Homework #7

1. **Singularity in density of states**. (a) From the dispersion 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 dimension. Show that \( D(\omega) = \left( \frac{L}{2\pi} \right)^3 \cdot \frac{2\pi}{A^{3/2}} (\omega_0 - \omega)^{1/2} \) for \( \omega < \omega_0 \) and \( D(\omega) = 0 \) for \( \omega > \omega_0 \). Here the density of modes is discontinuous.

**Solution:**

(a) \( \omega = \sqrt{\frac{4C}{m}} \sin \frac{ka}{2} = \omega_m \sin \frac{ka}{2} \quad k \geq 0 \), with \( \omega_m = \sqrt{\frac{4C}{m}} \) being the maximum frequency.

With positive \( k \),

\[ D(\omega) d\omega = \frac{2L}{2\pi} dk = \frac{L}{\pi} \frac{dk}{d\omega} d\omega . \]

Thus \( D(\omega) = \frac{L}{\pi} \frac{dk}{d\omega} \).

\[ \frac{d\omega}{dk} = \frac{\omega_m a}{2 \cos \frac{ka}{2}} = \frac{\omega_m a}{2} \sqrt{1 - \sin^2 \frac{ka}{2}} = \frac{\omega_m a}{2} \sqrt{1 - \frac{\omega^2}{\omega_m^2}} = \frac{a}{2} \sqrt{\frac{\omega_m^2 - \omega^2}{\omega_m^2 - \omega^2}} . \]

\[ \frac{dk}{d\omega} = \frac{2}{a \sqrt{\omega_m^2 - \omega^2}} . \]

\[ D(\omega) = \frac{L}{\pi} \frac{dk}{d\omega} = \frac{2L/a}{\pi \sqrt{\omega_m^2 - \omega^2}} = \frac{2N}{\pi \sqrt{\omega_m^2 - \omega^2}} . \]

(b) For \( \omega(K) = \omega_0 - AK^2 \),

\[ \left| \frac{d\omega}{dk} \right| = \left| -2AK \right| = -2A \sqrt{\frac{\omega_0 - \omega_0}{A}} = 2 \sqrt{A(\omega_0 - \omega)} . \]

In 3D, \( D(\omega) d\omega = \left( \frac{L}{2\pi} \right)^3 \cdot \frac{2\pi}{4\pi k^2} dk = \left( \frac{L}{2\pi} \right)^3 \cdot \frac{4\pi k^2}{d\omega} d\omega \)

Then

\[ D(\omega) = \left( \frac{L}{2\pi} \right)^3 \cdot \frac{4\pi k^2}{d\omega} \frac{dk}{d\omega} = \frac{L}{2\pi} \cdot \frac{2\pi}{A} \cdot \frac{1}{\sqrt{A(\omega_0 - \omega)}} = \left( \frac{L}{2\pi} \right)^3 \cdot \frac{4\pi}{A^{3/2}} \sqrt{\frac{\omega_0 - \omega}{\omega_0}} . \]

For \( \omega > \omega_0 \), there is no normal modes, so that \( D(\omega) = 0 \).

2. **Zero point lattice displacement and strain**. (a) In the Debye approximation, show that the mean square displacement of an atom at absolute zero is
\[ \langle R^2 \rangle = 3h\omega_0^2/8\pi^2\rho v^3, \] where \( v \) is the velocity of sound. Start from the result \( u_0^2 = 4(n+1/2)\hbar/\rho V \omega \) summed over the independent lattice modes: \[ \langle R^2 \rangle = (\hbar/2\rho V) \sum \omega^{-1}. \] We have included a factor of \( 1/2 \) to go from mean square amplitude to mean square displacement. (b) Show that \( \sum \omega^{-1} \) and \( \langle R^2 \rangle \) diverge for a one-dimensional lattice, but that the mean square strain is finite. Consider \( \langle (\partial R/\partial x)^2 \rangle = (1/2) \sum K^2 u_0^2 \) as the mean square strain, and show that it is equal to \( \hbar \omega_0^2 L/4\pi MNv^3 \) for a line of \( N \) atoms each of mass \( M \), counting longitudinal modes only. The divergence of \( R^2 \) is not significant for any physical measurement.

Solution:
(a) For the motion of frequency \( \omega \), the average kinetic energy should be half of the total energy: \[ N \cdot \frac{m}{2} \langle v_\omega^2 \rangle = \frac{E_\omega}{2} = \frac{1}{2} \cdot \frac{\hbar \omega}{2} \text{ or } \langle v_\omega^2 \rangle = \frac{\hbar \omega}{2Nm}. \]

On the other hand, \( v_\omega^2 = \omega^2 R^2_\omega \) and \( Nm = M = \rho V \). Therefore, we have
\[ \langle R^2_\omega \rangle = \frac{\langle v_\omega^2 \rangle}{\omega^2} = \frac{\hbar}{2\rho V \omega}. \]

Then \( \langle R^2 \rangle = \frac{\hbar}{2\rho V} \left( \frac{1}{\omega} \right) = \frac{\hbar}{2\rho V} \int_0^{\omega_0} D(\omega) d\omega / \omega \).

For 3D, there are three modes (two transverse and one longitudinal) for each \( \omega \), thus the density of states with the dispersion of \( \omega = vk \) is
\[ D(\omega) d\omega = 3 \times \frac{V 4\pi k^2 dk}{(2\pi)^3} = 3 \times \frac{V 4\pi \omega^2 d\omega}{(2\pi)^3 v^3} = \frac{3V \omega^2 d\omega}{2\pi^2 v^3}. \]

Then \( \langle R^2 \rangle = \frac{\hbar}{2\rho V} \int_0^{\omega_0} D(\omega) d\omega / \omega = \frac{\hbar}{2\rho V} \cdot \frac{3V}{2\pi^2 v^3} \int_0^{\omega_0} \omega d\omega = \frac{3h\omega_0^2}{8\rho \pi^2 v^3}. \)

(b) For 1D, \( D(\omega) d\omega = 3 \times \frac{2Ldk}{2\pi} = \frac{3Ld\omega}{\pi v} \).

\[ \langle R^2 \rangle = \frac{\hbar}{2\rho L} \int_0^{\omega_0} D(\omega) d\omega / \omega = \frac{\hbar}{2\rho L} \int_0^{\omega_0} \omega d\omega = \frac{\hbar}{2\rho L} \cdot \frac{3L}{\pi v} \ln \omega \bigg|_0^{\omega_0} \rightarrow \infty. \]

For 1D longitudinal wave, \( N \cdot \frac{C}{2} \langle R^2 \rangle = \frac{h\omega}{4} \) or \( \langle R^2 \rangle = \frac{h\omega}{2CN} \).

\[ \langle R^2 \rangle = \frac{\hbar}{2CN} \langle \omega \rangle = \frac{\hbar}{2CN} \int_0^{\omega_0} \omega d\omega = \frac{\hbar}{2CN} \cdot \frac{3L}{\pi v} \ln \omega \bigg|_0^{\omega_0} \rightarrow \infty. \]

\[ D(\omega) d\omega = 1 \times \frac{2Ldk}{2\pi} = \frac{Ld\omega}{\pi v}. \]

Then \( \langle R^2 \rangle = \frac{\hbar}{2CN} \int_0^{\omega_0} \omega D(\omega) d\omega = \frac{hL}{2CN \pi v} \int_0^{\omega_0} \omega d\omega = \frac{hL\omega_0^2}{4CN \pi v}. \)
Note the speed of sound \( v = \sqrt{\frac{C}{m} \cdot a} \), where \( a \) is the lattice constant, then we have
\[
\langle R^2 \rangle = \frac{\hbar \omega_D^3}{4C m \pi} = \frac{\hbar \omega_D^3}{4 \sqrt{\frac{m}{\pi}} N \pi} = \frac{\hbar \omega_D^3}{4 \pi m N \nu^3}.
\]
The strain is \( \varepsilon = R / a \), thus \( \langle \varepsilon^2 \rangle = \langle R^2 \rangle / a^2 = \frac{\hbar \omega_D^3}{4 \pi m N \nu^3} \).

3. **Gruneisen constant.** (a) Show that the free energy of a phonon mode of frequency \( \omega \) is \( k_B T \ln[2 \sinh(\hbar \omega / 2 k_B T)] \). It is necessary to retain the zero-point energy \( \hbar \omega / 2 \) to obtain this result. (b) If \( \Delta \) is the fractional volume change, then the frequency of the crystal may be written as
\[
F(\Delta, T) = \frac{1}{2} B \Delta^2 + k_B T \sum \ln[2 \sinh(\hbar \omega / 2 k_B T)],
\]
where \( B \) is the bulk modulus. Assume that the volume dependence of \( \omega_K \) is \( \delta \omega / \omega = - \gamma \Delta \), where \( \gamma \) is known as the Gruneisen constant. If \( \gamma \) is taken as independent of the mode \( K \), show that \( F \) is a minimum with respect to \( \Delta \) when
\[
B \Delta = \gamma \sum (\hbar \omega / 2) \coth(\hbar \omega / 2 k_B T),
\]
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.

**Solution:**

(a) \( Z_\omega = \sum_{n=0}^\infty e^{-(n+1/2)\hbar \omega / k_B T} = \frac{e^{-\hbar \omega / 2 k_B T}}{1 - e^{-\hbar \omega / 2 k_B T}} = \frac{1}{e^{\hbar \omega / 2 k_B T} - e^{-\hbar \omega / 2 k_B T}} = \frac{1}{2 \sinh \left( \frac{\hbar \omega}{2 k_B T} \right)} \).

\( F_\omega = -k_B T \ln \frac{Z_\omega}{k_B T} = k_B T \ln \left[ 2 \sinh \left( \frac{\hbar \omega}{2 k_B T} \right) \right] \).

(b) \( F(\Delta, T) = \frac{1}{2} B \Delta^2 + k_B T \sum \ln \left[ 2 \sinh \left( \frac{\hbar \omega_k}{2 k_B T} \right) \right] \).

\( F \) is minimized when \( \partial F / \partial \Delta = 0 \).

\[
B \Delta + k_B T \sum \frac{2 \cosh \left( \frac{\hbar \omega_k}{2 k_B T} \right)}{2 \sinh \left( \frac{\hbar \omega_k}{2 k_B T} \right)} = 0.
\]

From the given condition of \( \delta \omega / \omega = - \gamma \Delta \), there is \( d \omega / d \Delta = - \gamma \omega \).
Then the $\partial F / \partial \Delta = 0$ becomes $B\Delta - \gamma \sum_k \coth \left( \frac{h\omega_k}{2k_BT} \right) \frac{h\omega_k}{2} = 0$.

$$\Delta = \frac{\gamma}{B} \sum_k \frac{h\omega_k}{2} \coth \left( \frac{h\omega_k}{2k_BT} \right)$$

$$\sum_k \frac{h\omega_k}{2} \coth \left( \frac{h\omega_k}{2k_BT} \right) = \sum_k \frac{h\omega_k}{2} \frac{\exp \left( -\frac{h\omega_k}{2k_BT} \right) + \exp \left( \frac{h\omega_k}{2k_BT} \right)}{\exp \left( \frac{h\omega_k}{k_BT} \right) - 1} = \sum_k \frac{h\omega_k}{2} \frac{\exp \left( \frac{h\omega_k}{k_BT} \right) - 1}{\exp \left( \frac{h\omega_k}{k_BT} \right) - 1}$$

The first term is zero point energy and the 2nd term is thermal energy. If the zero energy can be ignored, we have $\Delta = \frac{\gamma}{B} U(T)$.

(c) With $\frac{\delta\omega_D}{\omega_D} = -\gamma \Delta = -\frac{V - V_0}{V_0} = -\gamma \frac{\delta V}{V}$, there is $\gamma = -\frac{\delta\omega_D}{\omega_D} / \frac{\delta V}{V} = -\frac{\partial \ln \omega_D}{\partial \ln V}$.

With $h\omega_D = k_\theta$, $\gamma = -\frac{\partial \ln \omega_D}{\partial \ln V} = -\frac{\partial \ln \theta}{\partial \ln V}$.

4. For $d$-dimensional crystal,
   (a) Show that the density of states varies as $\omega^{d-1}$.
   (b) Deduce from this that the low-temperature specific heat vanishes as $T^d$. Graphite has layered structure with very weak bonding between the layers. What temperature dependence of the specific heat would you expect for graphite at low temperature?
   (c) Show that if the dispersion were $\omega \sim k^n$, the low-temperature specific heat would vanish as $T^{d/n}$.

Solution:
(a) For $d$-dimensional system with $\omega = vk$,

$$D(\omega) d\omega \sim \frac{V k^{d-1} \frac{d}{dk}}{(2\pi)^d} \omega^{d-1} d\omega \omega^{d-1} \sim \frac{V \omega^{d-1} d\omega}{(2\pi)^d \omega^{d-1}}.$$  Thus $D(\omega) \propto \omega^{d-1}$

(b) The energy of the system is $U = \int_0^{\infty} \frac{h\omega}{e^{\hbar\omega/k_BT} - 1} D(\omega) d\omega \sim \int_0^{\infty} \frac{h\omega^d}{e^{\hbar\omega/k_BT} - 1} d\omega$

Let $x = \frac{\hbar\omega}{k_BT}$, $U \sim T^{d+1} \int_0^{h\omega_D/k_BT} \frac{x^d}{e^x - 1} dx$.  

At low temperature \((k_B T \ll \hbar \omega_D)\), the upper limit of the integral can be replaced by \(\infty\).

Then \(U \sim T^{d+1} \int_0^\infty \frac{x^d}{e^x - 1} dx \propto T^{d+1}\), and \(C = \frac{\partial U}{\partial T} \propto T^d\).

The layered structure of graphite behaves like a 2D system \(\Rightarrow C \sim T^2\).

(c) For \(\omega \sim k^\alpha\), \(D(\omega) d\omega \sim \frac{V_k^{d-1} dk}{(2\pi)^d} = \frac{V \omega^{(d-1)/\alpha} d\omega^{1/\alpha}}{(2\pi)^d \nu^d} \sim \omega^{d-1} d\omega\).

\[ U = \int_0^{\hbar \omega} \frac{\hbar \omega}{e^{\hbar \omega/k_B T} - 1} D(\omega) d\omega \sim \int_0^{\hbar \omega} \frac{\hbar \omega^{d/\alpha}}{e^{\hbar \omega/k_B T} - 1} d\omega \]

Let \(x \equiv \frac{\hbar \omega}{k_B T}\), \(U \sim T^{d+1} \int_0^{\hbar \omega/k_B T} \frac{x^d}{e^x - 1} dx\).

At low temperature \((k_B T \ll \hbar \omega_D)\), the upper limit of the integral can be replaced by \(\infty\).

Then \(U \sim T^{d+1} \int_0^\infty \frac{x^d}{e^x - 1} dx \propto T^{d+1}\), and \(C = \frac{\partial U}{\partial T} \propto T^{d/\alpha}\).