Names:

EXERCISE 7A: DEBYE THEORY OF PHONONS

Objectives:

- Understand the limitations of the Einstein model of the solid
- Calculate the heat capacity of **phonons** in a solid (Debye theory)

Useful past results:

- Planck distribution: $\langle s \rangle_\omega = \frac{1}{e^{\hbar\omega/\tau} - 1}$
- Wave equation: $\nabla^2 u = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2}$
- A definite integral: $\int_0^\infty dx \frac{x^3}{e^x - 1} = \frac{\pi^4}{15}$

1. *Law of Dulong and Petit.* Early in the term, we encountered the **Einstein's model of the solid**, which treated each atom as an independent 3D harmonic oscillator of frequency ω.

   a. In the Einstein model, you showed that high-temperature limit of the heat capacity of a solid consisting of N atoms is $C_V \to 3Nk_B$. Give a simple argument for this limit, specifying what constitutes "high temperature."

   b. In reality, atoms that are near each other interact, so that their motion is coupled (Fig. 1a). Remind yourself of the physics of coupled harmonic oscillators by considering just $N = 2$ such oscillators cofined to move in the xz-plane (Fig. 1b).

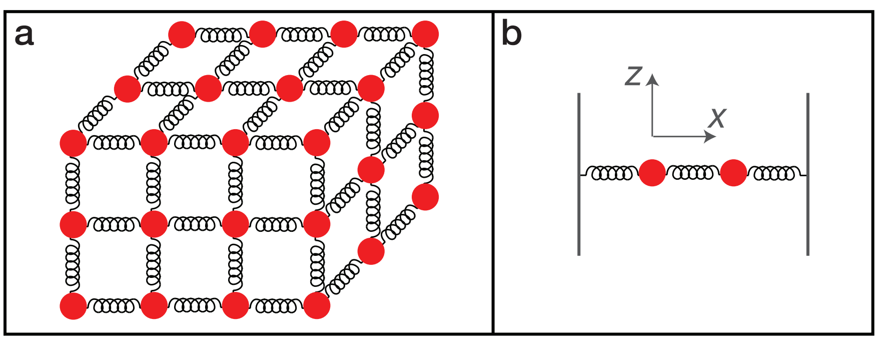

FIG. 1. (a) Debye model of a solid as a set of N coupled harmonic oscillators. (b) Minimal instance, consisting of just $N = 2$ two coupled harmonic oscillators.

i. How many normal modes are there for the system of $N = 2$ coupled oscillators? Illustrate them in a set of sketches with arrows indicating directions of motion.

ii. Consider the normal modes involving motion along $\hat{\mathbf{x}}$. Are their frequencies the same or different?

c. Now return to a solid of $N \gg 1$ atoms modeled as coupled harmonic oscillators.

i. How many normal modes are there in this system?

ii. How should we define the high-temperature limit for the system of N coupled oscillators? Does the result $C_V \to 3Nk_B$ still hold in the high-temperature limit? Why or why not?

2. *Acoustic waves.* In the thermodynamic limit, the normal modes of the solid are acoustic waves. The quantized excitations of these normal modes are called *phonons* (by analogy with the photons constituting electromagnetic waves). The acoustic waves in a solid of dimensions $L \times L \times L$ take the form

$$\boldsymbol{\xi}(x, y, z, t) = \boldsymbol{\xi}_0 \sin(\omega t + \phi) \sin(n_x \pi x/L) \sin(n_y \pi y/L) \sin(n_z \pi z/L), \tag{1}$$

where $\boldsymbol{\xi}$ denotes the displacement of an atom from its equilibrium position (x, y, z).

a. Find a relationship between the frequency ω, the indices (n_x, n_y, n_z), and the speed of sound v_s.

b. How many basis vectors are required to describe the polarization of the acoustic wave (i.e., the direction of oscillation $\boldsymbol{\xi}$) for a fixed direction of propagation? How does your answer compare with the case of an electromagnetic wave?

3. *Debye Model.* In a solid composed of a discrete lattice of N atoms, the discretization places an upper bound on the frequency of the acoustic modes, $\omega \leq \omega_D$. The maximum frequency ω_D is called the **Debye frequency**.

   a. Calculate the Debye frequency:

      i. First find a general expression for the total number of modes $\mathcal{N}(\omega)$ with frequency $\leq \omega$.

      ii. The Debye frequency is given by $\mathcal{N}(\omega_D) = 3N$. Why?

      iii. Find ω_D in terms of N, the volume $V = L^3$, and the speed of sound v.

iv. The Debye frequency is associated with a minimum possible wavelength $\lambda_D = 2\pi v_s/\omega_D$. Find λ_D in terms of N and V.

v. Give a physical interpretation for the lower bound λ_D. (Don't worry about details of the numerical pre-factor.)

b. Determine the density of phonon modes $\mathcal{D}(\omega) = d\mathcal{N}/d\omega$ for frequencies $\omega < \omega_D$.

c. Determine the energy spectral density u_ω of phonons at frequency $\omega < \omega_D$ in a solid at temperature τ, using the Planck distribution for the average occupation of each phonon mode.

d. Write down an integral representing the vibrational energy density U/V of the solid at temperature τ. Express the definite integral $\mathcal{I}$ in terms of a dimensionless parameter $x = \hbar\omega/\tau$ and a cutoff $x_D = \tau_D/\tau$.

e. Give the value of the **Debye temperature** $\theta_D \equiv \tau_D/k_B$ and explain its physical significance.

f. Give the total vibrational energy U in terms of N, τ, τ_D, and $\mathcal{I}$. Your answer should include no other dimensionful quantities.

g. Sketch the integrand from d., shading in the region of integration, for two cases:
   i. Low temperature: $T \ll \theta_D$
   ii. High temperature: $T \gg \theta_D$

h. Evaluate the integral $\mathcal{I}$ and determine the heat capacity:
   i. ...in the low-temperature limit $T \ll \theta_D$
   ii. ...in the high-temperature limit $T \gg \theta_D$

i. Sketch the dependence of the heat capacity on temperature T (interpolating between the high- and low-temperature results.

   i. Draw a solid curve showing the Debye model
   ii. On the same plot, add a dashed curve illustrating the Einstein model

$$\frac{C_V}{3Nk_B} = \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2}. \tag{2}$$

   iii. Give physical explanations for the similarities and differences between the two models.

j. What other degrees of freedom, not considered above, might modify the heat capacity of a real solid?