Solutions to the Radial Equation

To bring us back to where we were when we left the radial equation behind, we are looking for the wavefunction where it is separable into radial and angular parts:

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

and we have found the angular part to be the spherical harmonics. The radial part of the TISE is given by:

$$\frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{2m}{\hbar^2} \left[ V(r) - E \right] R = l(l + 1) R$$

and, if we define:

$$u(r) \equiv rR(r) \Rightarrow$$

$$R(r) = \frac{u(r)}{r}$$

then the equation becomes:

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

which is exactly of the form of the one-dimensional TISE with an effective potential of:

$$V_{\text{eff}} = V(r) + \frac{\hbar^2}{2m} \frac{l(l + 1)}{r^2}$$

We now have to choose a potential before we can proceed.

Infinite Spherical Well

As a first example, let’s consider now the central potential 3-D analogy to the 1-D infinite square well:

$$V(r) = \begin{cases} 0, & r < a \\ \infty, & r > a \end{cases}$$

Then, outside of the well, the wavefunction must be zero, and inside the potential is zero so that the radial equation becomes:
As a first step towards the general solution, let’s examine the case where $l=0$:

$$\frac{d^2u}{dr^2} = -k^2u, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The solutions to this are easy:

$$u(r) = A \sin kr + B \cos kr$$

Now, we have to remember what we are trying to obtain, and what the boundary conditions are. We want

$$R(r) = \frac{u(r)}{r} = A \frac{\sin kr}{r} + B \frac{\cos kr}{r}$$

and the boundary conditions tell us that $R(r)$ must be zero at $r = a$ and $R(r)$ must be finite (actually, normalizable) everywhere, so that $B = 0$ and:

$$R(r) = A \frac{\sin kr}{r}$$

$$R(a) = A \frac{\sin ka}{a} = 0 \Rightarrow$$

$$ka = n\pi \Rightarrow$$

$$E_{n0} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1,2,3 \ldots$$

The complete, normalized wavefunction is:

$$\psi_{n00} = \frac{1}{\sqrt{2\pi a}} \frac{\sin(n\pi r/a)}{r}$$

This is just $R(r)$ times $Y_0^0$ with the appropriate normalization. The wavefunction is defined by three quantum numbers $n$, $l$ and $m$. We will find next that for this potential, the energy depends upon both $n$ and $l$, but not on $m$. Later for the hydrogen atom, we find that this is not always the case.

The general solution for the radial equation, with an arbitrary value of $l$ is more complicated and I will only show the answer:
\( R(r) = A j_l(kr) \)

where \( j_l(x) \) are the spherical Bessel functions, the first few of which are listed below along with their partners, the spherical Neumann functions (the general solution includes these, but they also blow up at \( r=0 \) so that the coefficient of these are set to zero).

<table>
<thead>
<tr>
<th>( j_0 )</th>
<th>( n_0 )</th>
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</thead>
<tbody>
<tr>
<td>( \frac{\sin x}{x} )</td>
<td>( -\frac{\cos x}{x} )</td>
</tr>
<tr>
<td>( j_1 )</td>
<td>( n_1 )</td>
</tr>
<tr>
<td>( \frac{\sin x}{x^2} - \frac{\cos x}{x} )</td>
<td>( -\frac{\cos x}{x^2} - \frac{\sin x}{x} )</td>
</tr>
<tr>
<td>( j_2 )</td>
<td>( n_2 )</td>
</tr>
<tr>
<td>( \frac{3}{x^3} - \frac{1}{x} ) ( \sin x - \frac{3}{x^2} ) ( \cos x )</td>
<td>( -\left( \frac{3}{x^3} - \frac{1}{x} \right) ) ( \cos x - \frac{3}{x^2} ) ( \sin x )</td>
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</tbody>
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and the graphs of these are shown below:

The boundary condition now must be applied:

\( j_l(ka) = 0 \)

but, the spherical Bessel functions have many zeros and they are not at the familiar \( n\pi \) locations, and have to be found numerically or graphically. In any case, we just label
them \( \beta_n \), which just stands for the \( n^{\text{th}} \) zero of the \( l^{\text{th}} \) spherical Bessel function. Then, the allowed energies are just:

\[
E_{nl} = \frac{\hbar^2}{2ma^2} \beta_{nl}^2, \quad n = 1, 2, 3 \ldots
\]

and where for a particular value of \( n \), there is a corresponding value of \( l \). There are, however, the usual \( 2l+1 \) values of \( m \), each having the same energy, so for each value of \( n \) and \( l \), the state is \( 2l+1 \)-fold degenerate. The wavefunctions are given by the product of the radial and angular parts:

\[
\psi_{nlm}(r, \theta, \phi) = A_{nl} R(r) Y_l^m(\theta, \phi) \\
= A_{nl} j_l(kr) Y_l^m(\theta, \phi) \\
= A_{nl} j_l\left(\beta_{nl} \frac{r}{a}\right) Y_l^m(\theta, \phi)
\]