10

The Radial Functions for the Hydrogenic Atom

Because we have solved the angular part of the one-body problem for a spherically symmetric V(r) (or, equivalently, the angular part for the relative motion of a two-body problem), it would be good to provide a detailed example for a particular potential, V(r). Because the Coulomb problem is soluble via the factorization method, let us solve the radial problem for the general hydrogenic atom, i.e., the one electron atom (with $Z = 1, 2, 3, \dots$) for hydrogen, once-ionized Helium, twice-ionized Lithium, and so on,where

$$V(r) = -\frac{Ze^2}{r}. \tag{1}$$

The one-dimensionalized radial equation is

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \left[-\frac{Ze^2}{r} + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]\right)u(r) = Eu(r), \tag{2}$$

where the coordinate r in this equation is the "physical" r, measured in centimeters or Angstrom units and E is the energy measured in eV, for example. Let us first switch to dimensionless quantities, and let the $r_{phys.}$ and E of the above equation be replaced by dimensionless quantities r, and ϵ

$$r_{phys.} = \frac{a_0}{Z}r, \qquad \text{with} \quad a_0 = \frac{\hbar^2}{\mu e^2}, \qquad E = \frac{\mu Z^2 e^4}{\hbar^2}\epsilon, \tag{3}$$

leading to the radial equation in dimensionless quantities

$$\left(-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2}\right)u_{\lambda l}(r) = 2\epsilon u_{\lambda l}(r) = \lambda u_{\lambda l}(r). \tag{4}$$

This equation is factorizable via the factors

$$O_{\pm}(l) = \left(\mp\frac{d}{dr} + \frac{l}{r} - \frac{1}{l}\right), \tag{5}$$

with

$$O_{+}(l)O_{-}(l)u_{\lambda l} = \left(-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2} + \frac{1}{l^2}\right)u_{\lambda l} = \left[\lambda + \frac{1}{l^2}\right]u_{\lambda l}, \tag{6}$$

$$\begin{aligned} O_{-}(l+1)O_{+}(l+1)u_{\lambda l} &= \left(-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2} + \frac{1}{(l+1)^2}\right)u_{\lambda l} \\ &= \left[\lambda + \frac{1}{(l+1)^2}\right]u_{\lambda l}, \end{aligned} \tag{7}$$

so the factorization works, and

$$\mathcal{L}(l) = -\frac{1}{l^2}. \tag{8}$$

Because $\mathcal{L}$ is an increasing function of l for positive l, and because ϵ and, hence, λ must be a negative quantity for bound states, $[\lambda - \mathcal{L}(l+1)]$ will be a positive quantity only up through a maximum l-value. Thus,

$$\lambda = \mathcal{L}(l_{max} + 1) = -\frac{1}{(l_{max} + 1)^2} = 2\epsilon. \tag{9}$$

Renaming the integer l_{max}: $\quad l_{max} + 1 = n, \quad$ or $\quad l_{max} = (n-1)$, we obtain the hydrogen result

$$\epsilon = -\frac{1}{2n^2}, \qquad E = -\frac{\mu Z^2 e^4}{\hbar^2}\frac{1}{2n^2}. \tag{10}$$

The starting function is obtained from

$$O_{+}(l_{max} + 1)u_{\lambda l_{max}} = O_{+}(n)u_{n,l=(n-1)} = \left(-\frac{d}{dr} + \frac{n}{r} - \frac{1}{n}\right)u_{n,n-1} = 0, \tag{11}$$

leading to the normalized solution

$$u_{n,l=n-1} = N_n r^n e^{-\frac{r}{n}}, \qquad \text{with} \qquad N_n = \sqrt{\left(\frac{2}{n}\right)^{2n+1}\frac{1}{(2n)!}}. \tag{12}$$

The radial functions for the lower l values for a definite n can be obtained from these by action with the normalization-preserving step-down operators, $\mathcal{O}_{-}(l)$,

$$\mathcal{O}_{-}(l) = \frac{1}{\sqrt{[\lambda - \mathcal{L}(l)]}}\left(\frac{d}{dr} + \frac{l}{r} - \frac{1}{l}\right) = \frac{nl}{\sqrt{(n-l)(n+l)}}\left(\frac{d}{dr} + \frac{l}{r} - \frac{1}{l}\right). \tag{13}$$

For example, for $n = 2$, the starting function with $l = 1$ is given by

$$u_{n=2,l=1}(r) = \frac{1}{2\sqrt{6}}r^2 e^{-\frac{r}{2}}. \tag{14}$$

The eigenfunction with $l = 0$ is obtained via

$$u_{n=2,l=0}(r) = \frac{2}{\sqrt{3}}\left(\frac{d}{dr} + \frac{1}{r} - 1\right)\frac{1}{2\sqrt{6}}r^2 e^{-\frac{r}{2}}$$
$$= \frac{1}{2\sqrt{2}}r(2-r)e^{-\frac{r}{2}}. \tag{15}$$

We tabulate a few of the radial eigenfunctions obtained in this way for the lower n values. With $rR(r) = u(r)$, the $R(r)$ are given by

$$\begin{aligned}
&\text{For} \quad n = 1, l = 0 : R_{10}(r) = 2e^{-r},\\
&\text{For} \quad n = 2, l = 1 : R_{21}(r) = \frac{1}{2\sqrt{6}}re^{-\frac{r}{2}},\\
&\text{For} \quad n = 2, l = 0 : R_{20}(r) = \frac{1}{2\sqrt{2}}(2-r)e^{-\frac{r}{2}},\\
&\text{For} \quad n = 3, l = 2 : R_{32}(r) = \frac{2\sqrt{2}}{3^4\sqrt{15}}r^2 e^{-\frac{r}{3}},\\
&\text{For} \quad n = 3, l = 1 : R_{31}(r) = \frac{2\sqrt{2}}{3^4\sqrt{3}}r(6-r)e^{-\frac{r}{3}},\\
&\text{For} \quad n = 3, l = 0 : R_{30}(r) = \frac{2}{3^4\sqrt{3}}(27 - 18r + 2r^2)e^{-\frac{r}{3}}.
\end{aligned} \tag{16}$$

Here, the dimensionless r is $r = (Zr_{\text{phys.}}/a_0)$. To convert to a normalization in physical space $\int_0^\infty dr_{\text{phys.}} r_{\text{phys.}}^2 |R(r_{\text{phys.}})|^2 = 1$, the above results must be multiplied with the additional normalization factor $(Z/a_0)^{\frac{3}{2}}$.