PHYS 3317 Fall 2012
Homework 4 Atomic spectra & many-particle states

I had the full intention to have you solve multi-electron atomic energy levels in MATLAB for this homework. However, given that a number of people are struggling with the numerics (even though overall you guys are doing great!), we'll have a shorter homework this time to allow us to catch up with the intended homework deadline (Friday in your section). Regarding the computation of the multi-electron atomic energy levels — this would make a great final computer project instead. Detailed steps to this approach (the so-called *self-consistent field* method) can be found in Datta's book, sections 3.1 and 3.2.

1. Spin-orbit splitting

Using first-order perturbation theory (you will only need the basic result I gave you in lecture; but if you want to read more, refer to Griffiths Chapter 6), calculate the energy difference in eV between the $3\,^2P_{3/2}$ and $3\,^2P_{1/2}$ states of the hydrogen atom, which results from the spin-orbit interaction term in the Hamiltonian (considered to be a small perturbation):

$$\hat{V}_{so} = \frac{e^2}{8\pi\varepsilon_0(mc)^2}\frac{\hat{\mathbf{s}}\cdot\hat{\mathbf{L}}}{\hat{r}^3}.$$

(a) Start out by arguing that

$$\langle\frac{\hat{\mathbf{s}}\cdot\hat{\mathbf{L}}}{\hat{r}^3}\rangle = \langle\hat{\mathbf{s}}\cdot\hat{\mathbf{L}}\rangle\langle\frac{1}{\hat{r}^3}\rangle.$$

(b) Next, show that the expectation value

$$\langle\hat{\mathbf{s}}\cdot\hat{\mathbf{L}}\rangle = \frac{1}{2}\langle\hat{J}^2 - \hat{L}^2 - \hat{s}^2\rangle,$$

and, therefore, can be expressed in terms of quantum numbers l, j, and s. Find this expression.

(c) Finally, evaluate the difference $\Delta E_{so}(3P_{3/2}, 3P_{1/2}) = \langle V_{so}\rangle_{3P_{3/2}} - \langle V_{so}\rangle_{3P_{1/2}}$ for the two given $3p$ states:

$$\psi_{31m_l}(r,\theta,\phi) = R_{31}(r)Y_1^{m_l}(\theta,\phi).$$

You will need the explicit expression for the radial part of the wave-function, which can be found in most standard QM textbooks. I give the expression here for your convenience (a_0 is Bohr's radius).

$$R_{31}(r) = \left(\frac{1}{3a_0}\right)^{3/2}\frac{4\sqrt{2}}{9}\left(1 - \frac{1}{6}\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}.$$

Be sure to specify which state is higher in energy, and which is lower. Feel free to use Mathematica or `http://www.wolframalpha.com/` to evaluate the final integral.

Multiple-particle basis functions

Suppose we have three particles, labeled 1, 2, and 3, and three single-particle states or modes, a, b, and c. We presume the particles are essentially not interacting, so the state of the three particles can be written in terms of products of the form $|1a\rangle\,|2b\rangle\,|3c\rangle$, though we do insist that the states obey appropriate symmetries with respect to interchange of particles when the particles are identical. For the purposes of this problem, we are only interested in situations where each particle is in a different single-particle state or mode. For example, if the different states correspond to substantially different positions in space, we presume that we are considering states in which we would always find one and only one particle near each of these three positions if we performed a measurement. Write out all the possible states of the three particles:

(a) if the particles are identical bosons;

(b) if the particles are identical fermions;

(c) if the particles are each different (e.g., one is a neutron, one is a proton, and one is an electron).