Physics 270, Computational Physics

Problem No. 7

Quantum Physics: The Radial Schröedinger Equation

1. References

Your undergraduate quantum physics text book or Modern Physics textbook.

2. Goals

To explore how to use a spreadsheet to solve the Schroedinger equation for the hydrogen atom.

3. Theory

We wish to solve the Schröedinger Equation for an electron in a spherically-symettric time-independent potential. The specific example will be for the hydrogen atom. The form of the solution in three-dimensions can be written

$$y\left(r,q,j\right) = R_{nl}(r)Y_{lm}\left(q,j\right) \quad [1]$$

where

n=1,2,....

l=0,1,...n-1,

-l<=m<=l.

The radial part of the wavefunction is $R_{nl}(r)$. It depends on two quantum numbers, n and l, which specify the energy level of the electron E_n , and the total angular momentum $L = \sqrt{l(l+1)}\hbar$. The angular part of the wavefunction in a spherical potential is given by the "spherical harmonics" $Y_{lm}(\theta,\phi)$, which can be found tabulated in a quantum mechanics textbook.

To find the radial function $R_{nl}(r)$, we first make the substitution

$$R_{nl}(r) = \frac{u_{nl}(r)}{r}, \text{ where}$$

$$u(0) = 0 \text{ and}$$

$$\frac{du(r)}{dr} \equiv u'(r) = 1 \qquad [2].$$

The last two assignments define the *boundary conditions* for the solution, in terms of the value of the wavefunction and its first derivative at $r=0$.

In terms of the new function $u_{nl}(r)$, Schröedinger's equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + \left[\frac{\hbar^2}{2mr^2}l(l+1) + V(r) - E_n\right]u(r) = 0, \quad [3]$$

which we can write in more compact form as

$$u''_{nl}(r) = F_{nl}(r)u_{nl}(r),$$
$$F_{nl}(r) = \left[\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left(V(r) - E_n\right)\right] \quad [4].$$

We will use units in which length is given in Å, and energy in electron volts (eV). Then the constants can be combined as

$$A = \frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} = \frac{2\times 0.51\times 10^6}{(1973)^2} = 0.262\frac{1}{eV - \overset{o}{A}^2}.$$

The potential for an electron in the field of a single proton (hydrogen atom) is given by

$$V(r) = -\frac{Ze^2}{r} = -\frac{e^2}{\hbar c}\hbar c\frac{1}{r} = -\frac{1973}{137}\frac{1}{r}[eV],$$

where r is in units of Ångströms.

4. Assignment

Solve the SE using a spreadsheet, by turning the second-order differential equation (4) into two first order equations solved by the Euler method, as follows:

$$u(r_{i+1}) = u(r_i) + u'(r_i)\Delta r$$
$$u'(r_{i+1}) = u'(r_i) + F(r_i)u(r_i)\Delta r \quad [5]$$

The starting values of the function and derivative are given by eq. [2] above.

Be sure to include a column for calculating the actual radial wavefunction $R_{nl}(r)$. You will need to calculate the wavefunction out to a distance of about 5 Å, with at least 100 points.

5. Tasks

Only precise, discrete (quantized) values of energy E_n will produce wavefunctions that are finite at large radius. You will use your spreadsheet to find these energy *eigenvalues*.

1. The lowest energy solution for the hydrogen atom has an energy of E= -13.6 eV , corresponding to (n,l)=(1,0) . Plot the radial wave-function for energies near (above and below) this value. Determine the best value of the ground-state (lowest) energy for the hydrogen atom from your spreadsheet model (it might not be the same as the exact value).
2. Find the next highest energy eigenvalue by trial and error (next smallest negative number), for (n,l)=(2,0) . Plot the radial wave-function for the best value of energy.
3. Find the energy eigenvalue for the case (n,l)=(2,1) .
4. Plot the *radial probability density* for the (n,l)= (1,0), (2,0), and (2,1) cases. The radial probability density is given by $P_{nl}(r) = r^2 R^2_{nl}(r)$. The maximum value of $P_{nl}(r)$ determines the most-likely radius for the electron.
5. Tabulate your results for the energy eigenvalues and most-likely radius in the three cases of (n,l) studied.