To model a quantum particle in a radial potential, we addressed the derivation of the wave function parallel with the development in Griffiths, pg. 145, and in Dr. Crawford's course notes, and some various online sources.

The potential V(r) = 1/r in spherical coordinates describes the system as having constants of motion in the angular coordinates theta and phi, thus conserving angular momentum. Still, it admits an effective potential that includes a centrifugal factor,

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

The Schrodinger Equation with this potential may be solved using separation of variables. In this development, we focus on the radial wave function. The Schrodinger equation reads

$$-\hbar^2/2m\ d^2/dr^2\ \psi + [-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = E\ \psi.$$

$$[-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = E\ \psi + \hbar^2/2m\ d^2/dr^2\ \psi.$$

$$1/-E\ [-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = -\psi + \hbar^2/-2mE\ d^2/dr^2\ \psi.$$

$$[1/rE + \hbar^2/-2mE\ l(l+1)/r^2]\ \psi + \psi = \hbar^2/-2mE\ d^2/dr^2\ \psi.$$

We can introduce the variable $\kappa = \sqrt{(-2mE)}/\hbar$, giving

$$[1 + 2m/\hbar^2\kappa\ 1/\kappa r + l(l+1)/(\kappa r)^2]\ \psi = 1/\kappa^2\ d^2/dr^2\ \psi.$$

Set $\rho = \kappa r$, revealing $\rho_0 = 2m/\hbar^2\kappa$, which now gives

$$[1 + \rho_0/\rho + l(l+1)/\rho^2]\ \psi = d^2/d\rho^2\ \psi.$$

Note that by scaling ρ, we can translate this problem from the problem V(r) = 1/r to that of the hydrogen atom, with its specific radius. This is planned for later in the development.

Using an asymptotic breakdown, we can find the solution in three parts,

$\rho \to \infty$: $d^2/d\rho^2\ \psi = \psi$,
with solution $\psi(\rho) = A\ \exp(-\rho) + B\ \exp(\rho)$,
and since the second factor is not normalizable,
$\psi(\rho) = A\ \exp(-\rho)$.

$\rho \to 0$: $d^2/d\rho^2\ \psi = l(l+1)/\rho^2\ \psi$,
with solution $\psi(\rho) = C\ \rho^{l+1} + D\ \rho^{-l}$,
but $D\rho^{-l}$ disobeys normalizability, so
$\psi(\rho) = C\ \rho^{l+1}$.

The complete solution is then constructed assuming a power series v(ρ),

$$\psi(\rho) = A\ \exp(-\rho)\ C\ \rho^{l+1}\ v(\rho),$$

$$\text{where } v(\rho) = \sum_{j=0}^{\infty} c_j\ \rho^j.$$

The recursion relationship for the c_j coefficients is given by

$$c_{j+1} = \left\{\frac{2(j + l + 1) - \rho_0}{(j + 1)(j + 2l + 2)}\right\} c_j,$$

where c_0 is normalized by total probability equal to one.

In general, this power series does result in unnormalizable states. There must be a maximum value of j, then, above which the coefficients are all zero. This jmax is related to the quantum numbers n and l by

$$jmax = n - l + 1.$$

Looking back at the recursion relationship, it becomes clear that

$$2(j + l + 1) - \rho_0 = 2n - \rho_0, \text{ and } \rho_0 = 2n.$$

This gives us a relationship between the principle quantum number n and the energy of a state n, recalling that the angular momentum is conserved and so the energy value does not rely on the quantum numbers l or m.

$$E_n = -\hbar^2\kappa^2/2m.$$

$$\kappa = 2m/\hbar^2\rho_0.$$

$$E_n = -2m/\hbar^2\rho_0^2 = -m/2\hbar^2n^2 = E_1/n^2, \; n = 1,2,3\ldots,$$
where $E_1 = -m/2\hbar^2$.

Actually, this is not an energy. The scaling factor bringing this to solutions of the hydrogen atom would make it an energy. It comes back to the units of V(r) = 1/r. This of course has units of energy, but what are the constants that make it that way? We've used no constants here. This should at least be $V(r) = E_0/r$, for some energy.

This reveals the dependence on the principle quantum number of the previous quanties,

$$\kappa = 2m/\hbar^2\rho_0 = a/n,$$
where $a = m/\hbar^2$ is the Scrodinger constant factor relating the action and mass of this system (or if scaled to the correct units, the inverse of the Bohr radius of the Hydrogen atom);

$$\rho = \kappa r = ar/n.$$

This is where it becomes obvious the scaling would be good, because here we would see that the form reveals r/(bohr radius).

The spatial wave function is defined by three quantum numbers n, l, and m, and as previously stated, can be solved by separation of various such that

$$\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi),$$

where we have already found the radial function R,

$$R_{nl}(r) = 1/r \exp(-\rho)\, \rho^{l+1}\, v(\rho).$$

The model we've developed is nearly capable of handling the associated LaGuerre polynomials, but they become difficult to plot. So, for now, we focus on the radial function, only.

Substituting our new information back into the recursion relationship gives us the recursion in terms of the quantum numbers,

$$c_{j+1} = \left\{\frac{2(j + l + 1 - n)}{(j + 1)(j + 2l + 2)}\right\} c_j .$$

This is sufficient information to model the radial component of the wave function, except for normalizing the coefficient c_0. This is done using the expression of probability conservation

$$\int_0^\infty |R_{nl}|^2 \, r^2 \, dr = 1.$$

We want to simulate the hydrogen atom, where $V(r) \neq -1/r$, but instead $V(r) = -e^2/(4\pi\varepsilon_0)\ 1/r$. This changes some of our parameters, i.e.,

$\rho = \kappa r = r/an$ and $\rho_0 = m\, e^2/(2\pi\ \varepsilon_0\ \hbar^2\ \kappa)$,

where a now represents the Bohr Radius,

$a = 5.29 \times 10^{-2}$ nm.

The rest of the development is essentially the same.

In general, the normalization is given by

$$\left(\frac{(2/na)^3\ (n-l-1)!}{2n\ [(n+l)!]^3} \right)^{1/2}.$$

We will notate this normalization as α. If we also notate the generalized Laguerre polynomials of x as $L[q,p](x)$, then our model is

$$\alpha\ \exp(-r/na)\ (2r/na)^l\ L[n-l-1,2l+1](2r/na)\ Y_l^m(\theta,\phi).$$

We have not plotted this, but here Y_l^m refers to the spherical harmonics, which have the form (to within a normalization constant)

$Y_l^m(\theta,\phi) = \exp(i\ m\ \phi)\ P_l^m\ (\cos\theta)$,

where $P_l^m(x)$ are the Legendre Polynomials in x.

This model is implemented in mathematica, and will be presented to the Physics 520 class on Dec. 8, 2017.