PHYS 3317 Fall 2012
Homework 4 Atomic spectra and Multi-Particle States

I had a full intention to have you solve multi-electron atomic energy levels in MATLAB for this homework. Given that a number of people are struggling with numerics, we'll have a shorter homework instead 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. 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 (if unsure what that is — 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 you can find in any standard QM text. I give the expression here for your convinience

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

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.