Applied Physics 195 / Physics 195 — Assignment #4

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Date: October 9th, 2015
Due: **5pm SHARP (4:50pm + 10 min grace period)**, October 16th, 2015; slide your work under through the door at Maxwell-Dworkin Room 131.

Problem 1 (50 pt): Density of phonons

Consider a bulk solid with one atom per unit cell and with atom density per volume, n_0. By using the Debye theory with $\omega(\vec{k}) = v_0 k$ for all lattice wave dispersion relation branches (v_0: speed of sound), evaluate the phonon density per volume, n_{ph}. Show that for $T \gg \Theta_D$ (Θ_D: Debye temperature), $n_{ph} \sim T$ and for $T \ll \Theta_D$, $n_{ph} \sim T^3$. These are useful results; we will use them later in class to determine the temperature dependency of the electrical resistivity due to electron-phonon scattering.

Problem 2 (100 pt): 1D metal with tight binding

Consider the 1D crystal of Lecture Note #6 (length: L; lattice constant: a; number of atoms: N) in the tight-binding approximation, with one valence electron per atom. As we have studied, in the tight-binding approximation, the matrix element of the Hamiltonian H for an electron in the periodic potential due to the 1D crystal lattice may be written as

$$\langle n|H|m\rangle = \epsilon_0 \delta_{nm} - t[\delta_{n-1,m} + \delta_{n+1,m}] \tag{1}$$

in the basis of atomic ground states $\{|n\rangle\}$ ($n = 1, 2, 3, \cdots, N$). ϵ_0 and t (> 0) are as we defined in class/note.

(a) Show that a single-electron state with a state index k

$$|\psi_k\rangle = A \sum_{n=1}^{N} e^{-ikna} |n\rangle \tag{2}$$

is a single-electron energy eigenstate (A: normalization constant) and calculate the corresponding single-electron energy eigenvalue $\epsilon(k)$. Determine the normalization constant A. Check the orthogonality of the energy eigenstates, *i.e.*, $\langle \psi_k | \psi_{k'} \rangle = 0$ for $k \neq k'$ (you may find Poisson summation formula useful).

(b) Calculate the density of states $D(\epsilon)$.

(c) Argue that this crystal is a metal. How much total electronic energy lowering is achieved by brining together the N atoms into the 1D crystal? That is, what is the cohesive energy contributed by the valence electrons? For this calculation, assume $T = 0$.

(d) Calculate the chemical potential $\mu(T)$ and the total electronic energy $U(T)$ both to the second order of T, assuming $k_B T \ll t$. From the expression of $U(T)$, calculate the specific heat $C(T)$.

(e) Calculate the effective electron mass m^* and the plasmonic mass m_p (for the latter, assume $T = 0$).

Problem 3 (50 pt): Blackbody radiation vs. thermal lattice waves

The calculation of the total thermal photon energy in blackbody radiation (V in the equation right below is the volume that confines the electromagnetic radiations)

$$U_{bbr} = V \times \frac{\pi^2}{15} \frac{(k_B T)^4}{(c\hbar)^3} \sim T^4 \qquad \text{(Stefan-Boltzmann law)} \tag{3}$$

is procedurally a lot like the calculation of the total thermal phonon energy we studied. In either case: 1) we first solve the (electromagnetic or lattice) wave equation within the finite real-space volume that confines

the waves and thus discretizes the wave vector $\vec{k}$, identifying all available normal modes indexed with $\vec{k}$, their associated frequency $\omega(\vec{k})$, and all available dispersion relation branches (including polarizations); 2) we then calculate, for each mode, the mean number—and thus mean energy—of thermally excited particles (photons or phonons) according to the Bose-Einstein statistics, where the chemical potential is zero, as the total number of these particles is not fixed; 3) we then sum this mean thermal energy of each mode across all available modes along all available dispersion relation branches.

But then the two calculations are not exactly the same. First, the total number of branches is 2 in the blackbody radiation case but it is 3 or more in the lattice wave case (can you explain why?). Second, whereas all available modes to sum the energy over lie within the first Brillouin zone—which Debye tricked with the Debye sphere—in the lattice wave case, in the blackbody radiation case, there is no such $\vec{k}$-space zone and the energy summation is done across the entire $\vec{k}$ space (explain the origin of this difference).

(a) With all above in mind, derive Eq. (3), the Stefan-Boltzmann law.

(b) Recognizing the similarity and difference between the black body radiation and thermal lattice wave excitation, derive—in just a couple or so lines—the specific heat of solids in the low T case ($T \ll \Theta_D$) by making appropriate coefficient changes in Eq. (3) and taking an appropriate derivative, and explain why such simple conversion is not available for the high T case ($T \ll \Theta_D$).

The intention of this problem is to help understand the thermal phonon excitation from a broader point of view, by examining its similarity to and difference from black body radiation.