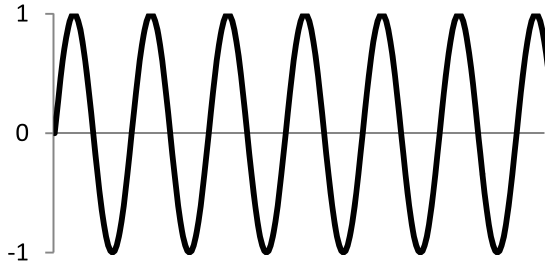
CHEM1101 Worksheet 4: Quantum Chemistry

Model 1: Light and Waves

The picture below shows a light wave. The wavelength is the distance between peaks (or the distance between troughs). The amplitude is the height of the wave.

We cannot see these waves. Instead, our eyes detect the *intensity* of the light which is given by the *square* of the wave.

Squaring means multiplying the wave at each point by itself, remembering that positive × positive and negative × negative are both positive.



Critical thinking questions

1. On the diagram, indicate the wavelength (λ) and the amplitude (A) of the wave.

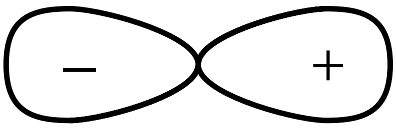
2. Put an asterisk (‘*”) to mark the positions where the wave is zero. These are ‘nodes’.

3. Peaks are where the wave is positive. Troughs are where the wave is negative. Labels these with “+” and “–“ signs respectively. *Lightly* shade the “–” areas.

4. On top of the picture, draw a sketch of the *intensity* of the light.

Model 2: Electron Waves

The picture below is a lobe representation of a 2-dimensional wave for an electron. The line encapsulates 90% of the electron density. We cannot see or measure the wave. Instead, the electron density can be measured and this is given by the *square* of the wave.



Critical thinking questions

5. Mark the position of the node and *lightly* shade the “–” area.

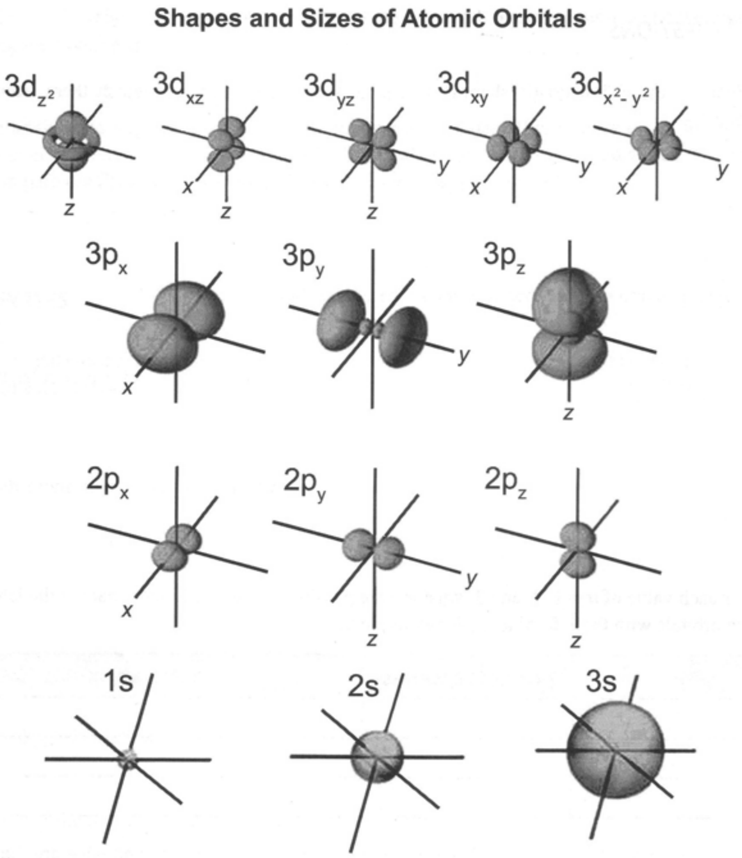
6. Draw a sketch of the electron density for this electron.

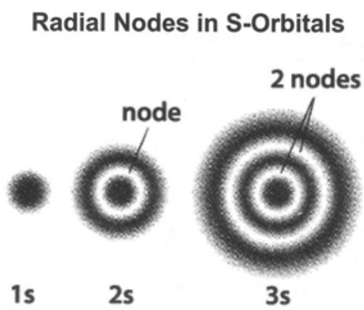
Model 3: Atomic Orbitals and Quantum Numbers

The wave functions for electrons in atoms are given the special name ‘atomic orbitals’.

As explored in Worksheet 3, the energy levels of hydrogen-like (one-electron)atoms are determined by a single quantum number, *n*. For other atoms, more quantities are involved in determining the shape and orientation of the atomic orbitals, these are the *angular momentum quantum number*, *l*, and *magnetic quantum number*, m_l.

Name	**Characterizes**	**symbol**	**Allowed values**
Principal	Size and Energy. Total *n* -1 nodes	*n*	***n* = 1, 2, 3,…**
Angular Momentum	Shape Energy in multi-electron atoms *l* planar nodes	*l*	***l* = 0, 1, 2,… *n*-1**
Magnetic	Orientation	m_l	**m_l = -*l*, 1-l,…0… *l*-1, *l***





Critical thinking questions

1. What are the characteristic shapes of *s*, *p*, and *d* orbitals?

2. Which quantum number identifies the shape of an orbital?

3. For each value of n = 1, 2, and 3, what are the possible values for l, and what labels correspond to these orbitals?.

n	**Possible *l* values**	**Orbital labels**
1		
2		
3		

4. For each value of l = 0, 1, 2, what are the possible values for m_l, and what are the labels for the orbitals with this set of m_l values?

l	**Possible m_l values**	**Orbital labels**
0		
1		
2		

5. Which orbitals have a plane where the probability of finding the electron is zero (a *nodal plane*)?

6. What is the relationship between the value of the angular momentum quantum number and the number of such *nodal planes*?

7. Which orbitals in the model have *radial nodes*?

Model 4: Electronic Configurations in Atoms

Critical thinking questions

1. Discuss with your group and write down definitions of

   a. The Aufbau Principle

   b. Pauli Exclusion Principle

c. *Hund's Rule*

2. Fill in the ground state electronic configuration for a carbon atom on the diagram below.

   a. Why isn't the electron configuration of carbon $1s^2\ 2s^3\ 2p^1$?

   b. Why isn't it $1s^2\ 2s^2\ 2p_x^2$?