Physics 249 Lecture 23, Oct 29th 2012  
Reading: Chapter 7.4, 7.5  
HW available on web site, due Nov 2nd

1) Predicting ionization energies.

In general when a subshell or shell is complete the distribution of electron probability for the completed shell is fairly spherical.

This makes the problem of predicting the probability distributions and observables such as the ionization potential tractable. A full shell will represent a spherically symmetric, though not 1/r, potential. Two methods exist to try and predict properties.

a) Solve the problem exactly. Possible in some spherically symmetric cases.

b) Perturbative series method. A good example of this is solving for ionization potentials. For this method you assume that the hydrogen atom like solution is correct. Then you determine the addition to the ionization energy over the hydrogen like solution by calculating the expectation value of the potential energy between the electron of interest and the other electrons using the hydrogen like wave functions. This already gives a fairly good approximation to the correct answer. This procedure can also be used to determine corrected wave functions and you can iterate this procedure multiple times using the new wave functions to achieve arbitrarily precise accuracy. (beyond the scope of this class).

2) Total angular momentum

To understand the total angular momentum we have to add the orbital and spin angular momentums. Understanding how they add will allow us to further understand the magnitude of the magnetic field that these angular momentums can produce and changes in energy level between states with the same n but different angular momentums and angular momentum projections on the z axis.

Note that once you have one electron in the system with angular momentum that defines an axis relative to which you can classify the angular momentum of all the other electrons. Electrons will tend to align or not depending on which configuration lowers the overall potential energy and obeying the Pauli exclusion principle. Even with only one electron the nucleus is composed of particles with spin and angular momentum which defines an axis. This gives a meaning the having an axis of interest, defined as the z axis in our systems.

Because of the quantization of angular momentum and the restrictions in how it is oriented imposed by the wave equation you can write simple rules for how it adds with. Define J as the total angular momentum and Jz as the projection such that:

\[ J^2 \rightarrow \hbar^2 j(j + 1) \]
\[ J_z \to \hbar m_j \]
\[-j \ldots m_j \ldots j \]

We like to understand how the orbital and spin components of the angular momentum add.

\( J \) can range through positive values defined by the following condition.

\[ |l-s| ... j ... l+s \]

There are multiple possibilities for \( j \) because \( l \) and \( s \) might have pointed in different directions and the vector sum could have a range of magnitudes.

\[ m_j = m_l + m_s \]

For \( m_j \) there are not multiple values since the direction of \( m_l \) and \( m_s \) are known so that you know exactly how much angular momentum is on along the z axis.

For \( l = 1 \) and \( s = \frac{1}{2} \)

\( j = 1/2, 3/2 \)
\[-j \ldots m_j \ldots j \]

If \( m_j = m_l + m_s = \pm 1 \pm \frac{1}{2} = \pm \frac{3}{2} \) then \( j \) must be \( 3/2 \)

If \( m_j = \pm \frac{1}{2} \) Then \( j \) might be \( 1/2 \) or \( 3/2 \).

A diagram explaining this is below.

The angular momentums in these diagrams has known values on the z axis but the total angular momentum might be pointed in various directions. These diagrams show directions such that when the angular momentums are combined where you get totals that correspond the quantized solutions for the total angular momentum. Note they must be aligned to achieve the maximum value addition. However, there are two ways they may be misaligned resulting in different \( j \) values but the correct \( m_j \) value.

We are using the ansatz that the total angular momentum should be quantized in a similar way to the individual momentums. In principle this can be proved by writing a full Schrodinger equation including both particles and the magnetic potential energy.
2) Spin orbit effect

Since both orbital and spin angular momentums cause magnetic fields there is the possibility of alignment between them. Also there is the possibility of alignment with the magnetic moment of the nucleus. Aligned states will have lower potential energy than anti-aligned states since $U = -\mu \cdot \vec{B}$. Overall magnetism will depend of the j and or more precisely the mj state which describes the projection of the total angular momentum on the z axis. We will use these concepts to understand ferromagnetism.

The magnetic moment is given classically as

$$\mu = \frac{q}{2m} \overrightarrow{L}$$

In a quantum system we replace L with the angular momentum operator. There can be angular momentum due to L, S or total angular momentum J and we can compute projections on the z axis. Just considering J

$$\mu = -\frac{e\hbar}{2m_e} \sqrt{j(j+1)} \hbar = -\mu_B \sqrt{j(j+1)} \hbar$$

Where we have defined the Bohr magneton:

$$\mu_B = \frac{e\hbar}{2m_e}$$
However, we are always measuring on some axis.

\[ \hat{\mu} = -\frac{e\hbar}{2m_e} m_j^2 \]

The alignments that create the lowest potential energy are a subtle effect of orbital considerations.