Problem Set PS04

ISSUED: 9/21/00 **Due: 9/28/00**

Prof. Darin J. Ulness Name _____

Instructions. Complete all questions before class on the due date. You are encouraged to work together. Be sure to struggle with the problem before seeking help. Many of the exercises are very similar to problems in the book. Understanding the solution to these problems will be helpful in completing the assigned exercises.

Mathematical Exercises

1. Sketch a graph of $f = -1/r$ for $0 \leq r < \infty$. If r is considered as a radius, what does this function look like in two dimensions?

Exercises

2. Using your handout on hydrogenic wavefunctions and average values, plot $\langle r \rangle$ for each value of n and l up through $n = 7$ (work in units of Bohr radius, i.e., set $a_0 = 1$). What does this say about the average radius of the hydrogen atom as the principle quantum number increases? How about as the angular momentum quantum number increases?

3. Using your handout on hydrogenic wavefunctions and average values, plot $\langle r \rangle$ for each value of n and l up through $n = 7$ (work in units of Bohr radius, i.e., set $a_0 = 1$). What does this say about the uncertainty in the position of the electron for the hydrogen atom as the principle quantum number increases? How about as the angular momentum quantum number increases?

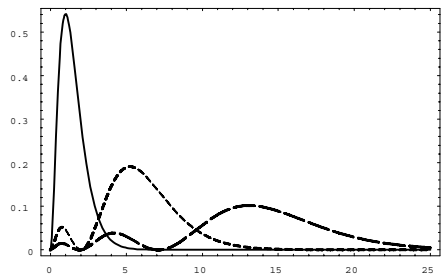
4. Derive the $3p_x$ and $3p_y$ wavefunctions from the $3p_1$ and $3p_{-1}$ wavefunctions. Derive the $3p_1$ and $3p_{-1}$ wavefunctions from the $3p_x$ and $3p_y$ wavefunctions.

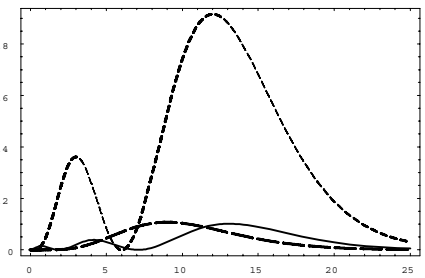
Conceptual Problems

5. Much of general chemistry and particularly inorganic chemistry can be explain using two simple ideas: i) penetration and ii) shielding. Penetration deals with the fact that outer shell electrons which are normally found far from the nucleus have a non-zero probability of being found near the nucleus and in fact inside inner shell electrons. Shielding arrises in atoms that have more than one electron and is a result of the interaction between the electrons. Each electron "shields" each of the other electrons from feeling the full nuclear charge. Electrons that are closer to the nucleus shield electrons that are farther from the nucleus. The figures below shows the so-called radial probability distribution functions for various numbers. This represents the probability of finding an electron at a given distance r from the nucleus irrespective of angle.

   (a) Considering the s electrons can the 3s electrons penetrate inside the average radius of the 2s electrons? How about inside the 1s electron radius.

   (b) Considering the figure showing the $n = 3$ electrons, which type of electrons do you think are more effective shielders s, p or d?.





Computer Problems

6. Use MATHEMATICA to make a density plot of the $|\psi_{1s}|^2$ and $|\psi_{2s}|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$ and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

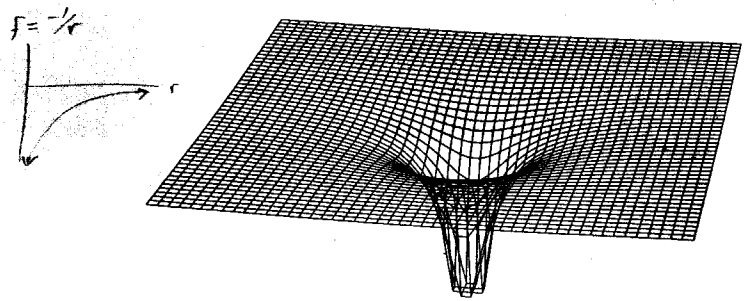
7. Use MATHEMATICA to make a density plot of the $\left|\psi_{2p_x}\right|^2$ and $\left|\psi_{2p_y}\right|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$, $\phi = \arctan\frac{y}{x}$, $\theta = \pi$ (this puts us on the x-y plane) and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

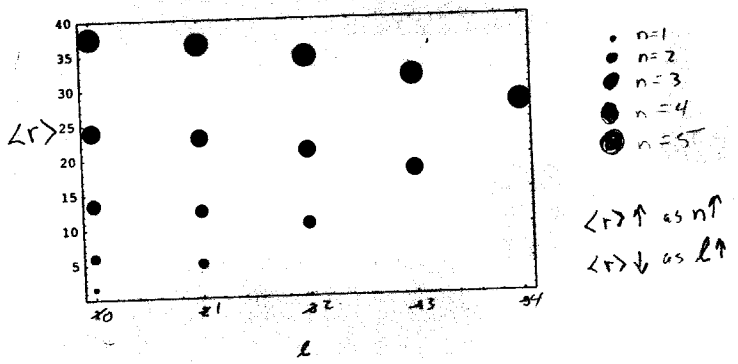
8. Use MATHEMATICA to make a density plot of the $\left|\psi_{2d_{xy}}\right|^2$ and $\left|\psi_{2d_{x+y}}\right|^2$. What do these plots tell us? (Hint: Define $\sigma = \sqrt{x^2 + y^2}$, $\phi = \arctan\frac{y}{x}$, $\theta = \pi$ (this puts us on the x-y plane) and plot versus x and y. Turn the `Mesh` to false and use a sufficient number for `PlotPoints` and appropriate ranges to make the plots look like the ones you've seen in freshman chemistry.)

Reflective Exercises

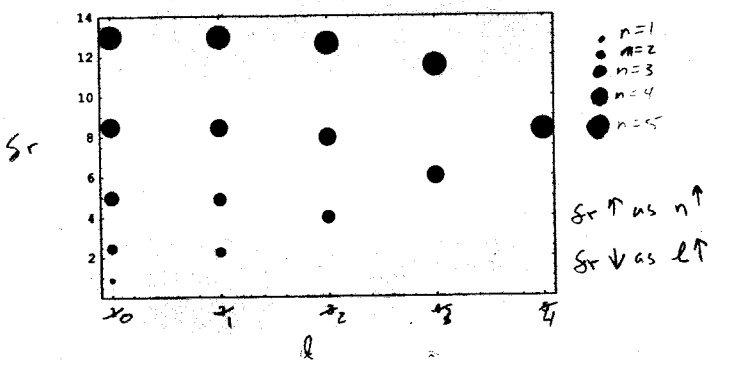
9. A popular play called *Copenhagen* deals with a mysterious visit of Heisenberg to his mentor Bohr that occurred during World War II. At the time Heisenberg was head of the German nuclear project and Bohr was in German occupied Denmark. Heisenberg claimed that the German nuclear project was focussed on creating nuclear power for use by Germany rather then focussed on the atomic bomb. Anyway the question is raised as to whether or not it is ethical to work on nuclear power of any reason. Suppose that at some point in the future your job required you to use your training to work on something that may be of tremendous benefit to society (such as nuclear power) but could potentially be very destructive (such as the atomic bomb). Also suppose that it was out of your control as to how your results would be used. How would you react to this situation?

10. What are the five traditional areas of chemistry? What do these areas deal with? Make all possible pairs of areas (e.g., biochemistry + inorganic chemistry = bioinorganic chemistry) and think of one modern problem that each of the 24 hybrid fields might tackle.

① 

② 

⟨r⟩ ↑ as n ↑
⟨r⟩ ↓ as ℓ ↑

③ 

δr ↑ as n ↑
δr ↓ as ℓ ↑

④ $3p_x = \frac{1}{\sqrt{2}}(3p_1) + \frac{1}{\sqrt{2}}(3p_{-1})$

$3p_y = \frac{1}{i\sqrt{2}}(3p_1) - \frac{1}{i\sqrt{2}}(3p_{-1})$

$3p_1 = \frac{1}{\sqrt{2}}(3p_x) + \frac{i}{\sqrt{2}}(3p_y)$

$3p_{-1} = \frac{1}{\sqrt{2}}(3p_x) - \frac{i}{\sqrt{2}}(3p_y)$

⑤ (a) yes definitely inside the 2s and probably inside the 1s

(b) s electrons are the best shielders, but the p electrons aren't too bad. The d electrons are poor.

⑥–⑧ see last year's solutions to PS04

⑨ your response

⑩ Analytical — chemical analysis and quantitation

Inorganic — chemical synthesis involving any of the atoms of the periodic table

Organic — chemical synthesis centered on carbon based molecules

Physical — physical processes behind chemical principles

Biochemistry — chemistry of biological organisms.