

MS 131, Problem Set #2

assigned 10/05/05

due 10/12/05

1. Consider the hydrogen atom. Beginning with the time independent Schroedinger equation and the form of the Coulombic potential,
 - (a) derive the partial differential equations that yield $R(r)$, $\Theta(\theta)$ and $\Phi(\phi)$.
 - (b) derive the solutions to $\Phi(\phi)$ and show that these solutions imply the quantum number m_l .
2. Continue to consider the hydrogen atom. Use the hand-out of hydrogenic orbitals given in class on 10/3/05, or any other source for those wavefunctions.
 - (a) Derive the expectation value of the radial distance of the electron from the nucleus, $\langle r \rangle$, for an arbitrary state.
 - (b) Derive the value of the maximum in the electron probability density for the 1s state.
 - (c) Compare the expectation value and the maximum probability density position for the 1s state. Why do they differ?
3. Continue to consider the hydrogen atom.
 - (a) Show that the 1s and 2s wavefunctions are (each) normalized to unity..
 - (b) Show that the 1s and 2s wavefunctions are orthogonal.
4. Continue to consider the beloved hydrogen atom. Take the electron to be in the 1s state.
 - (a) What is the electron density (electron/ \AA^3) at a point 0.37 \AA from the hydrogen nucleus of an isolated hydrogen atom?

Now suppose that two hydrogen atoms are brought together to form an attractive bond with 1s wavefunctions. Their inter-nuclear separation is 0.74 \AA .
 - (b) What is the electron density midway between the two nuclei? You need not normalize the molecular wavefunction.
 - (c) Explain in words why there is a difference between the results of parts a and b.
 - (d) Make a semi-quantitative estimate of how a proper normalization, including overlap effects, will alter the result of part b