## Physics 555 Fall 2011 Problem set # 4 due Friday Oct. 7

**1.** Kittel p.128 problem 1

**1. *Singularity in density of states.*** (a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of $N$ atoms with nearest-neighbor interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{(\omega_m^2 - \omega^2)^{1/2}} \ ,$$

where $\omega_m$ is the maximum frequency. (b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = (L/2\pi)^3(2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

**2.** Kittel p.129 problem 5

**5. *Grüneisen constant.*** (a) Show that the free energy of a phonon mode of frequency $\omega$ is $k_BT \ln [2 \sinh (\hbar\omega/2k_BT)]$. It is necessary to retain the zero-point energy $\frac{1}{2}\hbar\omega$ to obtain this result. (b) If $\Delta$ is the fractional volume change, then the free energy of the crystal may be written as

$$F(\Delta, T) = \tfrac{1}{2}B\Delta^2 + k_BT \sum \ln [2 \sinh (\hbar\omega_{\mathbf{K}}/2k_BT)] \ ,$$

where $B$ is the bulk modulus. Assume that the volume dependence of $\omega_{\mathbf{K}}$ is $\delta\omega/\omega = -\gamma\Delta$, where $\gamma$ is known as the Grüneisen constant. If $\gamma$ is taken as independent of the mode $\mathbf{K}$, show that $F$ is a minimum with respect to $\Delta$ when $B\Delta = \gamma\Sigma\frac{1}{2}\hbar\omega \coth (\hbar\omega/2k_BT)$, and show that this may be written in terms of the thermal energy density as $\Delta = \gamma U(T)/B$. (c) Show that on the Debye model $\gamma = -\partial \ln \theta/\partial \ln V$. Note: Many approximations are involved in this theory: the result (a) is valid only if $\omega$ is independent of temperature; $\gamma$ may be quite different for different modes.

**3. Scattering of phonons from a mass defect.** Suppose at the origin there is an isotopically defective atom of mass M', in an otherwise perfect crystal, with one atom per unit cell, and where all other atoms have mass M. The perturbation in the Hamiltonian is $H' = (P_0^2/2M)(M/M'-1)$, where $P_0$ means the momentum of the nucleus at the origin. Consider state |1> which has $N_Q$ phonons in mode Q (with frequency $\omega_Q$) and $n_{Q'}$ phonons in mode Q' (with frequency $\omega_{Q'}$); state |2> which has $N_Q-1$ in mode Q and $n_{Q'}+1$ in mode Q'; and state |3> which has $N_Q+1$ in mode Q and $n_{Q'}-1$ in mode Q'. **(a)** What is the transition rate 1 → 2? (It can be called $1/\tau(12)$.) What is the transition rate 1 → 3? (It can be called $1/\tau(13)$.) You should use the Fermi golden rule. **(b)** We now assume that $n_{Q'}$ is the equilibrium Bose-Einstein population of mode Q', whereas $N_Q$ is not, because mode Q is out of equilibrium. Derive a formula for the time-rate of change of the population of mode Q, defined as

$dN_Q/dt = -(N_Q - n_Q)/\tau_Q$, where $\tau_Q$ is the equilibration time (when only mode Q is out of equilbrium.) The idea is that all processes of type "12" (for all modes Q') contribute to diminishing the population of mode Q, whereas all processes of type "13" contribute in increasing the population of mode Q. Note that the rate of equilibration vanishes as $N_Q$ approaches equilibrium. **(c)** If you do this correctly, the result for $1/\tau_Q$ will have a (1/N-normalized) sum over modes Q', a delta function $\delta(\omega_Q - \omega_{Q'})$, another factor 1/N, and a factor $(\hat{\varepsilon}_Q \cdot \hat{\varepsilon}_{Q'})^2$. Show that (ignoring possible asymmetries of the polarizations) $1/\tau_Q$ can be written as proportional to $D(\omega_Q)\omega_Q^2$, where D is the phonon density of states, and $\omega_Q$ is the frequency of the mode Q. What does this have to do with Rayleigh scattering? The remaining 1/N is correct. If there are actually $N_{imp}$ isotopic impurities, the total scattering rate goes as $N_{imp}/N$.

**4. Curie *versus* Pauli paramagnetism**. (a) Oxygen molecules have spin 1. They are "paramagnetic," with a moment about 2 Bohr magnetons (the "g-factor" is slightly anisotropic, with $g_{zz} = 2.004$ and $g_{xx} = 2.001$; in this problem, you can assume magnetic isotropy). A field B causes a level splitting. Use classical statistical mechanics to derive the Curie law, $\chi = (N_A \mu_0)(\mu^2 / 3k_B T)$, where $N_A$ is Avogadro's number, $\mu_0 = 4\pi \times 10^{-7}$ N/A$^2$, $\mu^2 = S(S+1)g^2\mu_B^2$ is the magnetic moment of the $O_2$ molecule with S = 1, and $\mu_B = 9.27 \times 10^{-24}$ J/T is the Bohr magneton. The measured susceptibility of $O_2$ at low p and T = 293K is $4.3 \times 10^{-8}$ m$^3$/mole. (b) Rederive this result from quantum statistical mechanics for the spin 1 molecule. (c) Pauli worked out the susceptibility of a Fermi-degenerate gas of electrons ($k_BT$ is small compared with the Fermi energy. ) Do the derivation. (d) Explain the difference between the Pauli result and the Curie result.