PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 10 – Solution

10.1. Show that for a diatomic chain (two different masses M_1 and M_2 that interact with same force constant C, as given in Eq. (18) of Kittel Chapter 4), the ratio of the displacements of the two atoms u/v for the $k = 0$ optic mode is given by

$$\frac{u}{v} = -\frac{M_2}{M_1} ,$$

as shown in Eq. (26) of Kittel Chapter 4.

Solution:

From the first equation listed under Eq. (20) in Kittel Chapter 4, we get

$$\frac{u}{v} = \frac{C(1 + e^{-ika})}{2C - M_1\omega^2} . \tag{1}$$

For the optic mode with $k = 0$, we have

$$\omega_{opt}^2 = 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) . \tag{2}$$

Substituting the expression for ω from Eq. (2) in Eq. (1), we get for this mode

$$\frac{u}{v} = -\frac{M_2}{M_1} . \tag{3}$$

10.2. This problem is similar to Problem 10.1., but for zone boundary modes ($k = \pi/a$), and is based on Kittel Chapter 4, Problem #3. For the linear harmonic chain treated by Eqs. (18) to (26) in Kittel Chapter 4, find the amplitude ratios u/v for the two branches at $k_{max} = \pi/a$. Show that at this value of k the two lattices act as if they were decoupled: one lattice remains at rest while the other lattice moves.

Solution:

There are two zone boundary modes, namely $\omega_1^2 = 2C/M_1$ and $\omega_2^2 = 2C/M_2$. Assume $M_1 > M_2$. Therefore, $\omega_1 < \omega_2$.

For ω_1, use the the second equation of Eq. (20) in Kittel Chapter 4, i.e.

$$\frac{u}{v} = \frac{C(e^{ika} + 1)}{2C - M_2\omega^2} .$$

Thus, for $\omega = \omega_1$ and $k = \pi/a$ we get

$$\frac{v}{u} = 0 .$$

Consequently, only the masses M_1 move, while masses M_2 are at rest.

Similarly, for for $\omega = \omega_2$ and $k = \pi/a$, we can use the first equation of Eq. (20) in Kittel Chapter 4 and show that

$$\frac{u}{v} = 0$$

in that case, meaning that only the masses M_2 move, while masses M_1 are at rest.

10.3. This problem for a diatomic chain is based on Kittel Chapter 4, Problem #5. Consider the normal modes of a linear chain, in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(k)$ at $k = 0$ and $k = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

Solution:

We will call the alternating force constants C_1 and C_2. For one type of atoms, the force constant C_1 is on the right and the force constant C_2 is on the left. For the other type of atoms, C_2 is on the right and C_1 is on the left. The equations of motion for these two sites are

$$\begin{aligned} M\frac{d^2u_s}{dt^2} &= C_2(v_s - u_s) + C_1(v_{s-1} - u_s) = C_2v_s + C_1v_{s-1} - (C_1 + C_2)u_s \\ M\frac{d^2v_s}{dt^2} &= C_2(u_s - v_s) + C_1(u_{s+1} - v_s) = C_2u_s + C_1v_{s+1} - (C_1 + C_2)v_s\ . \end{aligned}$$

Try periodic solutions of the form

$$u_s = ue^{i(ksa-\omega t)} \quad \text{and} \quad v_s = ve^{i(ksa-\omega t)}\ .$$

This leads to the eigenvalue equation

$$\begin{pmatrix} C_1 + C_2 - M\omega^2 & -(C_2 + C_1e^{-ika}) \\ -(C_2 + C_1e^{+ika}) & C_1 + C_2 - M\omega^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0\ .$$

The two solutions are

$$M\omega_\pm^2 = (C_1 + C_2) \pm (C_1^2 + C_2^2 + 2C_1C_2\cos ka)^{1/2}\ .$$

Now, chose $C_1 = C$ and $C_2 = 10C$. The solutions are

$$\begin{aligned} \omega_1(k = 0) &= 0 && \text{and} \quad \omega_2(k = 0) = \sqrt{22\ C/M}\ , \\ \omega_1(k = \pi/a) &= \sqrt{2\ C/M} && \text{and} \quad \omega_2(k = \pi/a) = \sqrt{20\ C/M}\ . \end{aligned}$$

The zero-frequency mode at $k = 0$ is called the Goldstone mode.

10.4. This problem on singularities in the density of vibrational states is based on Kittel Chapter 5, Problem #1.

(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 vibrational states is

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

where ω_m is the maximum frequency. The singularity at ω_0 is called a van Hove singularity.

(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 vibrational states is discontinuous.

Solution:

From Eq. (15) in Kittel Chapter 5 we get

$$D(\omega) = \frac{L}{\pi} \frac{1}{d\omega(k)/dk} ,$$

where $L = Na$. For the 1D chain we have

$$\begin{aligned} \omega(k) &= \sqrt{\frac{4C}{M}} \sin(ka/2) = \omega_m \sin(ka/2) \\ \frac{d\omega(k)}{dk} &= (\omega_m \; a/2) \cos(ka/2) = (\omega_m \; a/2) \sqrt{1 - \left(\frac{\omega(k)}{\omega_m}\right)^2} . \end{aligned}$$

Using $\omega(k) = \omega$ and combining all equations, we get

$$D(\omega) = \frac{2L}{\pi a} \frac{1}{\sqrt{\omega_m^2 - \omega^2}} \quad \text{for} \;\; 0 \le \omega \le \omega_m .$$

10.5. This problem on the heat capacity of a layered solid in the Debye approximation is based on Kittel Chapter 5, Problem #4.

(a) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2.

(b) Suppose instead, as in many layered structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?

Solution:

Thermal energy associated with phonons is given by

$$U = \int_0^{\omega_D} d\omega D(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} ,$$

where the density of states $D(\omega)$ depends on the type of the mode (acoustic or optic, longitudinal or transverse). For a particular mode in the 2D lattice we have

$$\begin{aligned} D(\omega) &= \left(\frac{L}{2\pi}\right)^2 2\pi k \frac{1}{d\omega(k)/dk} , \\ \omega(k) &= \omega = vk , \\ D(\omega) &= \frac{A}{2\pi v^2} \omega . \end{aligned}$$

Assuming that the one longitudinal and the two transverse modes have the same speed of sound v, we obtain

$$U = 3 \frac{A\hbar}{2\pi v^2} \int_0^{\omega_D} d\omega \frac{\omega^2}{e^{\hbar\omega/k_B T} - 1} .$$

The Debye frequency ω_D is obtained using

$$\int_0^{\omega_D} D(\omega) d\omega = N = \frac{A}{2\pi v^2} \int_0^{\omega_D} \omega \; d\omega \Rightarrow \omega_D = \sqrt{\frac{4\pi N}{A}} v \; .$$

We then can determine U by substituting

$$\begin{aligned} \frac{\hbar\omega}{k_B T} &= x \; ; \;\; x_D = \frac{\hbar\omega_D}{k_B T} = \frac{\Theta_D}{T} \; , \\ U &= \frac{3A\hbar k_B^3}{2\pi v^2 \hbar^3} T^3 \int_0^{x_D} \frac{x^2}{e^x - 1} \; dx \; . \end{aligned}$$

For $T << \Theta_D$, i.e. for temperatures much smaller than the Debye temperature, we find that $x_D \to \infty$. Then,

$$U = \frac{3A\hbar k_B^3}{2\pi v^2 \hbar^3} T^3 I \; , \;\; \text{where} \;\; I = \int_0^{\infty} \frac{x^2}{e^x - 1} \; dx \; .$$

Using this equation for the thermal energy associated with 2D phonons, we get the heat capacity

$$C_V = \frac{dU}{dT} = 18 N k_B I \left(\frac{T}{\Theta_D} \right)^2 \; .$$

This is the T^2 law in 2 dimensions.
