

Problems 3 and 4 are designated (⌘) as 'no collaboration' problems.

As usual, you must complete and be able to replicate your own work.

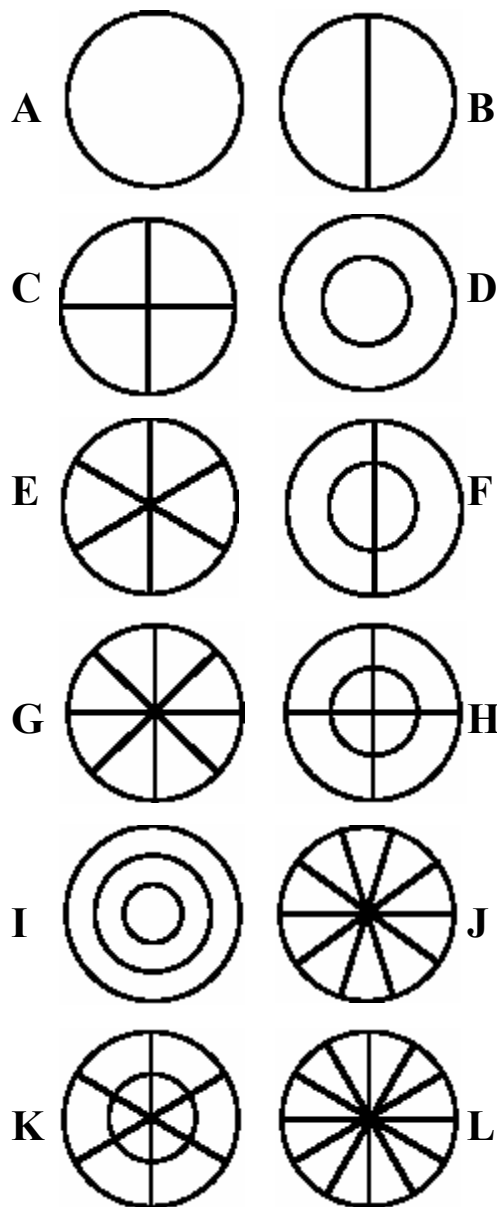
1. (25 Points) The symbols at right correspond to the twelve lowest energy standing wave patterns generated on the top surface of a kettledrum (T. D. Rossing in *Scientific American*, November 1982, pp. 172-178). The patterns A-L are labeled in order of increasing energy, with A representing the lowest frequency and L the highest. This circular two-dimensional system displays angular nodes akin to the square system we discussed in lecture. Its circular nodes are more analogous to the three-dimensional radial nodes in atomic orbitals.

- a. (10 Points) With the convention of nodes adopted above, assign each kettledrum pattern a corresponding atomic orbital. For example, pattern A would correspond to a 1s orbital, because it has no nodes while pattern B would be a 2p orbital because it has 1 angular node. Briefly show your reasoning for each pattern.

- b. (12 Points) Generate a figure similar to Figure 1-20 (p. 36) in Gray, placing the patterns A-L in their appropriate positions corresponding to the placement of the atomic orbitals above. Remember to re-order the relative heights of the patterns to conform with the energy ordering A through L.

- c. (4 Points) In the 3-D, multi-electron case of Fig. 1-20, energy increases with the angular momentum quantum number, l . However, your plot in part b. shows this is not true in the two-dimensional case. Explain, in terms of the relative contributions of circular and angular nodes, the relationship between energy and l in the kettledrum wave patterns.

- d. (4 Points) For the three-dimensional multi-electron case, explain briefly (in two or three sentences) why energy increases with l for a given n .



2. (25 Points) The following is a wavefunction for a one electron atom with nuclear charge Z .

$$\psi = \frac{1}{81} \left(\frac{1}{6\pi} \right)^{1/2} \left(\frac{Z}{a_0} \right)^{3/2} \left(\frac{Zr}{a_0} \right)^2 e^{-\frac{Zr}{3a_0}} (3\cos^2\theta - 1)$$

where a_0 is the Bohr radius and r is the distance from the nucleus.

- What is this orbital (such as 5d, 4p, etc., not 5d_{xy} or 4p_x)? Explain.
- How many radial nodes does this wavefunction have, and write a simple equation for the node(s) as a function of r . So report $r_{\text{node } n} = (\text{some distance})$ for each radial node.
- How many angular nodes does this wavefunction have and at what $\theta(s)$ are the node(s) (in degrees)?

3. (15 Points) Prof. Lewis discusses how electrons near the nucleus effectively screen the nuclear charge from other electrons in multi-electron atoms. In that case, why is it easier to remove an electron from a sodium atom than it is to remove an electron from a magnesium atom? After all, magnesium has more electrons to shield the nuclear charge, right?

4. (15 Points) In lab one day you measure the successive ionization energies of a single unknown element. You get the following data in arbitrary energy units.

1 st : 0.37	5 th : 2.56	9 th : 13.91	13 th : 23.98
2 nd : 0.89	6 th : 3.24	10 th : 16.44	14 th : 25.99
3 rd : 1.29	7 th : 10.33	11 th : 18.51	15 th : 118.47
4 th : 1.76	8 th : 11.97	12 th : 20.72	16 th : 128.40

Which element(s) are consistent with the ionization energy data above, given that you have several grams of it? Describe your reasoning. (*Hint: these are student-acquired numbers, and poorly acquired at that. Do not attempt to align these numbers to a data table!*)

5. (20 Points) Without that pesky electron-electron repulsion term, the Schrödinger equation can be solved exactly. But before we make up an alternate universe with aliens where atoms can only have one electron or something, let's just consider the boring He^+ case. We can compare the Bohr model to the Schrödinger model for this case and find useful information about the lone electron.

- Using the Bohr model, determine the distance from the nucleus of an electron in a 1s orbital of a He^+ ion. Use $a_o = 0.529 \text{ \AA}$.
- Using wavefunctions, we can't get a distance from the nucleus for where the electron *is*, because under quantum mechanics electrons have wave-like properties. We can, however, get the average distance from the nucleus at which it would be *observed*, and the most probable distance where it would be *observed*, using:

$$\psi_{1s} = 2 \left(\frac{Z}{a_o} \right)^{\frac{3}{2}} e^{-\frac{Zr}{a_o}} \quad \text{and} \quad P(r) = r^2 \psi^2(r) \quad \text{and} \quad \bar{r}_{nl} = \frac{n^2 a_o}{Z} \left(1 + \frac{1}{2} \left(1 - \frac{l(l+1)}{n^2} \right) \right)$$

where $P(r)$ is the probability function for finding the electron, and r_{nl} is the average distance from the nucleus for the one electron atom (from OGN), Z is the nuclear charge, a_o is the Bohr radius, and n and l are quantum numbers. Find the most probable distance and average distance at which the 1s electron for He^+ would be found.