Chem 260 Laboratory 6

This lab uses Excel sheets and plots to explore some features of H atom wavefunctions. The files are large, so it is best to open them one at a time. Start by copying the three files
                        260lab6a.xls, 260lab6b.xls and 260lab6c.xls
from the network drive (F) to your workstation's **local** hard drive (**C**).

RADIAL WAVEFUNCTIONS AND RADIAL DISTRIBUTION FUNCTIONS

1. Start Excel and open the file 260lab6a.xls.

2. View the 1s page and the associated plot. At what value of r is the probability of finding the electron a maximum?

3. Note that the normalization factor has been chosen to make

$$\int_0^\infty R(r)^2 r^2 \, dr = 1 .$$

   You can check this integration by summing column C and multiplying by dr, which can be approximated by the step size (A5-A4). Why is the result not *exactly* 1.00? Try extending the range of r to $6a_0$.

4. Add another column (D) which represents the probability of finding the electron within a sphere of a given radius, i.e. column D should contains the integral

$$\int_0^b R(r)^2 r^2 \, dr = 1 ,$$

   where b represents the current row value of r. One way to do this is to set a cell equal to the previous one + the next segment of area under the curve of $R^2 r^2$. For example, D5=D4+(A5-A4)*(C4+C5)/2.

5. Use column D to find the radius which encompasses 50% of the electron distribution. You may wish to reduce the step sizes to improve accuracy. The answer is not the same as the average value of r nor is it the radius at which the electron probability is a maximum.

6. Now find the radius which encompasses 90% of the electron distribution. This answer is over 1.4 Å! The bond length of H_2 is only half this, so it is easy to understand that the atomic orbitals overlap in the molecule.

7. Explore the effect of changing the nuclear charge. (The He^+ ion has one electron, like H, but $Z=2$.)

8. Inspect the plots for the other H atomic orbitals. Notice how the electron distribution moves away from the nucleus as the principal quantum number increases.

9. The radial distribution function for the 3s orbital suggests that the electron is distributed among three "shells" (there are two radial nodes). Use the integration method introduced in step 4 above to calculate what fraction of the electron is in the three shells. Write the answer in your lab report.

THE SHAPES OF H ATOM WAVEFUNCTIONS

10. Close 260lab6a.xls and open 260lab6b.xls. The plots in this spreadsheet file display the wavefunction and its square (probability plot) as a function of two coordinates (x and z). Since we can not display four dimensions the third co-ordinate is held constant ($y = 0$, or in polar coordinates $\phi = 0$).

11. Look at the 1s plot and the associated probability plot. The spike at the nucleus shows how an unpaired electron can interact with the nucleus even though the probability integrated over a sphere with non-zero radius is vanishingly small (as evident from the zero value of the radial distribution function at $r = 0$).

12. The spike is also to be seen in the 2s plots. It appears as the dominant feature but this is deceptive. Recall from the radial distribution function that most of the electron density is outside the first radial node. It is not obvious in the 2s plots displayed in this file as the density is well spread out over the "floor" of the 3-D plot.

13. The 2p plots should remind you of the (2, 1) function for a particle in a 2-D box. Remember, though, that the 2p plot displayed here is missing a dimension. To generate the dumb-bell shape you see in books you need to rotate this 2p plot about its long axis. However you would then lose the ability to display the amplitude of the wavefunction.

H ATOM 3d WAVEFUNCTIONS

14. Close 260lab6b.xls and open 260lab6c.xls.

15. The plot for $3d_{zx}$ also looks like a 2-D box function, and its relationship to the 2p function is obvious.

16. The usual book representation of the $3d_{z^2}$ function appears bizarre – a dumb-bell with a belt! The plot here looks more reasonable, but why is it so different from d_{zx}? The answer is that the $3d_{z^2}$ function shown here has the correct shape (in the limited dimensions available to us). The other ones (crossed dumb-bells) are not the shapes of actual wavefunctions but are symmetric and antisymmetric combinations of complex functions.