PHYSICS 715

Problem Set 1 **Due Friday, January 27, 2006**

Reading: Landau and Lifshitz, Chap. 1, Secs. 9—15, 23—25 (review of thermodynamics), Huang, Chap. 6 (suggested)

LD 1: Vacancies (Schottky defects) in solids.

(a) Determine the number of ways of putting $n = n_1 + n_2 + \cdots + n_m$ objects in m boxes without regard to order, with $n_1, \ldots, n_m$ in boxes $1, \ldots, m$. Give your reasoning in detail.

(b) Atoms can move under the influence of thermal agitation from the interior of a crystalline solid to new lattice sites on the surface, leaving behind unoccupied interior sites ("vacancies", "holes", or "Schottky defects") and increasing the size of the solid. The number of atoms is fixed; the number of holes is not, but is determined by the condition for equilibrium. We can ignore the fact that holes are not well-defined on the surface of the solid: surface effects vanish for a compact solid for $n \to \infty$.

Determine the statistical weight $\Gamma(n, m)$ for a configuration with n atoms and m holes, that is, the number of ways of distributing n atoms and m holes over a compact lattice. Explain your reasoning.

(c) Each vacancy increases the energy of the system by an amount $\Delta E > 0$. Find the Boltzmann entropy $S_B(E) = k \ln \Gamma$, and use the relation $\frac{1}{T} = \frac{\partial S_B}{\partial E}$ to determine m/n as a function of the temperature T. Stirling's approximation $\ln x! \approx x \ln x - x$, $x \gg 1$, will be useful.

LD 2: Statistics of large numbers and the Boltzmann factor.

A three-state system is occupied by $N = n_+ + n_0 + n_-$ independent particles, where n_+, n_0, n_- are the numbers of particles in the states with single-particle energies $+\epsilon$, 0, $-\epsilon$. N and E (the total energy of the system) are fixed.

(a) Determine the statistical weights $\Gamma(n_+, n_0, n_-)$ of the allowed configurations, taking n_0 as the free variable. Plot Γ carefully as a function of n_0/N for $0 \leq n_0/N \leq 1$, taking $N = 10$ (already a large number!) and $E = -2\epsilon$. Treat n_0 as continuous [Most scientific calculators give $x!$ for arbitrary real x, or you can use Stirling's approximation $\ln x! \sim (x + \frac{1}{2}) \ln x - x + \ln \sqrt{2\pi} + (1/12x) \cdots$.] Comment on the shape of the curve, possible fluctuations of n_0 around its most probable value, etc. What will happen as N is increased with E/N fixed? Try a case, e.g., $N = 40$, and show that the width of the peak decreases quantitatively in the variable n_0/N by the ratio you would expect.

(b) The *equilibrium* values of n_+, n_0, and n_- at a given total energy are the values which maximize the statistical weight Γ. Show that $n_0 = (n_+ n_-)^{1/2}$ at equilibrium for any E. The Boltzmann entropy of the system can be defined as $S_B = S_{\text{peak}} = k \ln \Gamma_{\text{peak}}$, with Γ_{peak} the statistical weight of the equilibrium configuration. Calculate S_{peak} with E/N fixed, and show that $S_{\text{peak}} \propto N$ for large N.

(c) A second definition of the entropy is $S_B = S_{\text{total}} = k \ln \Gamma_{\text{total}}$ where $\Gamma_{\text{total}} = \sum_{n_0} \Gamma(E, N, n_0)$ is the total statistical weight obtained by summing Γ over all allowed values of n_0. Calculate S_{total} numerically using Γ_{peak} and Γ_{total} for $N = 10$ and $N = 40$ and compare the results. What happens to the difference between the two forms of S_B for N very large? Use an appropriate estimate of the sum and be as quantitative as possible.

(d) Determine the equilibrium temperature of the system from the thermodynamic relation $\frac{1}{T} = \frac{\partial S_B}{\partial E}$. Use the result to determine the equilibrium ratios $n_+ : n_0 : n_-$ and the corresponding values n_+, n_0, n_- as functions of T rather than E.

LD 3: Pauli paramagnetism and negative temperature.

Consider a lattice of $N = N_\uparrow + N_\downarrow$ quantized distinguishable spin-1/2 atoms in a magnetic field (a Pauli paramagnet). The spins have two energy states, with energies $E_{\uparrow(\downarrow)} = \pm \mu_B \mathcal{H}$ for spin up (down), where $\mu_B = |e|\hbar/2m_e c$ is the Bohr magneton. (We use Gaussian cgs units; see the Appendix in Jackson, *Classical Electrodynamics*).

(a) Calculate the Boltzmann entropy of the system and determine the temperature from the thermodynamic relation

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_V \quad .$$

Assume $N_\uparrow$, $N_\downarrow \gg 1$, and use Stirling's approximation as appropriate. Is T always positive? Explain. [For a discussion and experiment, see N.F. Ramsey, Phys. Rev. **103**, 20 (1956), E.M. Purcell and R.V. Pound, Phys. Rev. **81**, 279 (1951). For a nice recent experiment using nuclear spins in metals, see P. Hakonen and O.V. Lounasmaa, Science **265**, 1821 (1994).]

(b) The individual spins are identical and independent, so the probability $w_\uparrow$ ($w_\downarrow$) that an individual spin is oriented up (down) is the same as the average probability $W_\uparrow = N_\uparrow/N$ ($W_\downarrow = N_\downarrow/N$) for spin $\uparrow(\downarrow)$ for the entire system. Show that this implies that the relative probability of finding a spin in the up or down state is given by the ratio of the corresponding Boltzmann factors $e^{-\beta E_{\uparrow(\downarrow)}}$, where $\beta = 1/kT$. Use the result to calculate the average magnetic moment per spin, $m = -\mu_B(w_\uparrow - w_\downarrow)$. Determine the high-temperature form of the magnetic susceptibility $\chi = (\partial m/\partial \mathcal{H})_T$. What quantitatively *is* a high temperature for a typical laboratory field, $\mathcal{B} = \mathcal{H} = 10^4$ gauss?