11/2/98

Lecture #26 H Atom

Heavy motionless proton orbited by electron of charge $-e$

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

Full wave function

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

B. Conditions $U_{n\ell}(r\to 0) \to 0$

$U_{n\ell}(r\to\infty) \to 0$ so normalizabl.

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

$$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi\; Y^*_{\ell m}(\theta,\phi)\, Y_{\ell m}(\theta,\phi) = 1$$

Drop $n\ell$ label on U for now

Radial equation

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

Look for bound states $E<0$

$$\kappa = \sqrt{\frac{-2mE}{\hbar^2}}$$

Divide by E

$$\frac{1}{\kappa^2}\frac{d^2 u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa^2 r} + \frac{\ell(\ell+1)}{\kappa^2 r^2}\right]u \qquad 1$$

Define $\rho = \kappa r$, $\rho_0 = \dfrac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa}$

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

Coulomb pot $\sim \frac{1}{r}$ centrifugal term $\propto \frac{1}{r}$

Power series solution
1. Pull out asym. behavior both as $\rho \to \infty$ and $\rho \to 0$
2. Expand what's left over in power series.

As $\rho \to \infty$

$$\frac{\partial^2 u}{\partial \rho^2} \simeq u \Rightarrow u = Ae^{-\rho} + \cancel{Be^{\rho}}$$

$B=0$

As $\rho \to 0$ centrifugal term dominates

$$\frac{\partial^2 u}{\partial \rho^2} \simeq \frac{l(l+1)}{\rho^2} u \quad \text{as } \rho \to 0$$

$$u = C\rho^{(l+1)} + \cancel{D\rho^{-l}}$$

Guess

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

and plug into radial eq. $(*)$

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

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

$$\frac{dv}{d\rho} = \sum_{j=0}^{\infty} (j+1) a_{j+1} \rho^j$$

$$\frac{d^2 v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1)\, a_{j+1}\, \rho^{j-1}$$

Plug into **

$$\sum_{j=0}^{\infty} j(j+1)\, a_{j+1}\, \rho^{j} + 2(l+1)\sum_{j=0}^{\infty} (j+1)\, a_{j+1}\, \rho^{j}$$

$$- 2\sum_{j=0}^{\infty} j\, a_j\, \rho^{j} + [\rho_0 - 2(l+1)] \sum_{j=0} a_j\, \rho^{j} = 0$$

$$[j(j+1) + 2(l+1)(j+1)]\, a_{j+1} - 2j\, a_j$$

$$+ [\rho_0 - 2(l+1)]\, a_j = 0$$

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

Again argue this power series must terminate or wave function will not be normalizable

Consider limit $j \to$ large

$$a_{j+1} \cong \frac{2}{j}\, a_j$$

or $\quad a_j \sim \dfrac{2^j}{j!} A$

$$V(\rho) = \sum_j a_j\, \rho^j = A \sum_{j=0} \frac{(2\rho)^j}{j!}$$

$$\sim e^{2\rho}$$

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

and this is not normalizable
so there must be a maximum j
such that

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

or $$2(j_{max} + l + 1) - \rho_0 = 0$$

Define principle quantum # n

$$n = j_{max} + l + 1$$

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

and $$\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$$

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

$$\boxed{E_n = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2} = \frac{E_1}{n^2}}$$

$n = 1, 2, 3, \ldots$ Bohr formula

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

$$= -\frac{1}{2} mc^2 \alpha^2 = \frac{1}{2} 0.511 \text{ MeV}\left(\frac{1}{137.036}\right)^2$$

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

$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ so $\frac{e^2}{4\pi\epsilon_0}$ has units energy - length

$\hbar c$ has units energy - length $= 197.33$ MeV-Fm

$\alpha \equiv \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c}$ is dimensionless

Fine structure constant $\alpha \simeq \frac{1}{137.036}$

Determines strength of E+M interaction

$\kappa = \left(\frac{m e^2}{4\pi\epsilon_0 \hbar^2}\right)\frac{1}{n} = \frac{1}{a n}$

$a = \frac{4\pi\epsilon_0 \hbar^2}{m e^2} = \frac{\hbar c}{m c^2}\left(\frac{4\pi\epsilon_0}{e^2}\hbar c\right) = \hbar c\left(\frac{\alpha^{-1}}{m c^2}\right)$

$= 197.33 \text{ MeV-Fm} \left(\frac{1}{137.036}\right)^{-1}\left(\frac{1}{0.511 \text{ MeV}}\right)$

$= 5.29 \times 10^4$ Fm $\qquad 1 \text{ Fm} = 10^{-15}$ m

$\boxed{a = 0.529 \times 10^{-10} \text{ m}}$ Bohr radius determines size of atom

$\rho = r/(a n)$

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

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

v is polynomial of degree

$j_{max} = n - \ell - 1$ in ρ

Ground state $n=1 \Rightarrow l=m=0$

$$v(\rho) = A \quad \text{const.}$$

$$\psi_{100} = A \frac{\rho^{l+1}}{r} e^{-\rho} \, Y_0^0(\theta,\phi)$$

$$\rho = \kappa r = r/a$$

$$\psi_{100} = \frac{A}{a} e^{-r/a} \, Y_0^0$$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$\int d^3r \, \psi_{100}^* \psi_{100} = 1 = \int_0^\infty r^2 dr \left(\frac{A}{a}\right)^2 e^{-2r/a} \underbrace{\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \, Y_0^{0*} Y_0^0}_{1}$$

$$= \int_0^\infty r^2 dr \, \frac{A^2}{a^2} e^{-2r/a} = A^2 \frac{a}{4} = 1$$

$$A = \frac{2}{\sqrt{a}}$$

$$\psi_{100} = \frac{2}{a^{3/2}} e^{-r/a} \, Y_0^0(\theta,\phi)$$

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