3/5/01

Lec. 23 Hydrogen Atom

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

Radial equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

$$\psi(r,\theta,\phi) = \frac{u(r)}{r} Y_l^m(\theta,\phi)$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$ look for bound states $E < 0$

Note also scattering states $E > 0$

Let $\rho \equiv \kappa r$ $\quad \rho_0 \equiv \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa}$

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

Procedure (1) Find large ρ and small ρ behavior of $u(\rho)$

(2) Expand remainder in a power series $\sum a_i \rho^i$

(3) Require series to terminate so that $u(\rho)$ is normalizable $\int_0^\infty dr\, |u|^2 = 1$

(4) This gives allowed energies

For large ρ $\quad \frac{d^2u}{d\rho^2} \simeq u \Rightarrow u = Ae^{-\rho} + Be^{\rho}$

Chose $e^{-\rho}$ since e^{ρ} blows up at large ρ.

For very small ρ

$$\frac{d^2 u}{d\rho^2} \simeq \frac{l(l+1)}{\rho^2} u$$

$$u(\rho) = C \rho^{l+1} + D\rho^{-l} \quad \text{as } \rho \to 0$$

but ρ^{-l} blows up so keep ρ^{l+1}

Guess

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

This defines remainder function $v(\rho)$.
Plug into

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

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)] v = 0 \quad (*)$$

Assume a power series

$$v = \sum_{j=0}^{\infty} a_j \rho^j$$

$$\frac{dv}{d\rho} = \sum_j j a_j \rho^{j-1}$$

$$\frac{d^2 v}{d\rho^2} = \sum_j j(j-1) a_j \rho^{j-2}$$

put into equation (*) and require each power of ρ vanish

$$a_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} a_j$$

For wave function to be normalizable and $\to 0$ as $\rho \to \infty$ need series to terminate

$$a_{j_{max}+1} = 0$$

let

$$n \equiv j_{max} + l + 1$$

$$\Rightarrow \quad \rho_0 = 2n = \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa}$$

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{me^4}{8\pi^2\epsilon_0^2\hbar^2\rho_0^2}$$

$$\boxed{E = -\frac{m}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \frac{1}{n^2} = \frac{E_1}{n^2}} \qquad n = 1, 2, 3, \ldots$$

Bohr Formula

$$\kappa = \frac{me^2}{4\pi\epsilon_0\hbar^2}\frac{1}{n} = \frac{1}{an}$$

$$a \equiv \left(\frac{4\pi\epsilon_0\hbar^2}{me^2}\right) = 0.529 \times 10^{-10}\ \text{m}$$

Bohr radius

Note $\rho = r/an$

$$\alpha = \text{Fine structure constant} \equiv \frac{e^2}{4\pi\epsilon_0\hbar c}$$

$$\cong \frac{1}{137.036}$$

$$E = -\frac{mc^2}{2}\alpha^2\frac{1}{n^2}$$

$mc^2 = 0.511$ MeV rest mass of electron

$\hbar c = 197.33$ MeV-fm $= 1973.3$ eV-Å

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\, Y_\ell^m(\theta,\phi)$$

$$R_{n\ell} = \frac{1}{r}\rho^{\ell+1} e^{-\rho} v(\rho)$$

$$a_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)} a_j$$

$$E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = -\frac{mc^2}{2}\alpha^2$$

$$= -13.6 \text{ eV}$$

Ground state $n=1 = j_{max} + \ell + 1$

let $\ell = j_{max} = 0$

$$a_1 = \frac{2(0+0+1-1)}{1\cdot 3} a_0 = 0$$

$$v(\rho) = a_0 \qquad a_2 = a_3 = \cdots = 0$$

$$R_{10} = \frac{a_0}{a} e^{-r/a}$$

Normalize $\displaystyle\int_0^\infty |R_{10}|^2 r^2\, dr = 1$

$$R_{10}(r) = \frac{2}{a^{1/2}}\frac{1}{a} e^{-r/a} \qquad Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$\psi_{100} = R_{10} Y_0^0$$

$$\boxed{\psi_{100}(r,\theta,\phi) = \frac{1}{(\pi a^3)^{1/2}} e^{-r/a}}$$