

The 3D radial equation



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- Recasting the radial equation

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- Particle in a bubble solution

Radial solution



Returning to the radial equation, where the potential is included

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

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$$r \frac{d^2 u}{dr^2} - \frac{2mr^2}{\hbar^2} [V(r) - E] \frac{u}{r} = l(l+1) \frac{u}{r}$$

Equation for $u(r)$



We can now obtain a differential equation for $u(r)$

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This looks like a time-independent Schrödinger equation with an effective potential $V_{\text{eff}}(r)$ whose solution is normalized as $\int_0^\infty |u(r)|^2 dr = 1$

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Example 4.1



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We must solve this for each value of l separately.
The $l = 0$ case is the simplest

Example 4.1 (cont.)



For $l = 0$, we need to impose the boundary condition $u(a) = 0$.

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thus, $ka = n\pi$ where n is an integer and the energies for the $l = 0$ case are

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Solutions for $l = 0$

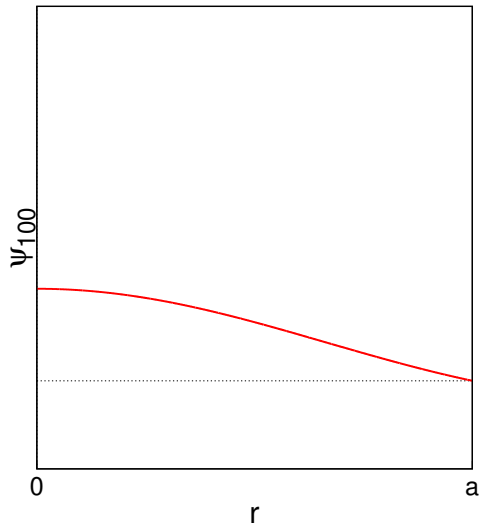


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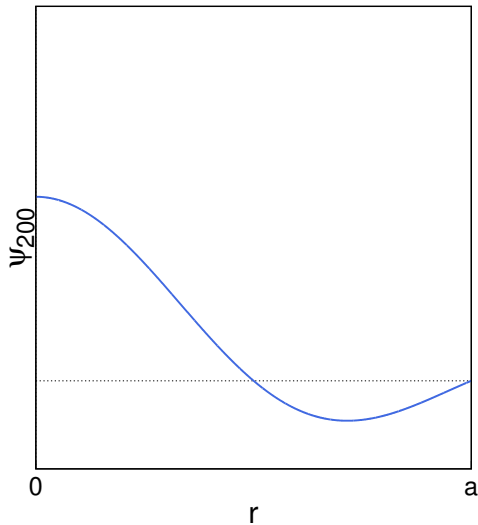
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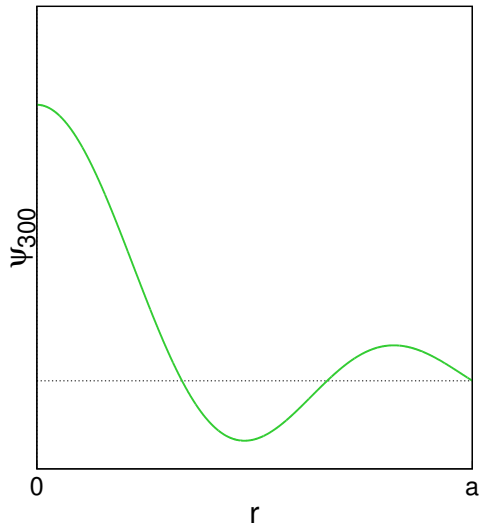
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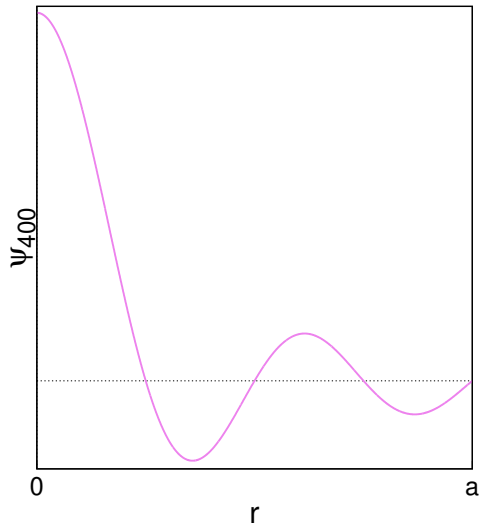
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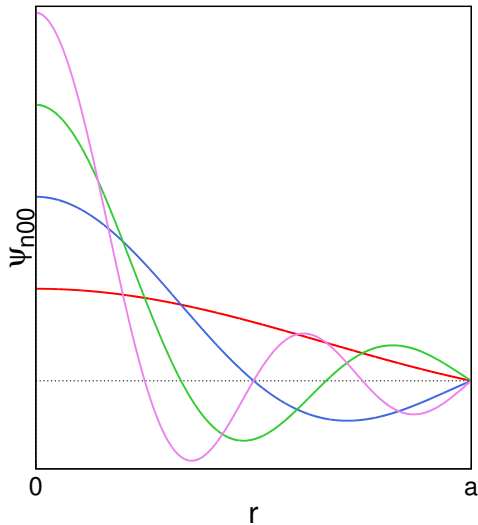
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$j_l(x)$ are spherical Bessel functions of order l

$$j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x}$$

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What about the solutions for $l \neq 0$?

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$j_l(x)$ are spherical Bessel functions of order l and
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while spherical Bessel functions are finite at the origin, spherical Neumann functions are infinite and thus we again set $B_l = 0$

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while spherical Bessel functions are finite at the origin, spherical Neumann functions are infinite and thus we again set $B_l = 0$

we still must apply the boundary condition that $j_l(ka) = 0$ but this is a bit more complex than for the $l = 0$ case

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$$R(r) = A_l j_l(kr)$$

Spherical Bessel functions



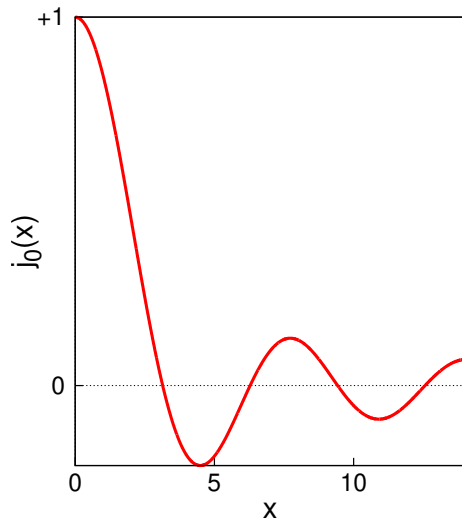
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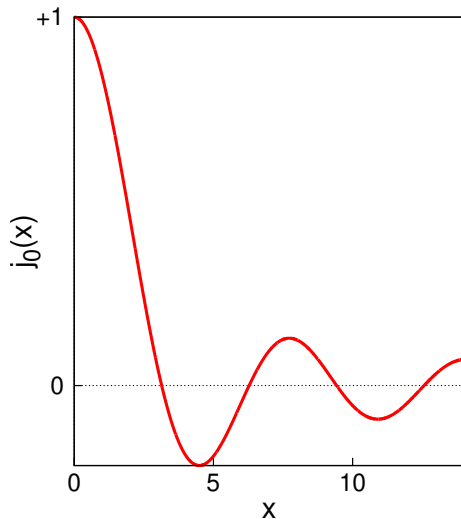
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$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = (-x) \frac{1}{x} \left(\frac{\cos x}{x} - \frac{\sin x}{x^2} \right)$$



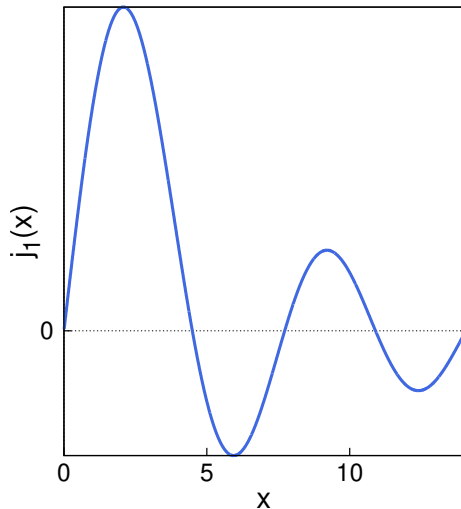
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Spherical Bessel functions

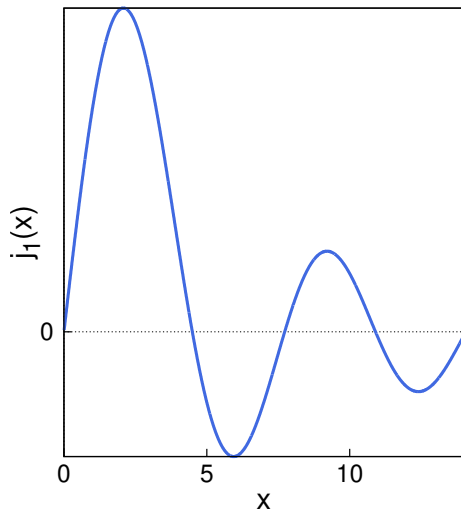


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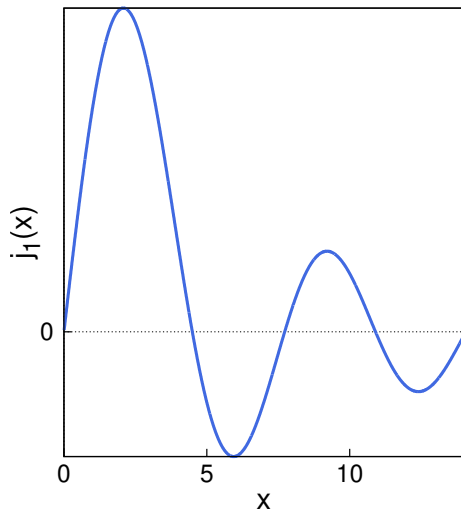


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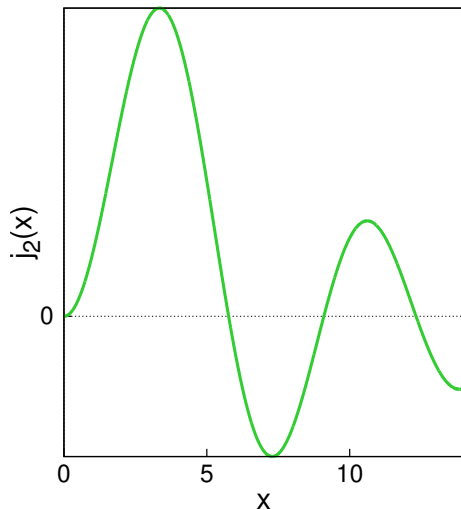


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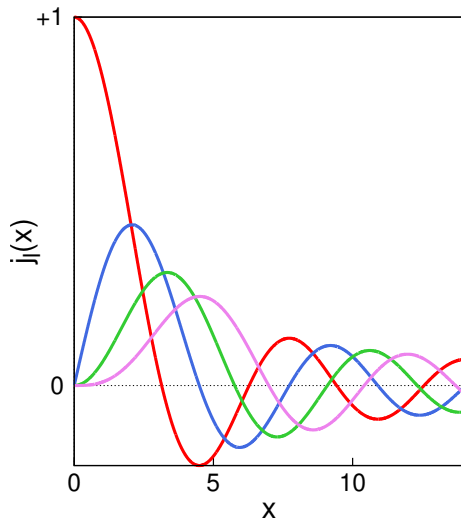


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Clearly the roots are not at nice, simple, locations!



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	β_{n1}	β_{n2}	β_{n3}
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j_1	4.493	7.726	10.904
j_2	5.762	9.906	12.325
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these are $(2l + 1)$ -fold degenerate states, that is, the energy does not depend on the quantum numbers which give rise to the degeneracy

Hydrogen atom: Part 1





- Hydrogen atom potential

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- Hydrogen atom potential
- Asymptotic solution

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- Hydrogen atom potential
- Asymptotic solution
- Differential equation for polynomial

Hydrogen atom



The potential of the hydrogen atom is simply the Coulomb potential, which is spherically symmetric

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$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

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where we assume that the nucleus (proton) is stationary because it is much more massive than the electron

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rewriting it with common terms

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initially we are only interested in bound states with $E < 0$ and so we can make the usual substitution $\kappa = \sqrt{-2mE}/\hbar$

Hydrogen atom (cont.)



$$\frac{1}{\kappa^2} \frac{d^2 u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa} \frac{1}{\kappa r} + \frac{l(l+1)}{(\kappa r)^2} \right] u$$

Hydrogen atom (cont.)



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$$\frac{d^2 u}{d\rho^2} \approx u$$

Hydrogen atom (cont.)



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As $\rho \rightarrow \infty$, the constant term dominates
and the solution is of the form

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Hydrogen atom (cont.)



$$\frac{1}{\kappa^2} \frac{d^2 u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa} \frac{1}{\kappa r} + \frac{l(l+1)}{(\kappa r)^2} \right] u$$

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but the second term is unbounded in the limit of $\rho \rightarrow \infty$, thus $B = 0$

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As $\rho \rightarrow \infty$, the constant term dominates

and the solution is of the form

$$\frac{d^2 u}{d\rho^2} \approx u$$

but the second term is unbounded in the limit of $\rho \rightarrow \infty$, thus $B = 0$

$$u(\rho)|_{\rho \rightarrow \infty} = Ae^{-\rho} + \cancel{Be^{\rho}}$$

however, in the limit of $\rho \rightarrow 0$, the centrifugal term is dominant

Hydrogen atom (cont.)



for $\rho \rightarrow 0$ the solution must satisfy

Hydrogen atom (cont.)



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$$u(\rho) = C\rho^{l+1} + \frac{D}{\rho^l}$$

Hydrogen atom (cont.)



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Hydrogen atom (cont.)



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$$\frac{d^2 u}{d\rho^2} = l(l+1)C\rho^{l-1} + l(l+1)\frac{D}{\rho^{(l+2)}}$$

$$u(\rho)|_{\rho \rightarrow 0} \sim C\rho^{l+1}$$

Hydrogen atom (cont.)



for $\rho \rightarrow 0$ the solution must satisfy

$$\frac{d^2 u}{d\rho^2} \approx \frac{l(l+1)}{\rho^2} u$$

this has a solution

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this solution can be shown to satisfy the equation

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but the second term blows up as $\rho \rightarrow 0$, so $D = 0$ and

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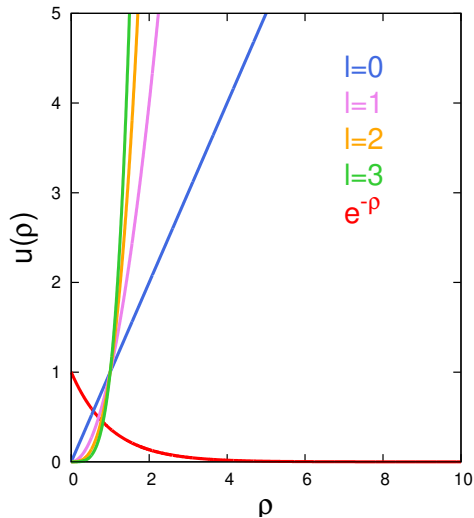
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where $v(\rho)$ is a polynomial in ρ

Asymptotic behavior



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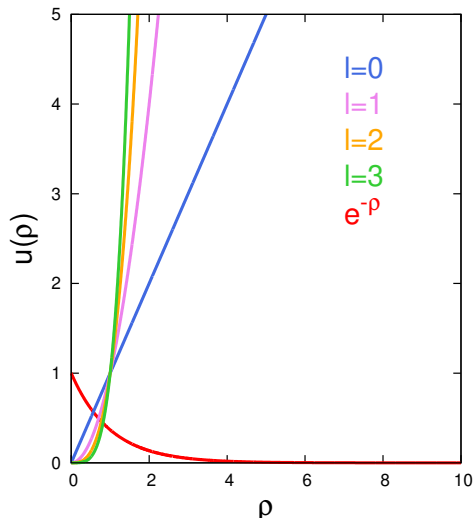


Asymptotic behavior



$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

The exponential term serves to limit the asymptotic behavior of the wavefunction

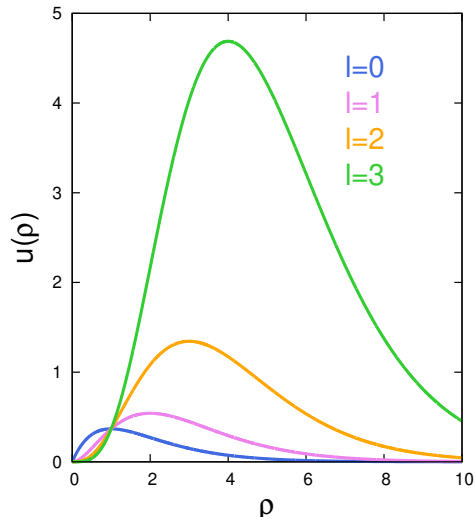


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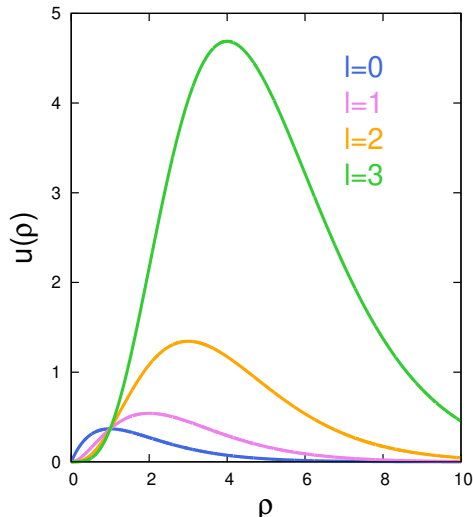
Asymptotic behavior



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The exponential term serves to limit the asymptotic behavior of the wavefunction

It remains only to determine the polynomial “wavy part” of the solution, $v(\rho)$. This is done in the same way as was the analytical solution of the harmonic oscillator.





The wavy part

The polynomial can be determined by substituting this solution into the original Schrödinger equation for $u(\rho)$

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

$$\frac{d^2 u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] u$$

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The Schrödinger equation for $v(\rho)$



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$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho), \quad \frac{d^2 u}{d\rho^2} = \rho^l e^{-\rho} \left\{ \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + \left[\rho - 2(l+1) + \frac{l(l+1)}{\rho} \right] v \right\}$$

Substituting into the Schrödinger equation for $u(\rho)$

$$\begin{aligned} 0 &= \frac{d^2 u}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] u = \frac{d^2 u}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] \rho^{l+1} e^{-\rho} v \\ &= \cancel{\rho^l e^{-\rho}} \left\{ \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + \left[\cancel{\rho} - 2(l+1) + \frac{l(l+1)}{\cancel{\rho}} \right] v - \left[\cancel{\rho} - \rho_0 + \frac{l(l+1)}{\cancel{\rho}} \right] v \right\} \\ 0 &= \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + [\rho_0 - 2(l+1)] v \end{aligned}$$

we will solve this in the same way as the harmonic oscillator, assuming that $v(\rho)$ is an infinite polynomial in ρ

The Schrödinger equation for $v(\rho)$



$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho), \quad \frac{d^2 u}{d\rho^2} = \rho^l e^{-\rho} \left\{ \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + \left[\rho - 2(l+1) + \frac{l(l+1)}{\rho} \right] v \right\}$$

Substituting into the Schrödinger equation for $u(\rho)$

$$\begin{aligned} 0 &= \frac{d^2 u}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] u = \frac{d^2 u}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] \rho^{l+1} e^{-\rho} v \\ &= \cancel{\rho^l e^{-\rho}} \left\{ \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + \left[\cancel{\rho} - 2(l+1) + \frac{l(l+1)}{\cancel{\rho}} \right] v - \left[\cancel{\rho} - \rho_0 + \frac{l(l+1)}{\cancel{\rho}} \right] v \right\} \\ 0 &= \rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + [\rho_0 - 2(l+1)] v \end{aligned}$$

we will solve this in the same way as the harmonic oscillator, assuming that $v(\rho)$ is an infinite polynomial in ρ

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

