


II-atom Radial Equation (Davydov # 38) & The Saga of the $F(a; b; z)^{15}$

3) To get down to cases with the H-like atom, put $V(r) = -Ze^2/r$ in Eq.(3), so...

$$\left[\frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} \left[E + \frac{Ze^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R = 0 \right]_{l=0,1,2,\dots} \quad \psi = \frac{1}{r} R Y_{lm} \quad (13)$$


The diagram shows a central nucleus represented by a black dot with a label (Ze, ∞) below it. A curved line represents the electron's orbit. A point on this orbit is labeled $(-e, m)$ with an arrow pointing to it. A radius vector r is shown from the nucleus to the electron.

It is traditional (and useful) to write this equation in dimensionless variables, adopting the following "atomic units" of length and energy...

LENGTH = Bohr radius : $a_0 = \hbar^2/m_e^2 = 0.529 \times 10^{-8} \text{ cm}$ (m =electron mass);

ENERGY = Hartree : $E_0 = e^2/a_0 = \alpha^2 mc^2 = 27.1 \text{ eV}$ ($2 \times \text{H-atom ionization}$);

Here : $\alpha = e^2/\hbar c = 1/137.036$ ($\pm 1 \text{ ppm}$) is the fine-structure const. (14)

In these units, we define dimensionless variables ρ & ϵ , and rewrite (13)...

$$\left\{ \begin{array}{l} \rho = r/a_0, \text{ radial position in units of Bohr radii,} \\ \epsilon = E/E_0, \text{ electron energy in units of Hartrees;} \\ \left\{ \frac{d^2}{d\rho^2} + \left[2\epsilon + \frac{2Z}{\rho} - \frac{l(l+1)}{\rho^2} \right] \right\} R(\rho) = 0. \end{array} \right. \quad (15)$$

We are not including reduced mass corrections [in (14), we've already let $\mu = \frac{mM}{m+M} \rightarrow m$, as for an only heavy nucleus], and -- in addition to ignoring electron & nuclear spins [meaning there are no magnetic energies in the problem] -- we assume the nucleus is a point, so the Coulomb potential holds all the way down to $\rho=0$.

For bound states $\epsilon < 0$, and we define : $\kappa^2 = -2\epsilon = 2|E|/E_0$. Asymptotics are :

$$\left. \begin{array}{l} \underline{\rho \rightarrow \infty} \Rightarrow \left\{ \frac{d^2}{d\rho^2} - \kappa^2 \right\} R(\rho) \approx 0, \text{ so } R(\rho) \propto e^{\pm \kappa \rho}. \\ \text{For } R(\infty) \rightarrow 0, \text{ choose only : } \underline{R(\rho) \propto e^{-\kappa \rho}, \text{ as } \rho \rightarrow \infty.} \\ \underline{\rho \rightarrow 0} \Rightarrow \left\{ \frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} \right\} R(\rho) \approx 0, \text{ so } R(\rho) \propto \rho^{l+1}, \text{ or } \rho^{-l}. \\ \text{For } R(0) = 0, \text{ choose only : } \underline{R(\rho) \propto \rho^{l+1}, \text{ as } \rho \rightarrow 0.} \end{array} \right\} \quad (16)$$

Factor out the asymptotic dependences, and rewrite the radial eqn (15) as...

$$\left\{ \begin{array}{l} R(\rho) = \text{const} \cdot \rho^{l+1} e^{-\kappa \rho} f(\rho), \\ \text{so } \rho \frac{d^2 f}{d\rho^2} + [2(l+1) - 2\kappa \rho] \frac{df}{d\rho} + [2Z - 2\kappa(l+1)] f = 0. \end{array} \right. \quad (17)$$