HW#5—Phys623—Spring 2016

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1. Use the variational principle to prove that any one-dimensional potential $V(x)$ with strictly finite range and $\int V(x)\,dx < 0$ has at least one bound state. *Hint*: For the simplest proof, consider a trial wave function that is constant in the region where the potential is non-vanishing and decreases linearly to zero outside this region. (This trial wavefunction has a kink, which contributes a delta function to the second derivative. Alternatively, you can integrate by parts in the energy functional, so as to express the kinetic energy contribution in terms of the integral of the square of the gradient.) The variational principle is discussed in Sec. 11.2 of Schwabl.

2. **(a)** Find an upper bound for the ground state energy of the hydrogen atom using a three-dimensional harmonic oscillator ground state wave function

$$\psi(r) = (\sqrt{\pi}\beta)^{-3/2}\exp(-r^2/2\beta^2)$$

as a trial function, with the width β as the variational parameter. Compare with the true ground state energy.

(b) Compute the relative error in the approximate energy, $(E_{\rm exact} - E_{\rm approx})/E_{\rm exact}$, and compare this number with the norm $||\psi_{\rm exact} - \psi_{\rm approx}||$ of the difference between the (normalized) exact and approximate wavefunctions. Explain the relation between these two numbers. (*Hint*: See Sec. 11.2.)

3. *Toy model of a helium atom*, Qualifier, January 1999, II-2.

Two particles, each of mass m, are confined in one dimension to a box of length L.

(a) First consider the case where the particles are spinless, not identical, and do not interact between themselves.

What are the normalized two-particle wave functions and energies of the three lowest-energy states of the system? Are any of these energy levels degenerate?

(b) Suppose the particles interact between themselves with the potential $V = \lambda\delta(x_1 - x_2)$, where x_1 and x_2 are the coordinates of the particles, $\delta(x)$ is the one-dimensional Dirac delta-function, and $\lambda > 0$.

In the lowest order of perturbation theory in V calculate the energies and two-particle wave functions for the three lowest-energy states of the system. Sketch how the energy levels shift relative to the energy levels of the noninteracting system.

(c) Formulate a condition on the coefficient λ for lowest order perturbation theory to be applicable.

(d) Now suppose that the particles are two identical fermions, each of spin 1/2, interacting via the potential V of part 3b. Explain how the Pauli principle determines the values of the total spin of the system for the three energy levels found in part 3b. Write the values of the total spin and the degeneracy next to the energy levels in the diagram of part 3b.

Possibly useful integrals:

$$\int_0^\pi d\phi\,\sin^4\phi = 3\pi/8 \qquad \int_0^\pi d\phi\,\sin^2\phi\,\sin^2 2\phi = \pi/4$$

4. *Thomas-Fermi model of an atom*, Adapted from Qualifier, Fall 1981, II-1.

This model treats the electrons as a degenerate Fermi gas, and is discussed in Sec. 13.4 of Schwabl. It is treated here using a variational principle for the energy functional. Suppose the electrons have a spherically-symmetric density $n(r)$. The energy of the electrons can be approximated as a functional of the electron density, $E\{n(r)\}$. The approximate electron density in the atom, $n_0(r)$, is determined as the density that minimizes the energy functional $E\{n(r)\}$.

(a) Write down the (approximate) energy functional $E\{n(r)\}$ for an atom with nuclear charge Ze and N electrons. The functional $E\{n(r)\}$ should contain three terms: (i) E_{ne} that describes the Coulomb interaction between the electrons and the nucleus, which is treated as a point charge Ze; (ii) E_{ee} that describes the Coulomb interaction between the electrons; (iii) T that describes the kinetic energy of the electrons. [*Hint*: To find T in terms of $n(r)$, use (13.18) divided by the (local) volume V.]

(b) i. By varying $n(r)$ in $E\{n(r)\}$, find an integral equation for $n_0(r)$. Take into account that we are looking for a minimum of energy with a given total number of electrons $\int n(r)\, d^3r = N$. This constraint can be handled with the help of a Lagrange multiplier. Show that the boundary condition at $r \to \infty$ implies that the Lagrange multiplier vanishes.

ii. By applying the Laplacian ∇^2 to the equation obtained in Problem 4(b)i, find a differential equation for $n_0(r)$. Show that this equation is equivalent to Eq. (13.63).

(c) Find the ratios E_{ne}/E_{ee} and $(E_{ne} + E_{ee})/T$ in the Thomas-Fermi atom (that is, when $n(r) = n_0(r)$ in E_{ne}, E_{ee} and T). Find these ratios by using the variational principle, but without explicitly finding the optimal density $n_0(r)$. Check whether the latter ratio is in agreement with the virial theorem. (*Hint*: Consider varying σ in $n(r) = (1 + \sigma)n_0(r)$ and $n(r) = n_0\left((1 + \sigma)r\right)$.)

(d) Does a neutral Thomas-Fermi atom have a well-defined radius R where $n_0(R) = 0$, or does $n_0(r)$ extend to infinity? What about a positively charged Thomas-Fermi ion? Can the Thomas-Fermi method describe a negatively charged ion?