MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I

Due on Wed., Nov. 1.

Problem set #6

1. Thermal Expansion Done Right

   The thermal expansion of a crystal lattice can be understood on the basis of the assumption (verified experimentally) that the phonon frequencies increase if the lattice spacing decreases. The simplest calculation assumes that all phonon frequencies behave in a similar way under compression of the lattice:

   $$\frac{d\omega(k)}{\omega k} = -\gamma \frac{dV}{V}.$$

   The positive parameter γ is known as Gruneisen's constant.

   For a crystal in vacuum at thermal equilibrium, the pressure is zero (the crystal contains its own shape in the absence of external influence). Thermodynamics tells us that $P = -\frac{\partial F}{\partial V}\big|_T$ where F is the total free energy. As far as we are concerned, F can be written as a sum of two terms: $F = \phi(V) + F_p(V, T)$. $\phi(V)$ is a structural energy associated with the geometric lattice of interacting atoms. If the atoms were stationary at their lattice sites (no degrees of freedom to be excited thermally), then volume of the crystal would be that for which $\phi(V)$ has a minimum:
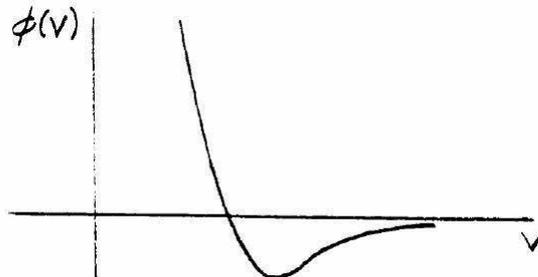
   $F_p(V, T)$ is the phonon contribution to the free energy and is a sum over the free energies of each individual phonon mode, $F_p(V, T) = \sum_k F_k$.

   (a) The link between thermodynamics and statistical mechanics is given by the relationship $F_k = -k_B T \ln Z_k(V, T)$, where Z_k is the partition function of the individual mode. Show that at equilibrium one must have the condition

   $$\frac{\partial \phi}{\partial V} = k_B T \sum_k \frac{1}{Z_k} \frac{\partial Z_k}{\partial V}.$$

   (b) In the canonical ensemble of statistical mechanics $Z = \sum_n e^{-E_n/k_B T}$, were the sum extends over all possible states of the subsystem being considered, in this case one phonon mode. Show that the equilibrium condition becomes

$$\frac{\partial \phi}{\partial V} = \gamma \frac{U_p}{V}$$

where U_p/V is the total thermal energy per unit volume in the phonon modes. This gives the following qualitative picture of thermal expansion: as T increases, the phonon energy increases, and the equilibrium point on the $\phi(V)$ shifts to larger V.

(c) The linear expansion coefficient α is defined as $\alpha \equiv \frac{1}{3}\frac{1}{V}\frac{\partial V}{\partial T}\big|_P$. If $\phi(V)$ is modeled by the leading terms in a Taylor series expansion about the minimum

$$\phi(V) = -\phi_0 + \frac{1}{2}K(V - V_0)^2,$$

find an expression for α. What is the temperature dependence of α at low temperatures?

2. Pressure and Bulk Modulus of an Electron Gas

(a) Show that the total energy E_{tot} of a three-dimensional gas of N free electrons at $T = 0$ is given by $\frac{3}{5}N\varepsilon_F$.

(b) Find the pressure of a free electron gas at $T = 0$. Show that $P(T = 0)$ can be expressed as $\frac{2}{3}E_{\text{tot}}/V$. (Hint: $P = -\frac{\partial E_{\text{tot}}}{\partial V}\big|_{N \text{ fixed}}$ at zero temperature.)

(c) Show that the bulk modulus $B = -V\frac{\partial P}{\partial V}$ of an electron gas at $T = 0$ is $\frac{5}{3}P$ or $\frac{10}{9}E_{\text{tot}}/V$. [Note that at $T = 0$ the isothermal (constant T on the partial derivative) and the adiabatic (constant entropy) bulk moduli are equal due to the third law of thermodynamics.]

(d) Use the data in table 6.1 of Kittel on page 139 to estimate the electron contribution to the bulk modulus of sodium.

3. Chemical potential of a Two-Dimensional Electron Gas

(a) Find the density of states as a function of energy for a non-interacting free electron gas in two dimensions.

(b) For this system, it is possible to find an analytic expression for the temperature dependence of the chemical potential. Show that

$$\mu(T) = k_B T \ln[e^{\varepsilon_F/k_B T} - 1],$$

where n is the number of electrons per unit area.

4. Energy transfer into a Fermion Gas

Consider a free, non-interacting gas of Fermions of mass M at $T = 0$. Assume that a momentum $\vec{P} = \hat{x}p_x$ is given to the system (by the scattering of a neutron for example), and it goes into the creation of a single hole-particle pair.

(a) For a given p_x, what is the *smallest* energy that can be imparted to the system by this process? Sketch this transition on a diagram of the Fermi sphere in momentum space.

(b) For a given p_x, what is the *largest* energy that can be imparted to the system by this process? Sketch this transition as well.

(c) On a graph of energy E versus p_x, show the band of energies that can be transferred to the system in this process. Show results for both $p_x < 2\hbar k_F$ and $p_x > 2\hbar k_F$.