Homework 11 – Thermodynamics of Materials

PHYS 324, Spring 2008, Longwood University

Due: April 21th

1. To model a semiconducting crystal we consider a lattice with N_0 sites, each of which may be occupied by either 0 or 1 electrons. There are N electrons distributed at random among the N_0 lattice sites. There is an occupation energy (ε) for each site, which is a function of the extensive variable X. Treat one lattice site as the system and the rest of the sites as a surrounding reservoir with temperature T and chemical potential μ. The site is either unoccupied ($\varepsilon = 0$) or occupied by $N = 1$ electrons $[\varepsilon = \varepsilon(X)]$.

   (a) Write down the grand partition function.

   (b) Determine the entropy.

   (c) Determine N as a function of μ, ε and T.

   (d) Show that the equation of state is as follows:

   $$Y = N\frac{d}{dX}\left[\varepsilon(X)\right]$$

   (e) Show that the internal energy is given by:

   $$U = N\varepsilon(X)$$

2. Repeat problem 1 including the possibility that the site may also be occupied by two electrons ($N = 2$) with opposite spins. Because of their Coulomb repulsion, the energy of occupation for two electrons (ε_2) is much larger than the energy of occupation for one electron (ε_1). Assume the following:

   $$\varepsilon_1 = \frac{A}{V}$$
   $$\varepsilon_2 = \frac{B}{V}$$

   where A and B are constants and V is the total volume of the semiconductor. The number of available electrons is temperature dependent so assume the following:

   $$N_{total} = < N > N_0 = CTV$$

   where C is another constant and N_0 is the number of sites.

   (a) Write the grand partition function.

   (b) Determine the entropy.

   (c) Determine N as a function of μ, V and T

   (d) Assume for this system that $\varepsilon_2 - 2\mu \gg kT$. Show that the equation of state is:

   $$P = \frac{AN}{V^2}$$

   (e) Show that the internal energy is given by:

   $$U = \frac{AN}{V} = \left(\frac{AC}{N_o}\right)T$$