Hydrogen Atom

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interested in the wavefunction of the electron

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

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

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

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

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

As $\rho\to\infty$, $\quad u'' = u \longrightarrow u(\rho) \overset{\rho\to\infty}{\approx} Ae^{-\rho} + \cancel{Be^{+\rho}}$ $\to\infty$

As $\rho\to 0$, $\quad u'' = \frac{\ell(\ell+1)}{\rho^2}u \longrightarrow u(\rho) \overset{\rho\to 0}{\approx} C\rho^{\ell+1} + \cancel{D\rho^{-\ell}}$ Boom!

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

$$\longrightarrow \rho v'' + 2(\ell+1-\rho)v' + [\rho_0 - 2(\ell+1)]v = 0$$

Let $v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j$

$$v'(\rho) = \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=1}^{\infty} j c_j\rho^{j-1}$$

$$v''(\rho) = \sum_{j=1}^{\infty} j(j-1)c_j\rho^{j-2} = \sum_{j=2}^{\infty} j(j-1)c_j\rho^{j-2}$$

$$\overbrace{\sum_{j=2}^{\infty} j(j-1)c_j\rho^{j-1}}^{\rho v''} + \overbrace{\sum_{j=1}^{\infty} 2(\ell+1)j c_j\rho^{j-1}}^{2(\ell+1)v'} \overbrace{- 2\sum_{j=1}^{\infty} j c_j\rho^j}^{-2\rho v'}$$

$$\underbrace{+ (\rho_0 - 2(\ell+1))\sum_{j=0}^{\infty} c_j\rho^j}_{+\rho_0 - 2(\ell+1)v} = 0$$

rewrite sums so all have ρ^j

$$\sum_{j=\cancel{1}\,0}^{\infty}(j+1)j\,c_{j+1}\rho^j + \sum_{j=0}^{\infty}2(\ell+1)(j+1)c_{j+1}\rho^j - 2\sum_{j=\cancel{1}\,0}^{\infty} j c_j\rho^j + (\rho_0 - 2(\ell+1))\sum_{j=0}^{\infty}c_j\rho^j = 0$$

make limits the same

$$\sum_{j=0}^{\infty}\underbrace{\left[(j+1)j\,c_{j+1} + 2(\ell+1)(j+1)c_{j+1} - 2jc_j + (\rho_0 - 2(\ell+1))c_j\right]}_{=0}\rho^j = 0$$

if that $= 0$ $\forall\rho$, then coefficients $= 0$

solve

$$\longrightarrow c_{j+1} = \frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)}c_j$$

Set c_0 & get others

For large j, $\quad c_{j+1} \approx \frac{2j}{j^2}c_j = \frac{2}{j}c_j$

$$c_j \approx \frac{2^j}{j!} \quad \text{for large } j$$

$$v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j = \sum_{j=0}^{\infty}\frac{2^j}{j!}\rho^j = \sum_{j=0}^{\infty}\frac{(2\rho)^j}{j!} = e^{2\rho}$$

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

blows up at $\rho\to\infty$!

Oh no!

There's some j_{max} so that

$$2\underbrace{(j_{max}+\ell+1)}_{n = 1,2,3,\ldots} = \rho_0 \quad \rho_0 = 2n \qquad \& \qquad c_{j_{max}+1} = \frac{\cancel{2(j_{max}+\ell+1) - \rho_0}}{\ldots}c_{j_{max}} = 0$$

But $\rho_0 = \dfrac{me^2}{2\pi\epsilon_0\hbar^2\left(\sqrt{-2mE}/\hbar\right)} = 2n$

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

Bohr formula

$E_1 = -13.6\,eV$ ground state energy of H electron

~~energy a~~ to remove an electron from H atom requires 13.6eV.. to send it to ∞.

Also

$$k = \overbrace{\frac{me^2}{4\pi\epsilon_0\hbar^2}}^{1/a}\frac{1}{n}$$

$a = 0.529 \times 10^{-10}\,m$

Bohr radius

$k = \dfrac{1}{an}$

$\rho = kr = \dfrac{r}{an}$