

561 Fall 2005 Homework 2

Passed out September 8, 2005; Due September 22, 2005

1. Problem 5.2 of Phillips. Note that the specific heat depends on the density of states in a range $\approx T$ around the Fermi energy. The Hartree-Fock approximation leads to a non-analytic form for the specific heat that is correction to well-known form for non-interacting particles. It is tricky to work out a detailed answer to this problem; you are asked to give the correct reasoning and an estimate for the temperature range below which the correction is $>\approx 10\%$.

2. Problem 8.3 of Phillips. In this problem assume that the Coulomb interaction is the usual 3d $1/r$ interaction, but the particles are confined to move in 2 dimensions. This is the actual problem for plasmons due to charged particles in a layer. [NOT REQUIRED: Also work out the last part of Problem 8.1 to show that the Thomas-Fermi screening length in 2 dimensions is independent of density.]

3. Phonons in metals

a. Derive the formula for the plasma frequency for the long-wavelength longitudinal oscillation frequency of charged particles of charge Ze , mass M , and density n ,

$$\omega_p^2 = \frac{4\pi n e^2 Z^2}{M}. \quad (1)$$

b. Show that if the interaction is screened according to the Thomas-Fermi approximation, then the frequency vanishes at long wavelength as it should for an acoustic mode in a metal, with a longitudinal velocity of sound v_L given by a simple formula in terms of the Thomas-Fermi screening constant k_{TF} .

c. Finally, using the relation of k_{TF} and the electron velocity at the Fermi surface v_F , derive the ratio of v_L to v_F . Does this appear to be a reasonable approximation?

4. Green's Functions for the Harmonic Lattice

There are many types Green's functions defined with different boundary conditions (as discussed in Mahan, Fetter, and Doniach). For a harmonic lattice with the hamiltonian,

$$H = \frac{1}{2M} \sum_I p_I^2 + \frac{1}{2} \sum_{I,J} D_{I,J} u_I u_J, \quad (2)$$

the retarded Green's functions for the displacements is

$$G_{I,J}^R(t) = -i\Theta(t)\langle [u_I^H(t), u_J^H(0)] \rangle, \quad (3)$$

and the time ordered Green's function is

$$G_{I,J}^T(t) = -i\langle T[u_I^H(t)u_J^H(0)] \rangle, \quad (4)$$

where $[a, b]$ is a commutator, $T[ab]$ is a time ordered product, and u^H means a Heisenberg operator. (In this case it is not important to distinguish between Heisenberg and interaction representations.)

a. Show that each of these Green's functions satisfies the equation

$$-M \frac{d^2}{dt^2} G_{I,J}(t) - \sum_K D_{I,K} G_{K,J}(t) = \delta_{I,J} \delta(t). \quad (5)$$

Hint: use the usual relation for Heisenberg operators $i\frac{dO^H}{dt} = [O^H, H]$. For commutators such as $[u, p^2]$, it may be convenient to use the identity

$$[A, BC] = ABC - BCA = [A, B]C + B[A, C] \quad (6)$$

b. Transform to normal modes labeled by wavevector k and give the equation obeyed by the Green's function $G_k(t)$ analogous to Eq. 5.

c. Give an explicit expression for the retarded function $G_k^R(t)$ valid for temperature $T \neq 0$.

d. Find an expression valid for temperature $T \neq 0$ for the dynamic correlation function

$$J_{1,q}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle u_q^H(t) u_{-q}^H(0) \rangle \quad (7)$$

which governs the intensity of scattering in an experimental measurement. (Leave the matrix elements which multiply the scattering intensity as unspecified multiplying constants. These depend upon the particular scattering problem. You need to give only the frequency dependent part given in equation 7.)

5. Relation of Structure factor, Interaction Energy, and Dielectric function

a. From the definition of ϵ^{-1} in terms of the density-density response function, derive the result that the Fourier transform $S(k)$ of the pair correlation function $g(r)$ is given by the following formula (and correct my errors if I have missed some factors). The purpose for this problem is for everyone to go through the derivation of this important result.

$$S(k) = -\frac{\hbar}{\pi} \frac{k^2}{4\pi e^2} \int_0^{\infty} d\omega \text{Im} \epsilon^{-1}(k, \omega) \quad (8)$$

b. Give the total potential energy of interaction between the electrons E_{int} in terms of $S(k)$, and derive the final expression for the total energy of an electron system in terms of integrals over the dielectric function

$$E = E^0 - \frac{\hbar}{\pi^3} \int d^3k \int_0^{e^2} \frac{d\alpha}{\alpha} \left[\int_0^{\infty} d\omega \text{Im} \epsilon_{\alpha}^{-1}(k, \omega) + \frac{2\pi n\alpha}{k^2} \right], \quad (9)$$

This formula is analogous to Pines A-39, but it is general and not restricted to the RPA approximation. Note that the dielectric function is a function of the coupling constant α . Also there may be errors in my formula of the factors of 2π , etc.

EXTRA - NOT REQUIRED TO TURN IN

Density Functional Theory (DFT)

These are small practice problems to make you think about the logic of DFT. (If you have trouble with these questions, Prof. Martin will be glad to discuss them with you. We will not treat DFT further in this course.)

a. The general proof of Hohenberg and Kohn is that the ground state density of any interacting electron system uniquely determines (except for a constant) the "external potential", i.e., the potential acting on the electrons from other sources. Give the proof explicitly for the simplest case, a non-interacting system of electrons.

b. For a non-interacting system of electrons, the "internal energy" of the electrons is just the kinetic energy. This is easily written in terms of the orbitals (as is done in the

notes in the section of Kohn-Sham theory). Show that the arguments of Hohenberg and Kohn applied to this case show that the kinetic energy is also a universal functional of the ground state density.

c. Not all densities are possible ground state densities. For example, show explicitly that the 2s state of hydrogen cannot be the ground state of any potential that does not have delta function singularities.