## Outline of the solution of Schrödinger equation for H-atom

The potential energy of the electron in H-atom is

$$E_p = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

where $r = \sqrt{x^2+y^2+z^2}$ is the distance between the electron and the proton. If the nucleus has more than a single positive charge we must include the additional charges in the Coulomb energy. We do this by a multiplicative term Z, called the atomic number.

$$E_p = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r} \tag{1}$$

Schrodinger equation for H-atom can be written as

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right]+E_p\left(x,y,z\right)\psi = E\psi$$

It is much simpler to solve the equation if we write it in spherical coordinates. In spherical coordinates the Schrodinger equation becomes

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

This equation can be solved by the standard technique of separation of variables; we try a solution of the form,

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

where $R$, $\Theta$, and $\Phi$ are functions of only one coordinate. On substitution into Eq. 2, rearrangement of terms, and division of both sides of the resulting equation by $R(r)$, $\Theta(\theta)$, and $\Phi(\phi)$, we obtain

$$-\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2m}{\hbar^2}r^2\sin^2\theta\left[E-E_p(r)\right]$$
$$-\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} \tag{3}$$

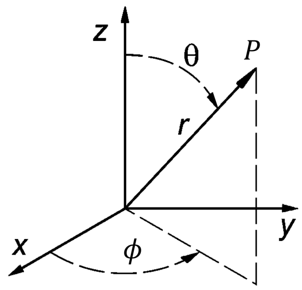


Figure 1: Spherical coordinates $r$, $\theta$, and $\phi$ of a point $P$.

The left side of Eq. 3 is a function of $r$ and $\theta$ alone, whereas the right side is a function of $\phi$ alone. The only way the equation can be valid is when both sides of the equation are equal to the same constant. For convenience, we let this constant be $-m_l^2$. The right side of the equation gives us equation

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m_l^2 \tag{4}$$

The left side of Eq. 3, after being set equal to the constant $m_l^2$ and rearranged, may be written as

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left[E-E_p(r)\right]=\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

Again, one side of this equation is a function of the variable $r$ only, whereas the other side is a function of the variable $\theta$ only. The only way the equality can be valid is when both sides are equal to the same constant. If we call this constant $l(l+1)$, $l$ will be an integer. We now get two differential equations, one for $R(r)$ and another for $\Theta(\theta)$.

$$\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = l(l+1) \tag{5}$$

and,

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left[E - E_p(r)\right] = l(l+1) \tag{6}$$

The next step is to solve the three differential equations (4, 5, and 6).

1. When we solve Eq. 4, we find that the only solutions for $\Phi$ that are single-valued are those for which

$$m_l = 0, \pm 1, \pm 2, ... \tag{7}$$

2. When we solve Eq. 5 for $\Theta$, we find that the only solutions that are valid only when

$$l = 0, 1, 2, .... \tag{8}$$

and

$$l \geq |m_l|$$

3. When we solve Eq. 6. we find the solution

$$E_n = -\frac{Z^2 e^4}{8\epsilon_0^2 h^2}\frac{1}{n^2} \qquad n = 1, 2, 3, ... \tag{9}$$

and

$$l < n$$

The restrictions on the values that $m_l$ and $I$ can take can now be restated as follows:

$$m_l = 0, \pm 1, \pm 2, ...., \pm l \tag{10}$$

and

$$l = 0, 1, 2, ..., n-1 \tag{11}$$

**Physical Significance of the Results**

The most important result of the solution of the Schrodinger equation for the H atom is the fact that the energy of the atom is quantized. The spectrum of energy levels is the same as the one postulated by Bohr. Because the energy depends only on the quantum number $n$, it is called the principal quantum number.

Similary it gives two more quantum number $l$ and $m_l$, and the wavefunction is written with the quantum numbers as subscripts, $\psi_{n,l,m_l}$.

The quantum number $l$ is called the orbital quantum number, because $l$ determines the magnitude of the angular momentum $L$ of the atom.

The quantum number $m_l$ is called the magnetic quantum number. It can be shown that if an atom is placed in a magnetic field directed along the $z$ direction, the $z$ component of the angular momentum L of the atom is given by

$$L_z = m\hbar$$