Physics 520
Problem Set 7

L. Sander, Fall 2005, Due 12/01/05.

In this problem set you will work out some of the things that I would have lectured on, but I ran out of time. All of them can be found in elementary books.

1. Screening: in the electron gas, there is screening: that is, a fixed positive charge will attract electrons, and a negative charge will repel them. This gives rise to a screening cloud around the fixed charge. This problem deals with the classical case (Debye Hückel). This theory is used in the chemistry of electrolytes.

a.) Consider a positive charge $\delta\rho_{ext}$ in a sea of mobile charges $-q$ of average density n_o and a neutralizing background qn_o. Suppose U is the electrostatic potential. Justify the following equations:

$$\nabla^2 U = -4\pi(\rho_{ext} + \rho_{ind}); \quad \rho_{ext} = qn_o + \delta\rho_{ext}; \quad \rho_{ind} = -qn_o \exp(qU/k_BT)$$

b.) Solve by a Fourier transformation for the case $\rho_{ind} = 0$, no screening. You should find for the 'bare' potential $U_b(k) = 4\pi\delta\rho_{ext}(k)/k^2$.

c.) Now turn on the screening, and assume U is small. Show that you get $U = U_b/\epsilon(k); \quad \epsilon(k) = 1 + \lambda^2/k^2$. You must find λ.

d.) Find $U(r)$, the screened potential in real space, for the case where $\delta\rho_{ext} = Q\delta(r)$, a point charge.

2. Do the same problem for a degenerate electron gas (Thomas-Fermi screening). All the steps are the same except that you can't use the Boltzmann distribution, but rather use a 'local' Fermi distribution where the energy of each electron is shifted by $-eU$, but the chemical potential is constant. You should find $\lambda^2 = 4\pi e^2 \frac{\mathcal{D}(E_F)}{\Omega}$.

3. In this problem you will work out the Hartree-Fock theory of the electron gas in the jellium model. You will need the interaction between electrons: suppose it is the Coulomb interaction. In k space it can be written (cf. Problem 1, 2) $v(k) = 4\pi e^2/\Omega k^2$. However, for $k = 0$ you should put $v = 0$ because of the positive background. a.) Suppose that the orbitals are plane wave states, $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{\Omega}$. Show that the two particle interaction term for v in second quantized notation can be written:

$$\frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},s,s'} v(q) \hat{c}^{+}_{\mathbf{k}+\mathbf{q},s} \hat{c}^{+}_{\mathbf{k}'-\mathbf{q},s'} \hat{c}_{\mathbf{k}',s'} \hat{c}_{\mathbf{k},s}.$$

b.) In the Hartree-Fock approximation we are interested in the expectation value of this operator in the ground state of the non-interacting Fermi gas, i.e., for the state: $|G\rangle = \prod_{k<k_F,s} \hat{c}^+_{\mathbf{k},s}|0\rangle$. Show that:

$$\langle G|\hat{\mathcal{H}}|G\rangle = 3NE_F/5 + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',s,s'} v(0)[\langle G|\hat{n}_{\mathbf{k},s}\hat{n}_{\mathbf{k}',s'}|G\rangle - \delta_{\mathbf{k},\mathbf{k}'}\delta_{s,s'}]$$

$$-\frac{1}{2}\sum_{\mathbf{k},\mathbf{q},s} v(q)\langle G|\hat{n}_{\mathbf{k+q},s}\hat{n}_{\mathbf{k},s}|G\rangle.$$

c.) Argue that the second term is 0. The third term, the exchange energy, is the decrease in the electron-electron interaction because of the Pauli principle (electrons avoid one another). Show that this term can be written:

$$E_x = -\frac{2\pi e^2}{\Omega}\sum_{k,K,s}\frac{f_{K,s}f_{k,s}}{|\mathbf{k}-\mathbf{K}|^2} = -\frac{3}{4\pi}Ne^2k_F.$$

d.) Plot the total ground state energy of the electron gas in the HF approximation as a function of density, n. Find the minimum in eV.

4. a.) The operator $\hat{\rho}(\mathbf{R}) = \sum_i \delta(\mathbf{R}-\mathbf{r}_i)$ measures the density of electrons. Show that in second-quantized notation $\hat{\rho}(\mathbf{R}) = \sum_{\mathbf{k},\mathbf{q},s} e^{i\mathbf{q}\cdot\mathbf{R}}\hat{c}^+_{\mathbf{k+q},s}\hat{c}_{\mathbf{k},s}$.
b.) The density correlation function, $g(R)$ measures the likelihood of finding an electron a $\mathbf{R}$ given that one is at 0. For the free electron gas (or Hartree-Fock) show that:

$$g(R) \equiv \frac{\Omega^2}{N(N-1)}\langle G|\hat{\rho}(\mathbf{R})\hat{\rho}(0)|G\rangle = 1 - \frac{9}{2}\left[\frac{\sin(k_FR) - k_Fr\cos(k_FR)}{k_F^3R^3}\right]^2$$

This is called the Hartree-Fock exchange hole: it is due to the statistical avoidance of electrons mentioned in the last problem.

5. Plasma oscillations: Suppose that a slab of metal is exposed to an external electric field perpendicular to the slab which varies at frequency ω. Write, as in electromagnetic theory, $E_{in} = E_{out}/\epsilon(\omega)$. Show that E_{in} becomes very large near $\omega = \omega_p = \sqrt{4\pi ne^2/m}$ where n is the number density of electrons. Find $\epsilon(\omega)$.

Hint: suppose the electrons in the slab move uniformly back and forth. Then there is an induced surface charge, and an induced electric field inside the slab as in an ordinary capacitor. Write Newton's equation for the electrons with the total field, induced plus external, as a restoring force.