CSC 335
Homework Set 4
Due 5:00 p.m., October 24, 2011

Problems from Burden and Faires:

Section 4.1: #21, #26

Section 4.2: #1(a), #1(c), #2(a), #2(c)

Section 4.3: #1(c), #1(h), #3(c), #3(h), #5(c), #5(h), #7(c), #7(h)

Section 4.4: #1(c), #1(h), #3(c), #3(h)

Section 4.5: #1(c), #1(e), #6, #16

Section 4.6: #1(a), #1(e), #2(a), #2(e)

Section 4.7: #1(a), #1(d), #4(a), #4(d),

Section 4.9: #3(b), #3(c), #4(a)

Problem from Dr. Pounds:

The *expectation value operator* is often used in quantum mechanics to return the average value of a quantum mechanical observable. In this problem we will compute the expectation value for the position of an electron trapped in a $2s$ orbital of the hydrogen atom. The expectation value for r is obtained by evaluating the integral:

$$\begin{aligned}
\langle r \rangle = \langle \psi^*_{2,0,0}|r|\psi_{2,0,0}\rangle &= \int_0^\infty \int_0^{2\pi} \int_0^\pi \psi^*_{2,0,0} r \psi_{2,0,0} r^2 \sin\theta d\theta d\phi dr \\
&= 4\pi \int_0^\infty \psi^*_{2,0,0} r \psi_{2,0,0} r^2 dr \\
&= 4\pi \int_0^\infty r^3 \psi^*_{2,0,0} \psi_{2,0,0} dr \\
&= 4\pi \int_0^\infty R(r) dr
\end{aligned}$$

Where $\psi_{2,0,0}$ is the wavefunction of the electron trapped in a $2s$ orbital and given by the equation:

$$\psi_{2s} = \psi_{2,0,0} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_o}\right)^{3/2} \left(2 - \frac{Z}{a_o} r\right) \mathrm{e}^{-\left(\frac{Z}{a_o} r\right)/2}$$

Z is the atomic number and, in this case, is equal to 1. The constant a_o is called the *Bohr radius* and takes on the value of 0.529×10^{-10} meters. The triple integral above can be reduced to one integral because the wavefunction does not depend on the angular variables. Write a program in either JAVA, C/C++, or Fortran employing 3-, 7-, and 15-point Gauss-Laguerre quadrature[1] to determine the expectation value for the position of the electron in the $2s$ orbital of the hydrogen atom. To make things easier to interpret, it is preferable to determine the expectation value in terms of a_o. The easiest way to accomplish this is to evaluate $R(a_o r)$ rather than $R(r)$. If you have questions, ask Dr. Pounds.

[1] The abcissas and weights needed for this will be placed on the class website. You will not have to generate them.