Hydrogen Radial Wave-Function Calculator

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From essentially any introductory Quantum Mechanics textbook, the radial wave-functions or hydrogen are one of the simplest wave-functions to visualize. The math involved is relatively "nice", meaning we can solve for the wave-functions analytically. However although the hydrogen atom yields analytic solutions, we require Bessel functions and Spherical Harmonics to depict the shape of the wave-functions. Furthermore, by introducing a numerical way to solve the Hydrogen wave-functions, we can generalize this technique to other atoms.

This program computes the radial component of the Hydrogen. To see what *radial_wavfn.m* is precisely calculating, we start with the Atomic Hamiltonian, $H = -\Delta + V(r)$, and the Schrodinger equation. For Hydrogen in spherical coordinates, the Schrodinger Equation becomes

$$\left[-\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right) - \frac{1}{r}\right]\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi) \tag{1}$$

Then using separation of variables, let $\Psi(r,\theta,\phi) = R(r)Y_{\ell,m}(\theta,\phi)$. Then the radial wave equation becomes

$$\left[-\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\ell(\ell+1)}{r^2} - \frac{1}{r}\right] R(r) = ER(r) \tag{2}$$

An analytic solution can be written down for $R_{n,\ell}$ where n is the principal quantum number and ℓ is the azimuthal quantum number. However, we will compute $R_{n,\ell}$ numerically using the Numerov Algorithm by following the approach found in [1].

The *plot_radwavfn(n,l,h)* function takes 3 inputs: n - principal quantum number, ℓ - azimuthal quantum number, and h - step size of the integration. See figure 1 for the output of *plot_radwavfn(15,2,0.001)*. Note that this program computes the radial wave function in both atomic units and a logarithmic scaled space. More specifically, it is achieved by the following transformation:

$$\begin{cases} x = \ln(r) \\ X(x) = R\sqrt{r} \end{cases}$$

The logarithmic scaling allowed us to use the Numerov Algorithm, since under this transformation, the equation in (2) become the correct form of ODE.

References

[1] M. L. Zimmerman, M. G. Littman, M. M. Kash, and D. Kleppner, Phys. Rev. A 20, 2251 (1979).

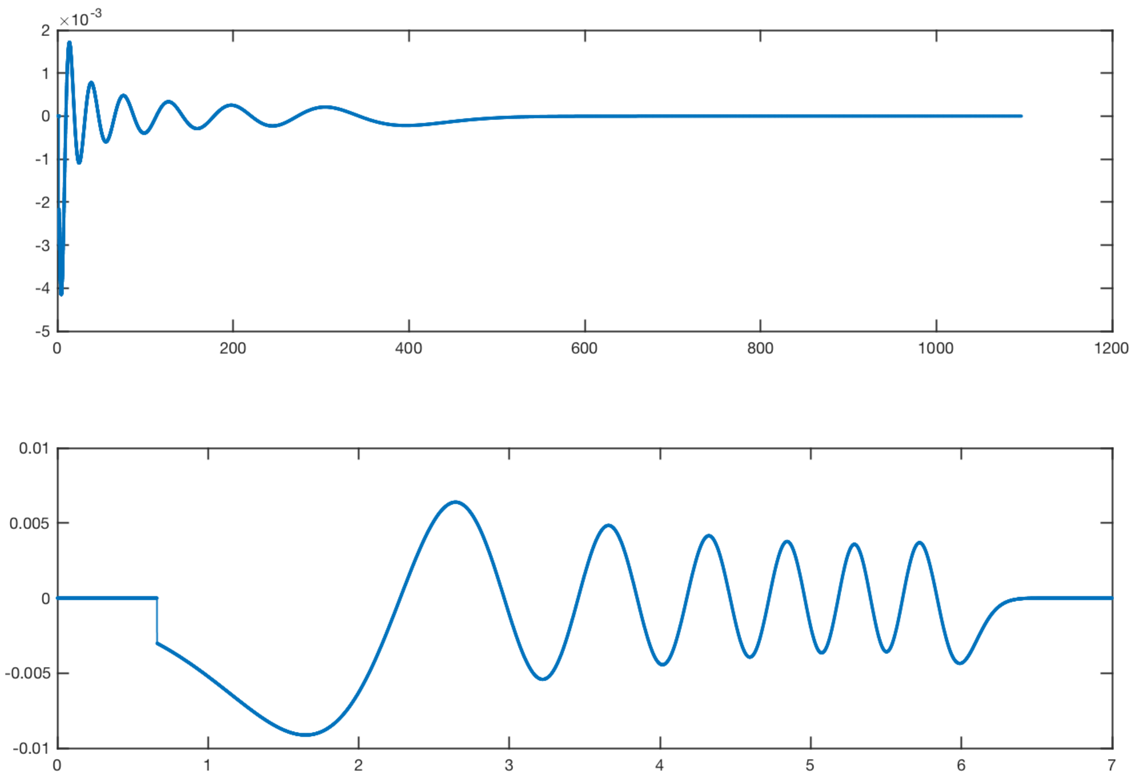

Figure 1: Top plot is the radial wave-function of hydrogen for level $n = 15, \ell = 2$ in atomic units. The bottom plot is of the same wave-function using logarithmic scaling.