

Lecture 8 -Title: Quantum Mechanical treatment of One-electron atoms : radial part

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In the previous lecture, we have solved the angular part of the Hamiltonian.

In this lecture, we will take up the radial part of the Hamiltonian.

We will also determine the total wavefunction of the Hydrogen atom and will calculate the energy levels.

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Now, let us solve the radial part (Eqn. 8.8)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{\ell(\ell+1)}{r^2} \right] R = 0$$

Let us first evaluate the ground state (lowest energy) of hydrogen atom.

Assuming the ground state and taking $\ell = 0$, we get

$$\begin{aligned} & \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) R = 0 \\ \Rightarrow & \frac{1}{r^2} \left[r^2 \frac{d^2 R}{dr^2} + 2r \frac{dR}{dr} \right] + \frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) R = 0 \\ \Rightarrow & \frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) R = 0 \end{aligned}$$

..... Eqn. (21)

Let us try a solution $R(r) = Ae^{-r/a_0}$, where A and a_0 are constants.

$$\begin{aligned} \frac{dR(r)}{dr} &= -\frac{A}{a_0} e^{-r/a_0} ; \quad \frac{d^2 R}{dr^2} = \frac{A}{a_0^2} e^{-r/a_0} \\ \frac{A}{a_0^2} e^{-r/a_0} - \frac{2A}{ra_0} e^{-r/a_0} + \frac{2A\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) e^{-r/a_0} &= 0 \\ \Rightarrow \left(\frac{1}{a_0^2} + \frac{2\mu E}{\hbar^2} \right) + \left(\frac{2\mu Ze^2}{4\pi\epsilon_0 \hbar^2} - \frac{2}{a_0} \right) \frac{1}{r} &= 0 \end{aligned}$$

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To satisfy this equation for any value of r ,

$$\frac{1}{a_0^2} + \frac{2\mu E}{\hbar^2} = 0$$

$$\Rightarrow E = -\frac{\hbar^2}{2\mu a_0^2}$$

.....Eqn. (22)

and

$$\frac{2\mu Ze^2}{4\pi\epsilon_0\hbar^2} - \frac{2}{a_0} = 0$$

$$\Rightarrow a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu Ze^2} = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} \quad [for Z=1]$$

.....Eqn. (23)

Let us calculate the values of a_0 and Ground State Energy E ,

$$\mu = \frac{m_e m_p}{m_e + m_p}$$

$$\approx 9.109 \times 10^{-31} \text{ Kg}$$

$$\left(\begin{array}{l} \text{where } m_e = 9.109 \times 10^{-31} \text{ Kg} \\ m_p = 1.672 \times 10^{-27} \text{ Kg} \\ \text{and } m_p \gg m_e \end{array} \right)$$

$$e = 1.6 \times 10^{-19} \text{ Coul}$$

$$\frac{1}{4\pi\epsilon_0} = 8.988 \times 10^9 \text{ nt-m}^2/\text{Coul}^2$$

$$\hbar = 1.055 \times 10^{-34} \text{ J-sec} = 0.6582 \times 10^{-15} \text{ eV-sec}$$

$$a_0 = \frac{(1.055 \times 10^{-34})^2}{8.988 \times 10^9 \times (1.6 \times 10^{-19})^2 \times 9.109 \times 10^{-31}}$$

$$= \frac{1.055 \times 1.055}{8.988 \times 1.6 \times 1.6 \times 9.109} \times 10^{-34-34+19+19+31-9}$$

$$= 0.00531 \times 10^{-8} \text{ m} = 0.529 \times 10^{-10} \text{ m} = 0.529 \text{ \AA}$$

which is same as Bohr Radius.

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Substituting value of a_0 in Eqn. (8.22),

$$\begin{aligned} E &= -\frac{\hbar^2}{2\mu a_0^2} \\ &= \frac{(1.055 \times 10^{-34})^2}{2 \times 9.109 \times 10^{-31} \times (0.529 \times 10^{-10})^2} = \frac{1.113 \times 10^{-68}}{5.098 \times 10^{-51}} \\ &= \frac{0.2183 \times 10^{-17}}{1.6 \times 10^{-19}} = 0.1364 \times 10^{+2} = -13.6 \text{ eV} \end{aligned}$$

This is the lowest energy state of Hydrogen obtained also from Bohr's calculation.

Now let us calculate the general radial equation,

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{\ell(\ell+1)}{r^2} \right] R = 0$$

The radial derivatives simplify if one factor $\frac{1}{r}$ out from function R , taking

$$R(r) = \frac{u(r)}{r}$$

.....Eqn. (24)

$$\begin{aligned} \frac{dR}{dr} &= \frac{r \frac{du}{dr} - u}{r^2} \\ \Rightarrow r^2 \left(\frac{dR}{dr} \right) &= r \frac{du}{dr} - u \\ \Rightarrow \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) &= r \frac{d^2u}{dr^2} + \cancel{\frac{du}{dr}} - \cancel{\frac{du}{dr}} \\ \Rightarrow \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) &= r \frac{d^2u}{dr^2} \end{aligned}$$

Substituting,

$$\frac{1}{r} \frac{d^2 u(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{\ell(\ell+1)}{r^2} \right] \frac{u(r)}{r} = 0$$

$$\Rightarrow \frac{d^2 u(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} \left(E + \frac{Ze^2}{4\pi\epsilon_0 r} \right) - \frac{\ell(\ell+1)}{r^2} \right] u(r) = 0$$

.....Eqn. (25)

This is the Schrödinger equation for the particle in one dimension, restricted to $r > 0$.

Rearranging

$$\frac{d^2 u(r)}{dr^2} + \left[\frac{2\mu E}{\hbar^2} - \underbrace{\left\{ -\frac{2\mu Ze^2}{4\pi\epsilon_0 \hbar^2 r} + \frac{\ell(\ell+1)}{r^2} \right\}}_{V_{\text{effective}}} \right] u(r) = 0$$

This is a kind of potential (*for* $\ell \neq 0$) with positive infinity at the origin, then negative potential and going to zero at large distances. So the minimum of the potential is at some positive r .

For bound states of proton-electron system, E will be a negative quantity.

Now, we will simplify by introducing dimensionless variable, ρ such as

$$\rho = +\alpha r$$

$$d\rho = +\alpha dr$$

$$d\rho^2 = \alpha^2 dr^2$$

$$\begin{aligned} & \frac{\hbar^2}{2\mu} \frac{d^2 u(r)}{dr^2} + \left[E + \frac{Ze^2}{4\pi\epsilon_0 r} - \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} \right] u(r) = 0 \\ \Rightarrow & \frac{\hbar^2}{2\mu} \alpha^2 \frac{d^2 u(\rho)}{d\rho^2} + \left[E + \frac{Ze^2 \alpha}{4\pi\epsilon_0 \rho} - \frac{\hbar^2}{2\mu} \frac{\alpha^2 \ell(\ell+1)}{\rho^2} \right] u(\rho) = 0 \\ \Rightarrow & -\frac{\cancel{\hbar^2}}{\cancel{2\mu}} \frac{\cancel{2\mu} E}{\cancel{\hbar^2}} \frac{d^2 u(\rho)}{d\rho^2} + \left[E + \frac{Ze^2 \alpha}{4\pi\epsilon_0 \rho} - \frac{\cancel{\hbar^2}}{\cancel{2\mu}} \frac{\cancel{2\mu} E}{\cancel{\hbar^2}} \frac{\ell(\ell+1)}{\rho^2} \right] u(\rho) = 0 \\ \Rightarrow & -\frac{d^2 u(\rho)}{d\rho^2} + \left[1 + \frac{Ze^2 \alpha}{4\pi\epsilon_0 E} \frac{1}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u(\rho) = 0 \\ \Rightarrow & \frac{d^2 u(\rho)}{d\rho^2} = \left[1 - \frac{Ze^2}{4\pi\epsilon_0 E} \frac{1}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u(\rho) \\ & = \left[1 - \frac{Z\mu e^2}{2\pi\epsilon_0 \hbar^2 \alpha} \frac{1}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u(\rho) \end{aligned}$$

Substituting $\rho_0 = \frac{Z\mu e^2}{2\pi\epsilon_0 \hbar^2 \alpha}$, we get

$$\frac{d^2 u(\rho)}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u(\rho)$$

.....Eqn. (26)

Here, we understand the asymptotic behavior of solution of the equation 8.26.

Case-I: when ρ is very large (at large separation between proton and electron), we can neglect the ρ terms in equation 8.26 and we get,

$$\frac{d^2 u(\rho)}{d\rho^2} = u(\rho)$$

The solution is of the type,

$$u(\rho) = Ae^{-\rho} + Be^{+\rho}$$

Since e^{ρ} becomes infinite for large ρ , we take $B = 0$ and hence,

$$u(\rho) \sim Ae^{-\rho}$$

Case-III: When ρ is very small, then $\frac{1}{\rho^2}$ is the dominant term, so,

$$\frac{d^2 u(\rho)}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2} u(\rho) \quad [Note \ell \neq 0]$$

The solution, $\frac{d^2 u(\rho)}{d\rho^2} = C\rho^{\ell+1} + D\rho^{-\ell}$

Again, as $\rho \rightarrow 0$; $\rho^{-\ell}$ becomes infinite.

So we take, $D = 0$

So, for small ρ ,

$$u(\rho) \sim C\rho^{\ell+1}$$

So, we have established that the solution $u(\rho)$ decays as $e^{-\rho}$ at large distance and goes as $\rho^{\ell+1}$ close to the proton (origin).

Now we write the general solution of equation as

$$u(\rho) = \rho^{\ell+1} e^{-\rho} \omega(\rho)$$

.....Eqn. (27)

where, $\omega(\rho)$ we have to define.

Let us substitute $u(\rho)$ into the Eqn. (8.26)

$$\begin{aligned} \frac{d u(\rho)}{d \rho} &= \rho^{\ell+1} e^{-\rho} \frac{d \omega(\rho)}{d \rho} + (\ell+1) \rho^{\ell} e^{-\rho} \omega(\rho) - \rho^{\ell+1} e^{-\rho} \omega(\rho) \\ &= \rho^{\ell} e^{-\rho} \left[\rho \frac{d \omega(\rho)}{d \rho} + (\ell+1-\rho) \omega(\rho) \right] \end{aligned}$$

and

$$\frac{d^2 u(\rho)}{d \rho^2} = e^{-\rho} \rho^{\ell} \left[\rho \frac{d^2 \omega(\rho)}{d \rho^2} + 2(\ell+1-\rho) \frac{d \omega(\rho)}{d \rho} + \left\{ \frac{\ell(\ell+1)}{\rho} - 2(\ell+1) + \rho \right\} \omega(\rho) \right]$$

Substituting in Eqn. (8.26)

$$\begin{aligned} & \cancel{e^{-\rho}} \rho^{\ell} \left[\rho \frac{d^2 \omega(\rho)}{d \rho^2} + 2(\ell+1-\rho) \frac{d \omega(\rho)}{d \rho} + \left\{ \frac{\ell(\ell+1)}{\rho} - 2(\ell+1) + \rho \right\} \omega(\rho) \right] \\ &= \rho \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] \cancel{e^{-\rho}} \rho^{\ell} \omega(\rho) \\ \Rightarrow & \rho \frac{d^2 \omega(\rho)}{d \rho^2} + 2(\ell+1-\rho) \frac{d \omega(\rho)}{d \rho} + \left\{ \frac{\cancel{\ell(\ell+1)}}{\cancel{\rho}} - 2(\ell+1) + \cancel{\rho} - \cancel{\rho} + \rho_0 - \frac{\cancel{\ell(\ell+1)}}{\cancel{\rho}} \right\} \omega(\rho) = 0 \\ \Rightarrow & \rho \frac{d^2 \omega(\rho)}{d \rho^2} + 2(\ell+1-\rho) \frac{d \omega(\rho)}{d \rho} + \{ \rho_0 - 2(\ell+1) \} \omega(\rho) = 0 \end{aligned}$$

.....Eqn. (28)

Now, we have to solve this equation 8.28. Let us take a solution of the form,

$$\omega(\rho) = \sum_{j=0}^{\infty} C_j \rho^j$$

$$\text{So, } \frac{d\omega(\rho)}{d\rho} = \sum_{j=0}^{\infty} j C_j \rho^{j-1}$$

$$\text{and } \frac{d^2\omega(\rho)}{d\rho^2} = \sum_{j=0}^{\infty} j(j-1) C_j \rho^{j-2}$$

Putting back to Eqn. (8.27)

$$\sum_{j=0}^{\infty} j(j-1) C_j \rho^{j-1} + 2(\ell+1) \sum_{j=0}^{\infty} j C_j \rho^{j-1} - 2 \sum_{j=0}^{\infty} j C_j \rho^j + (\rho_0 - 2(\ell+1)) \sum_{j=0}^{\infty} C_j \rho^j = 0$$

Shifting the summation of the ρ^{j-1} terms

$$\sum_{j=-1}^{\infty} (j+1) j C_{j+1} \rho^j + 2(\ell+1) \sum_{j=-1}^{\infty} (j+1) C_{j+1} \rho^j - 2 \sum_{j=0}^{\infty} j C_j \rho^j + (\rho_0 - 2(\ell+1)) \sum_{j=0}^{\infty} C_j \rho^j = 0$$

For, $j = -1$, the first two terms becomes zero. So, we start from $j = 0$

$$\begin{aligned} & \sum_{j=0}^{\infty} j(j+1) C_{j+1} \rho^j + 2(\ell+1) \sum_{j=0}^{\infty} (j+1) C_{j+1} \rho^j - 2 \sum_{j=0}^{\infty} j C_j \rho^j + (\rho_0 - 2(\ell+1)) \sum_{j=0}^{\infty} C_j \rho^j = 0 \\ \Rightarrow & \sum_{j=0}^{\infty} [j(j+1) C_{j+1} + 2(\ell+1)(j+1) C_{j+1} - 2j C_j + (\rho_0 - 2(\ell+1)) C_j] \rho^j = 0 \end{aligned}$$

This is valid, if all the coefficients of ρ^j are zero.

$$j(j+1)C_{j+1} + 2(\ell+1)(j+1)C_{j+1} - 2jC_j + (\rho_0 - 2(\ell+1))C_j = 0$$

$$\Rightarrow C_{j+1} = \frac{(2j+2(\ell+1)) - \rho_0}{(j+1)(j+2(\ell+1))} C_j$$

.....Eqn. (29)

Let us examine the behavior at large j value. For large j value, we ignore $(\ell+1)$ and ρ_0 , so,

$$C_{j+1} = \frac{2}{(j+1)} C_j$$

Taking the value C_0 for $j = 0$

$$C_1 = \frac{2}{1} C_0$$

$$C_2 = \frac{2}{2} C_1 = \frac{2^2}{1 \times 2} C_0$$

$$C_3 = \frac{2}{3} C_2 = \frac{2^3}{1 \times 2 \times 3} C_0$$

$$\therefore C_j = \frac{2^j}{j!} C_0$$

Thus,

$$\omega(\rho) = \sum_{j=0}^{\infty} C_j \rho^j = C_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j$$

$$= C_0 e^{2\rho}$$

Returning back in Eqn. (8.27), the general solution,

$$\begin{aligned} u(\rho) &= \rho^{\ell+1} e^{-\rho} \omega(\rho) \\ &= \rho^{\ell+1} e^{-\rho} C_0 e^{2\rho} \\ &= C_0 \rho^{\ell+1} e^{\rho} \end{aligned}$$

Again, the value of $u(\rho)$ increases exponentially for large ρ and cannot be accepted. The series has to terminate at finite number before reaching the large value of ρ .

So, we should expect, that at some finite value of j , Eqn. (8.29)

$$2(j + \ell + 1) = \rho_0$$

So, ρ_0 should be an even integer.

We define, $\rho_0 = 2n$

$$\frac{Z\mu e^2}{2\pi\epsilon_0 \hbar^2 \alpha} = 2n$$

$$\text{So, } \alpha = \frac{Z\mu e^2}{4\pi\epsilon_0 \hbar^2 n}$$

and,

$$\begin{aligned} \sqrt{-\frac{2\mu E}{\hbar^2}} &= \frac{Z\mu e^2}{4\pi\epsilon_0 \hbar^2 n} \\ \Rightarrow -\frac{2\mu E}{\hbar^2} &= \frac{Z^2 \mu^2 e^4}{(4\pi\epsilon_0)^2 \hbar^4 n^2} \\ \Rightarrow E &= -\frac{Z^2 \mu e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} \end{aligned}$$

This is same energy as Bohr formula for Hydrogen putting $Z = 1$.

Substituting $\rho_0 = 2n$ in Eqn.8.29 this

$$\begin{aligned} C_{j+1} &= \frac{2(j+\ell+1)-2n}{(j+1)(j+2(\ell+1))} C_j \\ &= -\frac{2(n-\ell-1-j)-2n}{(j+1)(2\ell+j+2)} C_j \end{aligned}$$

In fact, the solution of Eqn.8.28 is known as Associated Laguerre polynomials which is of the form

$$\begin{aligned} \omega(\rho) &= L_{n-\ell-1}^{2\ell+1}(2\rho) \\ &= \sum_{j=0}^{\infty} \frac{(-1)^j 2^j (n+\ell)!}{(n-\ell-j-1)!(2\ell+j+1)! j!} \end{aligned}$$

So, the coefficients

$$\begin{aligned} C_j &= \frac{(-1)^j 2^j (n+\ell)!}{(n-\ell-j-1)!(2\ell+j+1)! j!} \\ \frac{C_{j+1}}{C_j} &= -\frac{2(n-\ell-1-j)}{(j+1)(2\ell+j+2)} \end{aligned}$$

which is same as before.

In fact, rearranging Eqn. (8.28) we can get the solution as “Associated Laguerre Polynomials” of the differential equation of the form,

$$Z \frac{d^2}{dZ^2} L_{\bar{n}}^k(Z) + (k+1-Z) \frac{d}{dZ} L_{\bar{n}}^k(Z) + \bar{n} L_{\bar{n}}^k(Z) = 0$$

Substituting $Z = 2\rho$ in Eqn. (8.28), we get,

$$Z \frac{d^2}{dZ^2} \omega(Z) + [(2\ell+1)+1-Z] \frac{d\omega(Z)}{dZ} + \left[\frac{\rho_0}{2} - (\ell+1) \right] \omega(Z) = 0$$

$$\begin{aligned} \bar{n} &= \frac{\rho_0}{2} - (\ell+1) \\ \text{Here, } k &= 2\ell+1, \text{ and} \\ &= \frac{2n}{2} - (\ell+1) = n - (\ell+1) \end{aligned}$$

So the solution,

$$\omega(Z) = L_{n-(\ell+1)}^{2\ell+1}(Z) = L_{n-(\ell+1)}^{2\ell+1}(2\rho)$$

In this case, the solution (27) has to be rearranged and we get,

$$u(\rho) = (2\rho)^{\ell+1} e^{-\rho} L_{n-(\ell+1)}^{2\ell+1}(2\rho)$$

So,

$$\begin{aligned} rR_{n,\ell}(r) &= u(r) = \left(\frac{2r}{na_0} \right)^{\ell+1} e^{-r/na_0} L_{n-(\ell+1)}^{2\ell+1} \left(\frac{2r}{na_0} \right) \\ \Rightarrow R_{n,\ell}(r) &= N_{n,\ell} e^{-r/na_0} \left(\frac{2r}{na_0} \right)^{\ell} L_{n-(\ell+1)}^{2\ell+1} \left(\frac{2r}{na_0} \right) \end{aligned}$$

..... Eqn. (30)

Here we have added the normalization constant $N_{n,\ell}$ and absorbed the factor $\frac{2}{na_0}$ from the power term of r .

Now, we evaluate the normalization constant $N_{n,\ell}$ from the relation,

$$\int_0^\infty R_{n,\ell}^*(r) R_{n,\ell}(r) r^2 dr = 1$$

Substituting,

$$|N|^2 \left(\frac{na_0}{2} \right)^3 \int_0^\infty e^{-2r/na_0} \left(\frac{2r}{na_0} \right)^{2\ell+2} \left[L_{n-\ell-1}^{2\ell+1} \left(\frac{2r}{na_0} \right) \right]^2 d \left(\frac{2r}{na_0} \right) = 1$$

Here, we can use the orthogonality relation,

$$\int_0^\infty e^{-Z} Z^{k+1} L_n^k(Z) L_m^k(Z) dZ = \frac{\{(n+k)!\}^3}{n!} (2n+k+1) \delta_{mn}$$

So, we get, $|N_{n,\ell}|^2 \left(\frac{na_0}{2} \right)^3 \frac{2n\{(n+\ell)!\}^3}{(n-\ell-1)!} = 1$

So, $N_{n,\ell} = \sqrt{\left(\frac{2}{na_0} \right)^3 \frac{(n-\ell-1)!}{2n\{(n+\ell)!\}^3}}$

Normalized Radial Wavefunction,

$$R_{n,\ell}(r) = \sqrt{\left(\frac{2}{na_0} \right)^3 \frac{(n-\ell-1)!}{2n\{(n+\ell)!\}^3}} e^{-r/na_0} \left(\frac{2r}{na_0} \right)^\ell * L_{n-\ell-1}^{2\ell+1} \left(\frac{2r}{na_0} \right)$$

..... Eqn. (31)

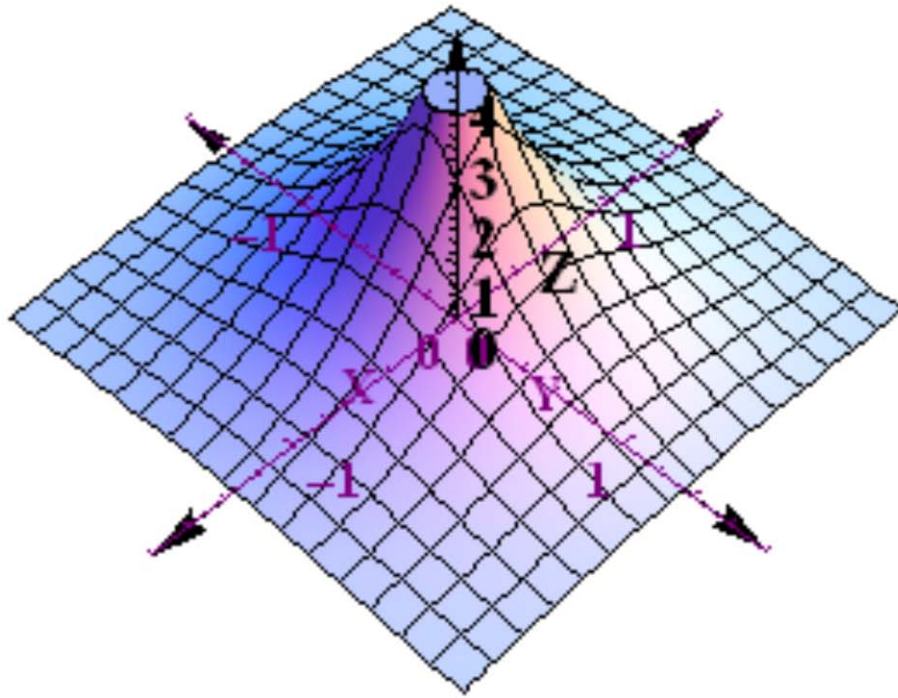
Some useful Associated Laguerre Polynomials

$$\begin{aligned} L_0^1(Z) &= 1 & ; & & L_0^3(Z) &= 6 \\ L_1^1(Z) &= 4 - 2Z & ; & & L_1^3(Z) &= 96 - 24Z \\ L_2^1(Z) &= 3Z^2 - 18Z + 18 \end{aligned}$$

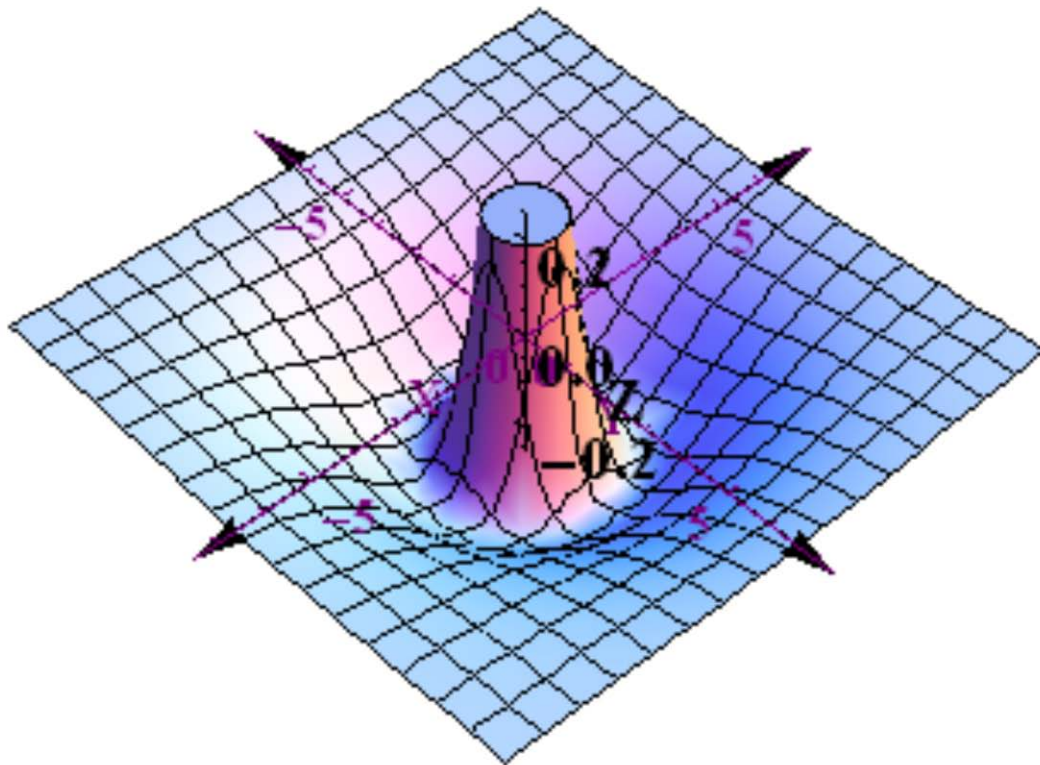
And the first few normalized radial wavefunction for Hydrogen,

Following figures show the plots of the radial function of the hydrogen atom.

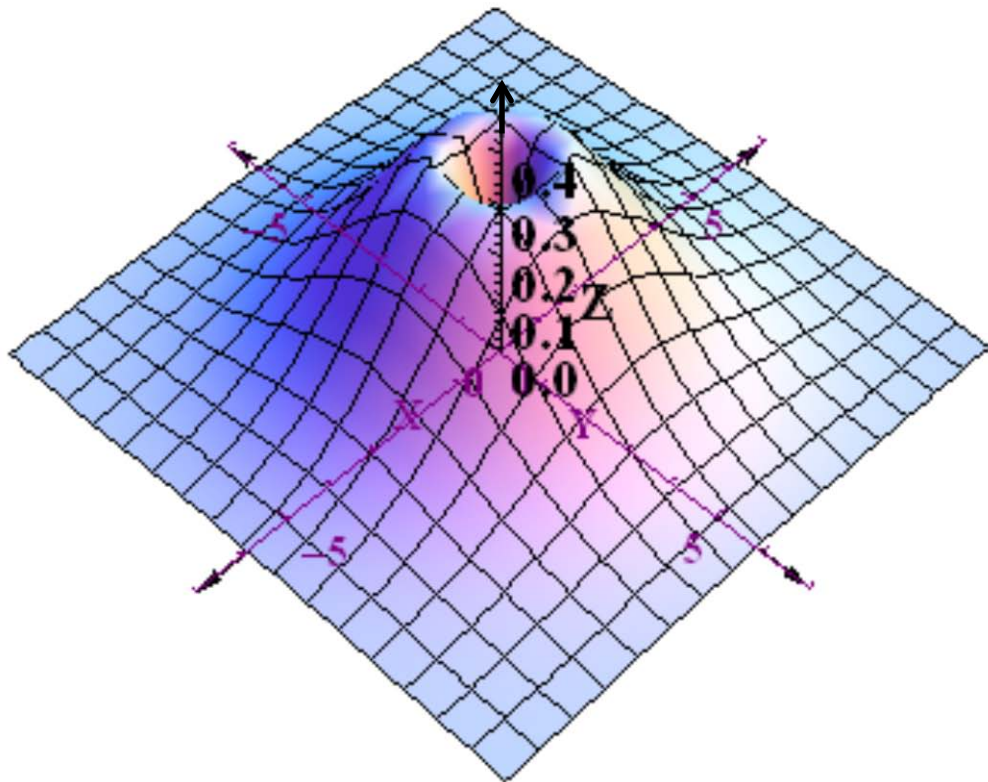
$$R_{1,0}(r) = 2a_0^{-3/2}e^{-r/a_0}$$



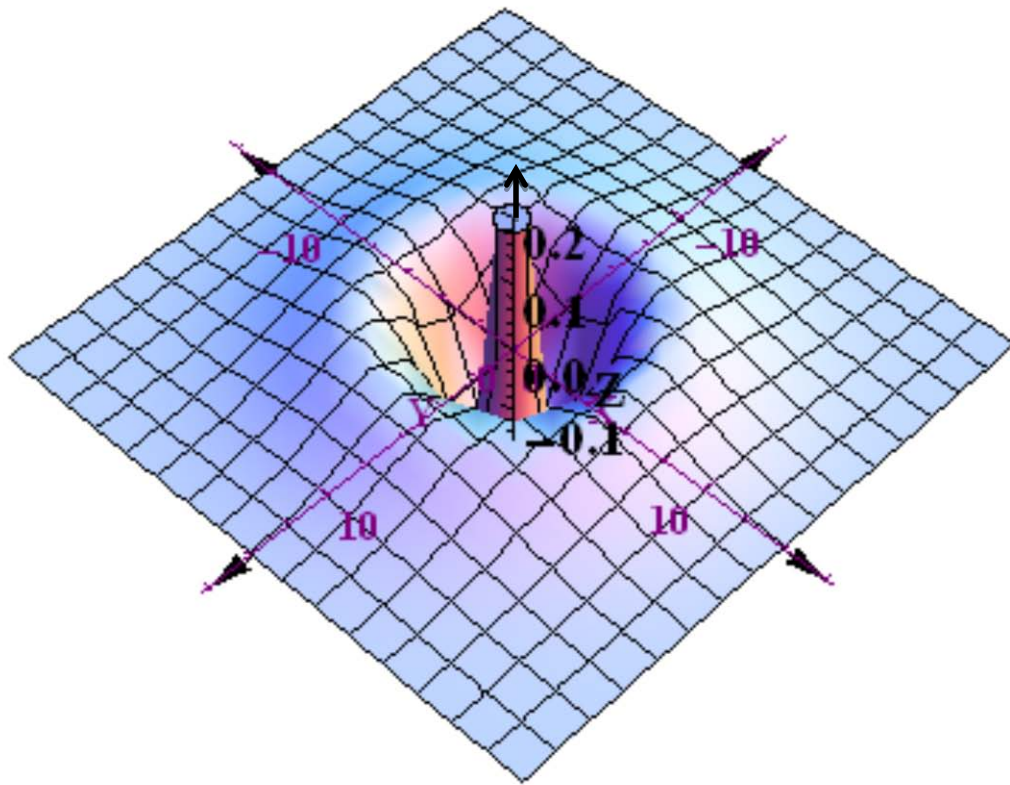
$$R_{2,0}(r) = \frac{1}{\sqrt{2}} a_0^{-3/2} \left(1 - \frac{r}{2a_0} \right) e^{-r/2a_0}$$



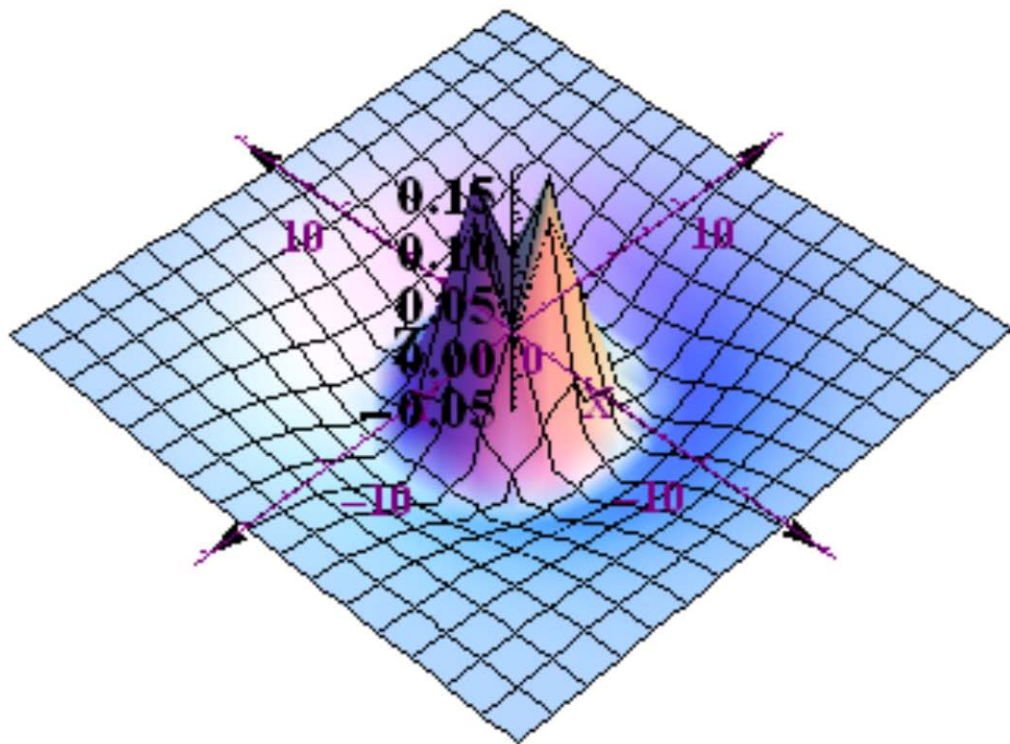
$$R_{2,1}(r) = \frac{1}{\sqrt{24}} a_0^{-3/2} \frac{r}{a_0} e^{-r/2a_0}$$



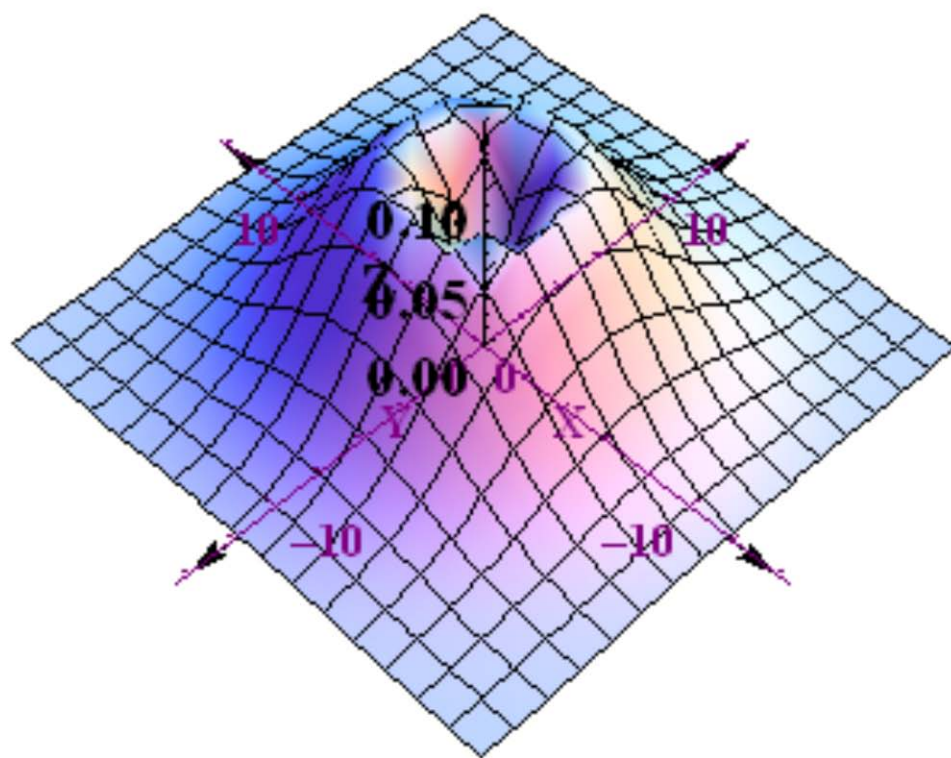
$$R_{3,0}(r) = \frac{2}{\sqrt{27}} a_0^{-3/2} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2} \right) e^{-r/3a_0}$$



$$R_{3,1}(r) = \frac{8}{27\sqrt{6}} a_0^{-3/2} \left(1 - \frac{r}{6a_0} \right) \frac{r}{a_0} e^{-r/3a_0}$$



$$R_{3,2}(r) = \frac{4}{81\sqrt{30}} a_0^{-3/2} \frac{r^2}{a_0^2} e^{-r/3a_0}$$



So the total wavefunction,

$$\Psi_{n,\ell,m} = R_{n,\ell}(r) \Theta_{\ell,m_\ell}(\theta) \Phi_{m_\ell}(\phi)$$

From Eqn. (8.20) and (8.31),

$$\Rightarrow \Psi_{n,\ell,m} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n\{(n+\ell)!\}^3}} e^{-r/na_0} \left(\frac{2r}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) \\ \times \sqrt{\frac{(2\ell+1)(\ell-m_\ell)!}{4\pi(\ell+m_\ell)!}} P_\ell^{m_\ell}(\cos\theta)$$

..... Eqn. (32)

Here, $n \Rightarrow$ Principle Quantum Number

$\ell \Rightarrow$ Azimuthal Quantum Number

$m_\ell \Rightarrow$ Magnetic Quantum Number

Recap

In this lecture, we have solved the radial part of the Hamiltonian.

We have also determined the total wavefunction of the Hydrogen atom.

The calculated energy levels depend on the principle quantum number n .

However, the total wavefunction of the electron is characterized by three quantum numbers, namely n , l , m_l .