Physics 140A: Homework Problem Set 6

Assigned 2/14/05. Due 2/22/05.

1. Realistic Phonon Density of States. 20 points.
A phonon dispersion curve that is more realistic than the Debye model is given by

$$\omega(k) = \Omega \ sin(\frac{\pi}{2}\frac{k}{k_D})$$

Here Ω is the maximum frequency (which occurs at the Debye wavevector k_D). Consider an elemental (one atom per cell) fcc Bravais lattice of lattice constant **a**.
(a) Determine the Debye wavevector k_D using Debye's considerations.
(b) Calculate the phonon velocity $v(k)$ and determine the sound velocity (denote it by c).
(c) In preparation for calculation of the density of states $\rho(\omega)$, calculate the wavevector $k(\omega)$ that satisfies $\omega - \omega(k)$=0.
(d) Evaluate the density of states *per primitive cell* $\rho(\omega)$. Assume that all three branches are "degenerate," that is, they all have the same energy, *i.e.* they are identical.
(e) Sketch the result, showing the correct behavior both at $\omega \to 0$ and $\omega \to \Omega$.

2. Bose-Einstein Thermal Occupation Function. 10 points.
From the Bose-Einstein thermal distribution function

$$n\Big(\frac{\hbar\omega}{k_B T}\Big) \equiv n(\beta\hbar\omega); \quad n(x) \equiv \frac{1}{e^x - 1},$$

(a) sketch $n(\beta\hbar\omega)$ vs. ω at fixed T and point out all limiting behaviors.
(b) calculate its temperature derivative (and put into as simple a form as possible). Again sketch this function vs. ω at fixed T.

3. Free Electron Gas. 20 points.
Do the following for the homogeneous "free electron gas" in *each* of **one**, **two**, and **three** dimensions, using the simplest cell (line; square; cube) of length **a**.
(a) Calculate the density of states *per unit cell* $\rho(E)$. Make a simple sketch, putting all three on the same graph with Fermi energies aligned.
(b) Calculate the average energy per particle at T=0.

4. Electronic Band Gaps in 3D. 10 points.
Consider a *bcc* structure crystal in the free electron approximation.
(a) Determine the magnitude k of $\vec{k}$ at the Brillouin zone boundary along each of the $< 110 >, < 110 >$, and $< 111 >$ directions. Using a diagram of the *bcc* BZ may be useful.
(b) From (a), determine the free electron energy at each of these boundaries. Using a lattice constant of a=3 Å, give these energies in eV.
(c) Since an insulating solid must have a gap in some range of energy *over the entire Brillouin zone*, argue that it might be more difficult for a solid to be insulating in 3D than in 1D.