

where  $\mu = \frac{m_{nucleus} m_e}{m_{nucleus} + m_e}$  is the reduced mass of the system.

Using separation of variable technique, one can find the solution of the above equation to be

$$\psi(r, \theta, \phi) = R_{nl}(r) \Theta_{lm}(\theta) \Phi_m(\phi)$$

where

$$R_{nl}(r) = \left[ \frac{\left(\frac{2z}{na_0}\right)^3 (n-l-1)!}{2n[(n+l)!]^3} \right]^{1/2} e^{-\frac{zr}{na_0}} \left(\frac{2zr}{na_0}\right)^l L_{n+l}^{2l+1}\left(\frac{2zr}{na_0}\right)$$

$$\Theta_{lm}(\theta) = \left[ \frac{(2l+1)(l-m)!}{2 \cdot (l+m)!} \right]^{1/2} P_l^m(\cos \theta)$$

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

**Table : Normalised radial wave functions:**

$n$	$\ell$	$R_{n\ell}(r)$
1	0	$2 \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
2	0	$\frac{1}{2\sqrt{2}} \left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	$\frac{1}{2\sqrt{6}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}$
3	0	$\frac{2}{81\sqrt{3}} \left(\frac{1}{a_0}\right)^{3/2} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	$\frac{4}{81\sqrt{6}} \left(\frac{1}{a_0}\right)^{3/2} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{4}{81\sqrt{30}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r^2}{a_0^2} e^{-r/3a_0}$