# Physics 195 / Applied Physics 195 — Assignment #9

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Date: Nov. 28, 2017
Due: 12:45pm + 10 min grace period, Dec. 8, 2017 at the dropbox outside Maxwell-Dworkin Room 131.

## Problem 1 (70 pt; <u>NO COLLABORATION</u>): Lattice waves in 1D diatomic crystal

(a) Consider a 1D diatomic crystal as shown on page 3 of Lecture #18. Assume $C_1 = C_2 \equiv C$ and $M_1 \neq M_2$. The entire crystal length is $L$, the length of the unit cell (containing two atoms) is $a$, the total number of unit cells is $L/a = N$, and the total number of atoms is $2N$. Calculate all possible lattice wave dispersion relations and sketch them in the 1st Brillouin zone. What is the total number of normal modes? What are the total degrees of freedom of the system?

(b) Show that the solution of part (a) collapses to one acoustical dispersion branch in the limit of $M_2 = M_1$. In this case, what is the total number of normal modes and what are the total degrees of freedom of the system?

## Problem 2 (100 pt; <u>NO COLLABORATION</u>): Lattice waves in 1D triatomic crystal

Extending from the 1D diatomic crystal on page 3 of Lecture #18, consider a 1D triatomic crystal, with $M_1 = M_2 = M_3 \equiv M$ and with $C_1$, $C_2$, and $C_3$ being all different from one another. Further assume that $\omega_{0,2}^2 = 2\omega_{0,1}^2$ and $\omega_{0,3}^2 = 3\omega_{0,1}^2$, where

$$\omega_{0,1} \equiv \sqrt{\frac{C_1}{M}}; \quad \omega_{0,2} \equiv \sqrt{\frac{C_2}{M}}; \quad \omega_{0,3} \equiv \sqrt{\frac{C_3}{M}}. \tag{1}$$

The crystal length is $L$, the length of the unit cell (containing three atoms) is $a$, the total number of unit cells is $L/a = N$, and the total number of atoms is $3N$. Show that the lattice wave dispersion relations manifest in one acoustical branch and two optical branches by examining the relevant eigen-equation at $k = 0$. Calculate the frequencies of the two optical branches at $k = 0$, and the approximate velocity of acoustical lattice wave modes at small $k$ near 0. Quantitatively determine the relative motions of the three atoms within a unit cell in each of the single acoustical and two optical modes at $k = 0$.

## Problem 3 (80 pt): Lattice waves in 2D monatomic crystal

Consider a 2D square monatomic crystal with a lattice constant of $a$. In equilibrium, atoms (single atomic mass: $M$) are located at $(na, ma)$ where $n, m = 1, 2, 3, ..., N$. Thus there are a total of $N^2$ atoms and a total of $N^2$ unit cells. Let the atom at equilibrium position $(na, ma)$ be displaced by $(x_{n,m}, y_{n,m})$. In the harmonic approximation and considering only the nearest neighborhood interactions, we can write the total potential energy of the crystal as

$$V = \sum_{n,m} \left[ \frac{1}{2} C_1 (x_{n,m} - x_{n+1,m})^2 + \frac{1}{2} C_2 (y_{n,m} - y_{n+1,m})^2 + \frac{1}{2} C_1 (y_{n,m} - y_{n,m+1})^2 + \frac{1}{2} C_2 (x_{n,m} - x_{n,m+1})^2 \right]. \tag{2}$$

The 1st term means that if any two atoms adjacent along the $x$ axis are perturbed along the $x$ axis, a harmonic restoring force acts along the $x$ axis. The 2nd term means that if any two atoms adjacent along the $x$ axis are perturbed along the $y$ axis, a harmonic restoring force acts along the $y$ axis. The former and latter harmonic forces differ in magnitude for the same degree of perturbation, and hence, the two different coefficients, $C_1$ and $C_2$. Furthermore, it is reasonable to assume that $C_1 > C_2$; for numerical concreteness, let's assume that $C_2$ is 10 percent of $C_1$. The 3rd and 4th terms can be similarly interpreted for any two atoms adjacent along the $y$ axis.

(a) Find all possible 2D lattice wave dispersion relations $\omega(\vec{k})$.

(b) Sketch, within the 1st Brillouin zone, these dispersion relations for the lattice waves propagating along the $x$ direction.

(c) Evaluate the speed of sound as a function of direction for every possible branch of dispersion relations. Along which direction does the sound propagate fastest?

(d) How many available $k$ states are there? What is the total number of normal modes? What are the total degrees of freedom of the system?

## Problem 4 (100 pt; <u>NO COLLABORATION</u>): Debye model for 2D and 1D crystals

(a) Consider a 2D crystal—2D both structurally and dynamically—with one atom per unit cell. Assume a crystal area of $A$ and a total of $N$ atoms in the crystal. We apply the Debye model to this crystal. For all possible branches of lattice wave dispersion relations, use the identical $\omega(\vec{k}) = v_0 k$, with $v_0$ serving as the speed of sound. Calculate the density of states for each branch. Calculate the specific heat due to the lattice waves at a general temperature $T$. Verify that for $T \gg \Theta_D$ ($\Theta_D$: Debye temperature), the specific heat converges to that described by the 2D version of Dulong-Petit law. Calculate the specific heat for $T \ll \Theta_D$, and show that it is proportional to $T^2$.

(b) Consider now a 1D crystal—1D both structurally and dynamically—with one atom per unit cell. Assume a crystal length of $L$ and a total of $N$ atoms in the crystal. We once again apply the Debye model to this 1D crystal. Let the lattice wave dispersion relation be approximated as $\omega(\vec{k}) = v_0 k$, with $v_0$ being the sound speed. Calculate the density of states. Calculate the specific heat due to the lattice waves at a general temperature $T$. Verify that for $T \gg \Theta_D$, the specific heat agrees with the 1D version of Dulong-Petit law. Show that the specific heat for $T \ll \Theta_D$ is proportional to $T$.

## Problem 5 (50 pt): Spectral range of acoustical lattice waves

From the Debye temperature table on page 7 of Lecture Note #19, estimate the spectral ranges of the acoustical lattice wave modes of the solids listed in the table.

## Problem 6 (150 pt): $T$-dependency of electrical resistivity due to electron-phonon scattering

(a) 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, $n_{ph}$, and show that

$$n_{ph} \propto \begin{cases} T^3 & (T \ll \Theta_D); \\ T & (T \gg \Theta_D). \end{cases} \qquad (3)$$

where $\Theta_D$ is Debye temperature. In connection with this, also show that the average energy per thermal phonon is given approximately by

$$\epsilon_{ph} \approx \begin{cases} k_B T & (T \ll \Theta_D); \\ k_B \Theta_D & (T \gg \Theta_D). \end{cases} \qquad (4)$$

while omitting the proportionality constants on the order of 1.

(b) **Metal resistivity (due to electron-phonon scattering) at low temperatures**: Assume $T \ll \Theta_D$. Argue that the average thermal phonon momentum $p_{ph} = \hbar k_{ph}$ is far smaller than the electron Fermi momentum $p_F = \hbar k_F$. Therefore, one-time electron-phonon collision will cause only a very small angle scattering, which is too small to be directly associated with the Drude momentum relaxation time $\tau$. These small-angle scatterings should accumulate through multiple collisions (say, $r$ times) to cause one *effective* large angle (say, 90°) electron scattering, which is directly associated with $\tau$. Since the number of individual collisions (that give small angle scatterings) is proportional to $n_{ph}$, $\tau \propto r/n_{ph}$. Show that $r$ is on the order of $\sim k_F^2/k_{ph}^2$,

and is proportional to $T^{-2}$. Prove $\rho \propto T^5$ for metal.

(c) **Metal resistivity (due to electron-phonon scattering) at high temperatures**: Assume $T \gg \Theta_D$. Show that $p_{ph} \sim p_F$, and hence, $r \sim 1$ and $\rho \propto T$ for metal.

(d) **Semiconductor resistivity**: In metals, $\rho$ increases with $T$ with characteristic power laws as seen above. Briefly discuss how $\rho$ changes with $T$ in semiconductors.

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**Bonus Problem (0 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)

$$U_{bbr} = V \times \frac{\pi^2}{15} \frac{(k_B T)^4}{(c\hbar)^3} \sim T^4 \qquad \text{(Stefan-Boltzmann law)} \tag{5}$$

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 black-body 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. (5), 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. (5) and taking an appropriate derivative, and explain why such simple conversion is not available for the high $T$ case ($T \gg \Theta_D$).

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.