Physics 249 Lecture 20, Oct 22nd 2012
Reading: Chapter 7.1, 7.2, 7.3
Homework due Friday Oct 26th. Available on web site.

1) Angular momentum

The momentum of the particle can be either radial or angular (perpendicular) to the radial direction.

\[ \vec{p} = p_r \hat{r} + p_\theta \hat{\theta} \]

where:

\[ p_r = \mu \frac{dr}{dt}, \quad p_\theta = \mu r \frac{d\alpha}{dt} \]

Consider the classical definition of angular momentum:

\[ \vec{L} = \vec{r} \times \vec{p} = r p_\theta \sin \alpha = r p_\theta \]

Then the kinetic energy term that goes in the Schrodinger equation can be written as:

\[ \frac{p^2}{2\mu} = \frac{p_r^2 + p_\theta^2}{2\mu} = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} \]

where we understand how to replace these equations with operators

\[ \frac{p_r^2}{2\mu} \rightarrow -\frac{\hbar^2}{2\mu r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) \]

If you want to try this is the easier of the two relationships to derive. Given that this is radial derivative term in the Schrodinger equation the other part of the momentum must give the angular part.

\[ \frac{L^2}{2\mu r^2} \rightarrow -\frac{\hbar^2}{2\mu r^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \]

Now consider the angular portion of the wave equation after partial separation of variables.

\[ - \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y_{lm}(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{lm}(\theta, \phi)}{\partial \phi^2} \right] = C_r Y_{lm}(\theta, \phi) \]

\[ = l(l+1)Y_{lm}(\theta, \phi) \]

Where the integer l characterized the quantized solutions to the theta wave equation. Now we can interpret l.
\[ L^2 Y_{lm}(\theta, \phi) = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] Y_{lm}(\theta, \phi) = \hbar^2 (l + 1) Y_{lm}(\theta, \phi) \]

The angular momentum is quantized by an integer \( l \) and has eigenvalues of: \( L^2 \rightarrow \hbar^2 l(l + 1) \).

Now consider angular momentum for the angle \( \phi \) around the \( z \) axis

\[ L_z \rightarrow -i\hbar \frac{\partial}{\partial \phi} \]

\[ L_z Y_{lm}(\theta, \phi) = m \hbar Y_{lm}(\theta, \phi) \]

Thus \( m \) is the projection of the angular momentum on the \( z \) axis. Note that the projections are never as large as the total angular momentum. The wave functions are quantized with different amounts of angular momentums projected on the \( z \) axis. We will see this qualitatively form pictures of the wave functions.

2) Visualizing the full wave function

Visualizing these can be fairly difficult. I suggest

http://hyperphysics.phy-astr.gsu.edu/hbase/hydwf.html
Radial wave functions

xz view

http://chemlinks.beloit.edu/Stars/images/orbitals.jpg
tilted z axis xz view

http://www.falstad.com/qmatom/
3D java app.

Some notation.
s: \( l=0 \)
p: \( l=1 \)
d: \( l=2 \ldots \)

Things to note.

a) \( n-l \) maximum of the radial wave functions.

b) The \( m=0 \) configuration are oriented vertically along the \( z \) axis such that there is nothing to rotate in the \( xy \) plane. They are static in terms of rotation in the \( xy \) plane.
c) The $m=1,2 \ldots$ configuration are oriented such that the lobes can rotate in the xy plane. Remember the phi wave function is that of a traveling wave in phi.

d) Point c implies a circularly rotating current which should cause a magnetic field. With several caveats on how orbitals are filled in multi electron atoms this is true.

e) The electrons have angular momentum, but do not radiate. The short answer is that the transitions are forbidden by conservation and exclusion principles. We will explore what this means as we consider multi-electron atoms.

f) Energy levels. Any change in the potential of the system can change the energy levels and break the degeneracy between states with the same energy. For instance,

i) The additional electric or magnetic field caused by other electrons in a multi-electron atom. Even if the field is spherically symmetric, such as an s wave electron it still modifies the form of the potential and can break degeneracies. For instance, states with different $l$ tend to have different characteristic radii which will be inside/outside different amount the shielding provided by an inner s wave orbit.

ii) An external electric or magnetic field.
Hydrogen Wave Function

\[ \psi_{nlm}(r, \theta, \phi) = \sqrt{\frac{2}{n^2 \pi}} \left( \frac{n - l - 1}{2n(n + l)} \right)^{\frac{1}{2}} \exp \left[ -\frac{r}{a_0} \right] \cdot L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\theta, \phi) \]