LAB 9: NUMERICAL WAVE FUNCTIONS FOR ATOMS

By: Hamilton Physics Department

LEARNING OBJECTIVES

Students will:

- Develop a numerical spreadsheet that can solve the Schrödinger equation to find wave functions and energy eigenstates for Hydrogen and the Helium He^+ ion.
- Compare and contrast the graphs and energy states with examples provided in the textbook.

PRELAB

PART I – GRADING ABSTRACTS:

You are going to grade us!

To hone your perspective, we would like you to read two of the abstracts below. Two are from journal articles that reported on ground-breaking new measurements. The others are from physicists in our department. For each of the TWO, please:

a) Review: Apply the rubric to two of these abstracts, assigning a grade for each category.
b) Summarize and annotate: Write a one or two sentence summary of the work focusing on "what" and "results". On or next to the abstract identify the sentences that describe the goals, comparison if relevant.

See the "Abstracts – Grading and Writing" document for the abstracts.

REVIEW – METHOD OF FINITE DIFFERENCES

In Lab 8, we learned how to find 1-D wave functions for any 1-D potential in Excel. In this lab, you will apply this method to find some Hydrogen wave functions and then explore the low levels of Helium. We learned how to convert the general 1-D Schrödinger differential equation, written in dimensionless units

$$-\frac{d^2u}{dx^2} + V(x)u = Eu$$

into a Finite Difference formula to find a new value of u given two old ones

$$u_{i+1} = 2u_i - u_{i-1} - (\Delta x)^2(E - V_i)u_i$$

where u_i and V_i are the values of $u(x)$ and potential $V(x)$ evaluated at the position x_i.

We organized the problem in columns in a spreadsheet like the image at right. The cells with blue backgrounds contain simple numbers. The rest contain formulae. The yellow backgrounds contain formulae of the form “=<cell above>+dx” to create the regularly spaced x values. The magenta cells contain the finite difference formula.

	A	B	C	D	E	F	G
1	dx	0.01		xi	Vi	E-Vi	ui
2	x0	-1		-1	100	-99	0
3	V0	100		-0.99	100	-99	0.001
4				-0.98	100	-99	0.00201
5	u0	0		-0.97	100	-99	0.00304
6	u1	0.001		-0.96	100	-99	0.0041
7				-0.95	100	-99	0.0052
8	E1	1		-0.94	100	-99	0.006352
9				-0.93	100	-99	0.007567
10				-0.92	100	-99	0.008857
11				-0.91	100	-99	0.010234

Figure 1: Example spreadsheet organization

There were some practical issues:

1. You had to pick the first two values of the wave functions (the two blue cells in the u column) to ensure that the wave function went to zero at the left edge and that it had some kind of sensible magnitude.
2. You had to pick dx to be small enough that the potential made very little change going from one row to the next.
3. You had to extend the domain (the list of x values) out far enough to give the wave function enough to go smoothly to zero in the negative KE region otherwise the energies were unreliable.

THE HYDROGEN RADIAL SCHRÖDINGER EQUATION

We start from the Hydrogen radial Schrödinger equation in the dimensionless form

$$-\left\{\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)\right\}+\left\{\frac{\ell\left(\ell+1\right)}{\rho^2}\right\}R-\frac{2Z}{\rho}R=\mathcal{E}R.$$

where the radial coordinate ρ is in units of Bohr radii ($\rho = r/a_0$) and the energy (curly E) is in *units* of 13.6eV. That is: energy E = 13.6*Ɛ (in eV).

The above equation is not in the correct form for our spreadsheet, but can be made so by a further change of variable, as follows.

Letting u(ρ) = ρR(ρ), we simplify to show that

$$-\frac{d^2u}{d\rho^2}+\left\{\frac{\ell\left(\ell+1\right)}{\rho^2}\right\}u-\frac{2Z}{\rho}u=\mathcal{E}u$$

which is of exactly the form that we need for the numerical method.

THE COMPUTATIONS

1. *Hydrogen without Angular Momentum*

   Your first task is to find the three lowest u radial functions, and their energies, for the Hydrogen levels without angular momentum (i.e. $\ell = 0$). That is, find the **lowest three** solutions to

$$-\frac{d^2u}{d\rho^2} - \frac{2Z}{\rho}u = \mathcal{E}u$$

and compare your results to theory. Please plot both the radial probability density $|u(\rho)|^2$ and the radial wave function $R(\rho)=u(\rho)/\rho$ to compare with the figures in the book for all three solutions. Make a new sheet in Excel for each solution. You might try using your Excel files from Lab 8 as a starting point.

The x-axis is in dimensional atomic units ($\rho=r/a_o$). Your domain for the solution is technically zero to infinity, but the spreadsheet cannot handle this. At the low end, ρ=0 will not work because of the divide by zero. You need to pick a tiny value such as 1E-10 for your first ρ and then a fairly small $d\rho$ such as 0.01. You will also need to pick a fairly large maximum radius ρ, something like 10 for the first energy level and larger for subsequent energy levels. (Remember, the exponential tail of your solution should smoothly decay to 0.) Don't try for high precision values of energy; 2 or 3 sig figs are quite sufficient.

2. *Hydrogen with Angular Momentum*

   Now repeat your computations, adding in the angular momentum term, for the two cases $\ell = 1$ and $\ell = 2$. Find two levels for $\ell = 1$ and $\ell = 2$. Again, compare your energies and plots with theory. Question: What are the n quantum numbers for your states?

   Lastly, use all your energy levels (from parts 1 and 2) to construct a portion of the energy level diagram for Hydrogen using the format found in Figure 6.7 on page 191 of the text, with energy on the vertical axis and the angular momentum quantum number on the horizontal axis.

3. *Helium + Ion*

   Make a new spreadsheet and find the lowest energy state for a singly-ionized He atom, He^+. Again, compare your result with what you expect and with the Hydrogen results.

PART II – WRITING AN ABSTRACT:

Now that you have read a few abstracts, thought about their structure, and gained some familiarity with the rubric, we would like you to write an abstract for your lab report submission. Your length limit is 200 words. Although writing a paragraph that is 200 words or less seems like a simple task, it is quite challenging. You need to capture quite a lot of information in a very succinct way. You should start the process by creating an outline for your abstract, sketching out the information that you need to include from your experiment that meet the requirements of categories 1-5. With the outline in hand, then try writing the abstract. It's normal to revise multiple times. You will likely find that your first attempt goes beyond 200 words. Think about the extraneous information that you can cut and how you can rephrase your statements to get right to the point.