CCB 421/521: Homework 4

Due in class on Thursday, Feb. 24. (Note: these are problems from the book; I'm posting them here because the electronic/Kindle version of the text seems to have lots of typos. Let's hope I don't make typos myself!)

(5-11) Compute the extremum points for the D_{2s} and D_{2p} radial distribution functions for hydrogen. Also compute $< r >$ for these states and compare. *Note:* you may use the result of Problem 5-13:

$$< r >= \frac{n^2}{Z}\left\{1+\frac{1}{2}\left[1-\frac{l(l+1)}{n^2}\right]\right\}$$

(6-4) Express the following in atomic units: 5 nm, Planck's constant, 50 kJ, 5×10^{-5} cm s^{-1}, and the mass of the benzene molecule. Provide both the numerical value, and the associated combination of m_e, e, $\hbar$, and a_0.

(6-6) Convert kT (k is Boltzmann's constant and T is the temperature on the absolute scale) to atomic units when the temperature is 300 K.

(6-7) Consider the following trial wavefunction for the particle in a box: $\xi = Nx$ (N is a normalization constant).

(a) Show that N=$\sqrt{3}$ (for a box of unit length)

(b) Show that the approximate energy due to this wavefunction is zero.

(c) The result in *(b)* appears to violate the upper-limit theorem. Explain the apparent discrepancy.

(6-9) Calculate the expectation value of the linear momentum p_x for the particle in a box using the following trial wavefunction from Eq. (6-65):

$$\xi(x) = N(x^{0.862} - x^{2.862})$$

(Note that N is given in Eq. 6-66.) Compare this with the exact result and explain what you find.