Physics 685 – Electronic Structure

Homework 11

Please read Martin, Electronic Structure, Chapter 5, sections 3-4, Chapter 6, sections 1 and 2. Come prepared to answer questions based on reading.

1. Martin, problems 5.16 and 5.17. I expect there maybe a typo in equation 5.32: 0.899 maybe should be 0.66.

2. **Review Project: 1D interacting homogeneous electron "gas"**

   This is the deal: take a 1 dimensional system of length L, and periodic boundary conditions, in a uniform (zero) external potential. A single particle in such a system has eigenstates

$$\phi_{k,\alpha}(\mathbf{r},\sigma) = \sqrt{\frac{1}{L}} \exp{(ikx)} \delta_{\sigma,\alpha} \tag{1}$$

   with allowed values of k of

$$k = \text{fillintheblanks } n \tag{2}$$

   with n any integer. The label α identifies the spin state and can either represent up or down spins: $\alpha = \uparrow, \downarrow$. The probability distribution in space is constant:

$$P(x) = \frac{1}{L}. \tag{3}$$

   Finally, the energy of the single particle is equal, up to a constant, to its kinetic energy, which is

$$KE = \frac{\hbar^2 k_n^2}{2m}. \tag{4}$$

   An ensemble of *noninteracting* particles can be modeled by a one-dimensional HEG, with particle density. We have density given in general by

$$n(x) = \sum_i f_i \left|\phi_i(x)\right|^2 \tag{5}$$

   where our state i is given by spatial quantum number n and spin quantum number α. The expectation here is over the *spatial* part of ϕ_i only – we assume the spin part is summed out. For the HEG this becomes

$$n(x) = \sum_{n,\alpha} f_{n\alpha} \left|\phi_{n,\alpha}(x)\right|^2 = N/L \tag{6}$$

   where the occupancy f can take a value of 0 or 1, and N is the total number of electrons.

For a one dimensional HEG, we need a few changes from the three-D case. The fermi wavevector in one-dimensional gas is

$$k_F = k_{F\sigma} = n_\sigma/\pi \tag{7}$$

(check the constant for me!) and the average energy for one dimension is

$$E/N = \langle KE \rangle/N = \frac{E_F}{2} \tag{8}$$

with E_F the energy at k_F (am pretty sure of the fraction here).

For our system, take two "electrons", both spin up, one with $k = 2\pi/L$ and the other with $k = -2\pi/L$, Add a positive "jellium" background of net charge $2e/L$ and have the electrons interact with it.

Then figure out:

(a) Start from the Hamiltonian 3.1-2 in Martin expressed for the two particle system, construct the HEG Hamiltonian 5.2 expressed for the two-particle system. That is starting with

$$H = T + U_{Ne} + U_{ee} + U_{NN} \tag{9}$$

find appropriate expressions equivalent or similar to those in Eq. 5.2 for each of the four terms on the right-hand side of the equation.

(b) The slater determinant wavefunction for the two particles, with both spin and space variables: $\psi_{SD}(x_1, \sigma_1; x_2, \sigma_2)$ This can be written as a function $F(x_1 - x_2)$ which you should check goes to zero as $x_1 - x_2 \to 0$.

(c) The expectation value of the single-particle density, given by:

$$n(x) = \sum_{i=1}^{N} \langle \delta(x - x_i) \rangle. \tag{10}$$

NOT given in Martin!!!!!!!!!!!!!!!!!!!!!! Refer to notes of Homework 5. The expectation value should be taken over ψ_{SD} and integrating/summing over the variables x, x', σ, σ'. Show this equals the form (Eq. **??**) that one expects for noninteracting particles. What should $f_{n\sigma}$ be for this system?

(d) What is the expectation value for the **pair density**:

$$n^{(2)}(x, x') = \langle \sum_i \sum_{j \neq i} \delta(x - x_i)\delta(x - x_j) \rangle \tag{11}$$

using the Slater determinant wavefunction ψ_{SD}. What is the expected density of pairs with $x = x'$?

For the **pair density fluctuation**:

$$\delta n^{(2)}(x, x') = n^{(2)}(x, x') - n(x)n(x') \tag{12}$$

(This is difference in the expectation of particle pair at x and x' from the expectation you'd get from completely independent measurements of particles at x and x' and is a measure of how much the measurements at x and x' are correlated.)

For the **exchange hole**:

$$n_x(x, x') = \frac{\delta n^{(2)}(x, x')}{n(x')} \tag{13}$$

which gives the change in density at x given you know one is at x'

For the **pair correlation function**:

$$g(x, x') = \frac{n^{(2)}(x, x')}{n(x)n(x')} \tag{14}$$

which is a function varying from 0 to 1 as the pair density goes from 0% to 100% of the uncorrelated pair density.

(e) Sketch the exchange-correlation hole versus $u = x_1 - x_2$ for u in the range 0 to L. Explain the values at 0 and L.

(f) Derive the average KE per-particle as an expectation of ψ_{SD} and show that it matches

(g) Find the expectation of the electron-electron interaction $\langle U_{ee} \rangle$ for the Slater-determinant wavefunction. Or at least in integral form.

3. **Project part 2: interacting fermions with delta-function potentials**

We would like to solve for the entire energy using the jellium Hamiltonian. There is one problem. In 1D, the *electron* gas is extremely strongly interacting. The problem is that if we use a Coulomb interaction, the integral that might describe the interaction energy between particles of opposite spins or between an electron and the jellium background would have a term roughly like the following:

$$\int_0^R dx \frac{1}{x} = \ln R/0 \to \infty, \tag{15}$$

with x standing for the distance between electrons, and R an appropriate range. This is an infinite energy for any finite R – but not in two or three dimensions – why? The result is that in one dimension, the *non*-interacting approximation is extraordinarily bad as a starting point for doing the interacting electron gas!

Lets have instead an interacting *fermion* gas with one or the other of two interactions:

$$V(x_1, x_2) = \lambda e^2 \delta(x_1 - x_2) \tag{16}$$

$$
\begin{aligned}
V(x_1, x_2) &= \frac{\lambda e^2 L^2}{2}\left[\frac{1}{4} - \left(\frac{x_1 - x_2}{L}\right)^2\right], |x_1 - x_2| < L/2 && (17)\\
&= 0, |x_1 - x_2| > L/2. && (18)
\end{aligned}
$$

The second should be an upside-down parabola and be finite in range. With either case, evaluate the expectation values for U_{ee} and U_{eN} and U_{NN} to get an overall energy expectation.