Physics 221B
Spring 2008
Homework 17
Due Friday, February 8 at 5pm

Reading Assignment: Lecture notes for 1/29/08; Notes 26, Notes 27, pp. 1–20. We only covered the elements of the Thomas-Fermi model in lecture, so you may just skim Notes 26 to get the general idea.

1. A continuation of problem 4 from last week. This problem is due to Professor Commins. See Eqs. (1) and (3) of that problem for the one-dimensional "hydrogen" and "helium" Schrödinger equations.

(a) For one-dimensional "helium," employ the variational method with a trial wave function analogous to that used in class for the ground state of 3-dimensional helium. Find the best value of $\langle H \rangle$ and compare to 3-dimensional helium.

(b) For one-dimensional "helium," take a trial wave function of the form

$$\psi(x_1, x_2) = u(x_1)u(x_2), \tag{1}$$

where $u(x)$ is the variational parameter (that is, the whole function, as in Hartree theory). Assume $u(x)$ is real; there is no loss of generality in this. Find an equation for $u(x)$. It will be a kind of Hartree equation, and it will contain a pseudo-energy eigenvalue, call it ϵ. Define ϵ so that the equation looks like

$$-\frac{1}{2}u''(x) + \ldots = \epsilon u(x), \tag{2}$$

where the ellipsis indicates omitted terms.

(c) The desired solution must be normalizable (in fact, we demand that it be normalized), so we must have

$$\lim_{x \to \pm\infty} u(x) = 0. \tag{3}$$

Show that this can only be satisfied if $\epsilon < 0$. Hint: To solve the equation, make the change of notation, $u \to x$, $x \to t$, and interpret it as a one-dimensional problem in classical mechanics.

(d) Find the normalized solution $u(x)$ and the pseudo-eigenvalue ϵ.

(e) Find the variational estimate of the ground state energy of one-dimensional "helium". Hint: Note that

$$\langle H\rangle = 2\epsilon - \langle\delta(x_1 - x_2)\rangle. \tag{4}$$

Does your new estimate improve on the results of part (a)? Would you expect it to do so?

2. For this problem you should review the lecture notes on the perturbation theory for the excited states of helium, in which the energy shifts were shown to be of the form $J_{n\ell} \pm K_{n\ell}$.

(a) The exchange integral $K_{n\ell}$ defined in lecture and in the lecture notes depends on two hydrogen-like orbitals. It is easily generalized to any two single-particle orbitals (recall that "orbital" means a single-particle wave function). Show that if the two orbitals have no spatial overlap, then the exchange integral vanishes. Then use your knowledge of hydrogen-like orbitals to explain the dependence of the exchange integral on n for fixed ℓ, and on ℓ for fixed n. This has certain implications for the energy levels of the excited states of helium.

(b) Go to `http://physics.nist.gov/PhysRefData/ASD/levels_form.html` and check your predictions using the experimental data on the first several excited states of helium. Enter "He I" for the atom (this is neutral helium). You will see that some of the levels have a fine structure, which we did not discuss in detail in class. This should not prevent you from checking your predictions.

3. Show that the Slater determinant $|\Phi\rangle$ is normalized if the orbitals $|\lambda\rangle$ are orthonormal. See Eqs. (27.41) and (27.42).