Problem Set 1

1. The root mean square speed of an O_2 molecule at 21°C is 479 m/s. Calculate the de Broglie wavelength for an O_2 molecule travelling at this speed. How does this wavelength compare with the approximate length of this molecule, which is about 242 pm. (For this comparison, state the wavelength as a percentage of molecular length)

2. A typical mass for a horse is 510 kg, and a typical galloping speed is 22 kilometers per hour. Use these values to answer the following questions.

a. What is the momentum of a galloping horse? What is its wavelength?
b. If a galloping horse's velocity and position are simultaneously measured, and the velocity is measured to within ± 1.0%, what is the uncertainty of its position?
c. Suppose Planck's constant was actually 0.01 J s. How would that change your answers to (a) and (b)? Which values would be unchanged?

3. How would you represent the wave function(s) in the $\psi_{n,l,m}$ format for electron in the H-atom that exists in the following orbitals (a) 6p and (b) 3s, Example, $\psi_{n,l,m}$ corresponding to 2p will be $\psi_{2,0,0}$; etc

4. What is an eigen function and what are eigen values? Explain with a specific example.

5. In a graph, show the position of a particle (x, y, z) in terms of the spherical co-ordinates (r, Θ, φ). What are the possible values of r, Θ, φ.

6. In quantum mechanics, what is meant by the wavefunction of a particle?

7. (a) How many values of the quantum number *l* are possible when n = 7? (b) How many values of ml are allowed for an electron in a 6d-subshell? (c) How many values of *m* are allowed for an electron in a 3p-subshell? (d) How many subshells are there in the shell with n = 4?

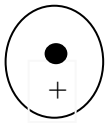
8. For a hydrogen atom (with Z = 1), calculate the energies, in kJ mol^{-1}, of the four lowest energy levels. Do the same for the He^+ ion, which has Z = 2. Plot the levels of He^+ to scale in a similar way to Fig. 2.13 on page 45 of Keeler and Wothers, labelling each with the value of the principal quantum number n. Discuss the choice of energy zero you have used.

9. The radial part of the 3p AO wave function is:

$$R_{3,1}(r) = N_{3,1}\left[6\left(\frac{r}{a_0}\right) - \left(\frac{r}{a_0}\right)^2\right]\exp\left(-\frac{r}{3a_0}\right).$$

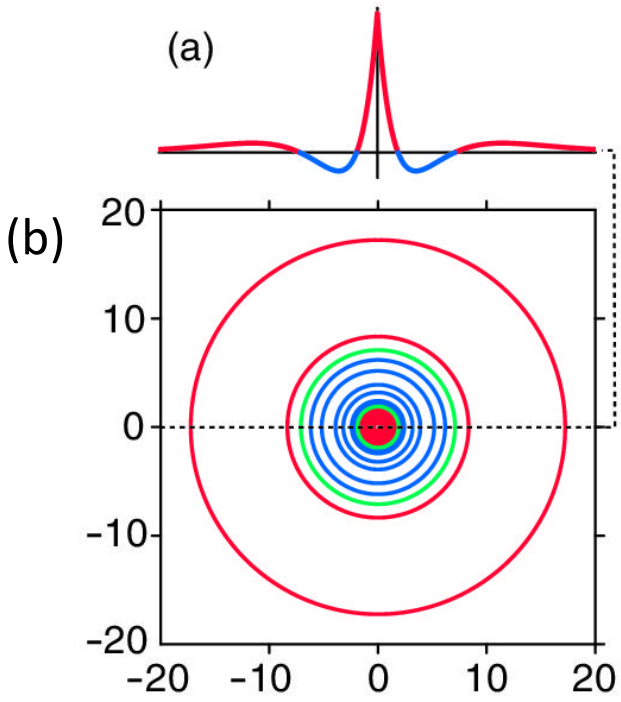
Determine the position of the radial node in the 3p orbital?

10. Sketch the 2s, 3s and 4s orbitals of H-atom (draw only one equal probability iso-surface; NOT contour plots, eg 1s should be sketched as shown below)



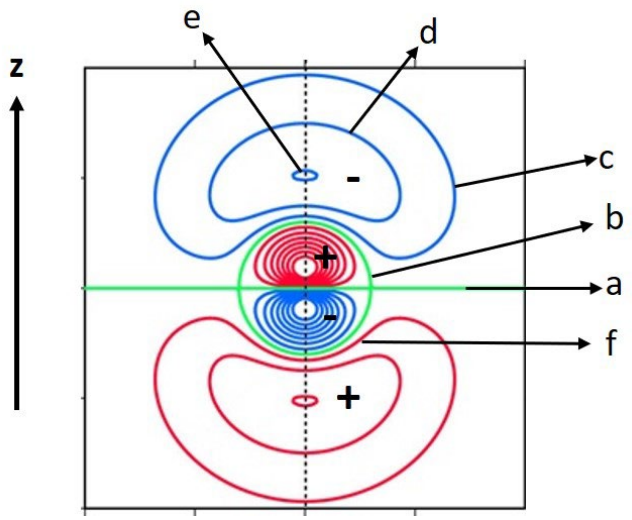
11. Sketch the $2p_x$, $2p_z$ and $3p_z$ (draw only one equal probability iso-surface; NOT contour plots). Label the axis, nucleus, radial node, nodal plane and sign of wavefunction wherever applicable).

12. The 2D plot of wavefunction ψ (figure a) and the contour plot of wavefunction ψ (figure b) are shown below for the 3s orbital. Consider that the contour plot of ψ^2 looks like the plot shown below (of course, there will be no "signs"). In such a scenario, answer the following:



(i) In figure b, what does the green circle represent.
(ii) Which contour has more probability of finding the elctron: outer red contours or the inner blue contour.
(iii) How many radial nodes are present.

13. The contour plot of wavefunction (ψ) shown below is of one of the p orbitals. Consider that the contour plot of ψ^2 looks like the plot shown below (of course, there will be no "signs"). In such a scenario, which of the following statements is true:



(A) Between "c", "d" and "e", the "probability of finding electrons" increases in the order c>d>e

(B) The circle "b" represents the angular node

(C) The line "a" represents the radial node

(D) The "probability of finding electrons" is higher in the point "d" in comparison to "f"