0.1 Energy eigenvalue equation

Today we will solve for the eigenstates of a particle in a central potential. To do this, we will solve the radial energy eigenvalue equation. I will not derive here the radial energy eigenvalue equation, which you have probably seen in the *Central Forces* paradigm:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(r)}{\partial r^2} + \left(\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + V(r)\right)u(r) = Eu(r) \tag{1}$$

where $u(r) = rR(r)$ is one way we look at the radial wave function and ℓ is the angular momentum quantum number (which takes non-negative integer values). The extra potential term is called the *centrifugal* potential, and represents the kinetic energy associated with the angular momentum. Remember, this is an eigenvalue equation just like you've been working with recently, but now we expect that the energy eigenvalues will be discrete rather than arranged in continuous bands, so they'll be harder to guess.

We can "shoot" this equation much like you have been donig for the past few weeks, with the sole difference being that I'm going to ask you to shoot *backwards* this time, starting at large radius and working your way inwards. This will minimize some numerical instability issues that would otherwise be a bit of a pain.

$$-\frac{\hbar^2}{2m}\frac{u(r+\Delta r) + u(r-\Delta r) - 2u(r)}{\Delta r^2} + \left(\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + V(r)\right)u(r) = Eu(r) \tag{2}$$

Now since we're going to shoot inwards from large radius, we'll solve for $u(r-\Delta r)$:

$$u(r-\Delta r) = 2u(r) - u(r+\Delta r) + \Delta r^2\left(\frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2}(V(r) - E)\right)u(r) \tag{3}$$

To find the energy eigenvalues, we will make use of the two boundary conditions we know for a bound state: the wave function $u(r)$ must approach zero at large r, and it must be zero at $r = 0$. The latter comes about because $u = rR$, and since the wave function itself ($R(r)$) is finite, when multiplied by zero you ($u(r)$, get it? a pun!) must be zero.

We will consider two potentials, but you probably won't have time for both of them. If the sum of your birthdays is even, then solve the hydrogen atom $V = -\frac{e^2}{r}$ where e is the electron charge. Otherwise solve the three-dimensional simple harmonic oscillator, $V = \frac{1}{2}kr^2$.

1. Choose a pretty large radius and give it a name like $r_{\max}$. We will assume the wave function has reached zero at this point. Later you may find you didn't pick a large enough radius and need to increase this. Also pick an angular momentum quantum number.

2. Create an array to hold $u(r)$, and initialize its final value to zero, and its penultimate (second to last) value to zomething non-zero.

3. Write a loop to come in from large radius, solving for each value $u(r)$ using the equation above, based on the next two larger radii values.

4. Plot your wave function versus radius.

5. Tweak your energy until you find a value that results in a $u(r)$ that never crosses zero (but reaches $u(r = 0) \approx 0$).
6. Solve for more energy eigenvalues. Try to get a few energy eigenvalues for several values of angular momentum.
7. When you have a few of them, visualize your energy eigenvalues as horizontal lines on a plot of the potential energy versus r.

Extra fun Write a function to count the number of nodes (zero crossings) of a radial function.

More fun Write a function that solves automatically for the lowest possible energy that has a specified number of nodes.