Please complete the following questions. You are allowed to work in groups but remember to show your own work.

Problem 1. (Diatomic Einstein Solid)

The Einstein model we studied in lecture assumed all the oscillators are oscillating at the same constant frequency ω_E. However, as you may already know, most solids are not pure elemental crystals and are instead made up of ≥ 2 species of atoms. There is no reason to assume that the two species of atoms will oscillate at the same frequency so let's extend the Einstein model and calculate the heat capacity for a diatomic Einstein solid.

Assume you have a diatomic crystal made up of atom 1 and atom 2 with masses m_1 and m_2, respectively, and total number of atoms $N = N_1 + N_2$. We will assume that all interatomic bonds have the same stiffness k.

(a) Explain why the frequency of the two different atom species must be different. What are these frequencies, ω_1 and ω_2?

(b) Write down the expected energy, E_1 and E_2 for each atom species at temperature T.

(c) What is the total energy of the entire diatomic solid? Use this energy to calculate the heat capacity.

(d) Going back to the monoatomic Einstein model, explain in your own words the physical significance of the Einstein temperature.

(e) In this diatomic model, there are two Einstein temperatures, $T_{\text{Einstein},1}$ and $T_{\text{Einstein},2}$. explain why there are two and predict what will happen to the energy of the atoms as we reduce temperature below these Einstein temperatures.

(f) If $T_{\text{Einstein},1} > T_{\text{Einstein},2}$, what will be the total energy of the system when the temperature drops below $T_{\text{Einstein},2}$?

Problem 2. (Density of States of the Debye Model)

Let's get some more practive calculating the density of states. Do the following for 1, 2, and 3 dimensions (We did the 3D case in class but you should redo it for practice).

(a) What is the dispersion relation used for the Debye model? (This should be the same for all dimensions)

(b) Assuming periodic boundary conditions, write down the total number of states N from 0 up to some k-value, k_0, as a sum and then turn this sum into an integral. Explain in your own words, the physical significance of the prefactor your get from turning the sum into an integral.

(c) Now change variables from k to ω using your dispersion relation so that you get your n-dimensional desnsity of states $g_n(\omega)$ in the form

$$N = \int g_n(\omega)\, d\omega$$

Keep in mind that your k integral may be multiple integrals (for $n > 1$ dimensions) so you need to pick the appropriate coordinate system to reduce the $d^n k$ integral to a single dk integral.

Problem 3. (2D Debye Solid)

Let's review the calculation for the Debye model by redoing it for 2D.

(a) Write down the assumptions of the Debye model.

(b) Find an expression for the Debye frequency of the 2D solid, ω_D.

(c) Show that the expected energy has the form

$$\langle E \rangle = KT^n \int_0^{\beta\hbar\omega_D} \frac{x^2}{e^x - 1}\, dx$$

where $x = \beta\hbar\omega$. Here, K is a constant and n is some whole number, both of which you should find.

(d) Show that in the high temperature limit, you recover the expected Heat capacity predicted by Dulong-Petit. That is, show that

$$C = 2Nk_B$$

for high T. (*Hint*: What is the high T limit in terms of x?)

(e) Show that in the low temperature limit, the heat capacity has the form

$$C = IT^m$$

where I is some integral expression independent of T (you don't have to solve the integral) and m is some whole number, both of which you should find.

Problem 4. (Monoatomic Chain of Atoms)

Let's do a few more things for the monoatomic chain that we didn't really talk about in detail during lecture.

(a) Write down the dispersion relation and explain how the Debye model can be recovered from this dispersion.

(b) Show that the oscillatory mode with wave vector k is equivalent to a mode with wave vector $k + \frac{2\pi}{a}$. In your own words, explain how this allows us to only focus on what happens only within the 1st Brillouin zone.

(c) Write down the displacement of two neighboring atoms, u_n and u_{n+1} and find the phase difference between the two atoms. What happens to this phase difference in the long wavelength limit? Sketch the corresponding motion of the atoms in the chain in the long wavelength limit.

(d) What is the phase difference at the smallest wavelength (the edge of the Brillouin zone)? Sketch the corresponding motion of the atoms.

(e) Find the expression for the density of states, $g(\omega)$, of the monoatomic chain. Plot your expression for $g(\omega)$ (you can set all constants to 1). Your plot should diverge at a specific value of ω. What is the significance of this value?

(f) Write down an integral expression for the heat capacity of the monoatomic lattice (This is a nasty integral that you can't solve). Show that this gives you the Dulong-Petit result in the high temperature limit.

Problem 5. (Diatomic Chain of Atoms)

In class, we setup the diatomic scenario and arrived to the following coupled system of equations

$$m_1 \ddot{u}_n = \gamma_2(v_n - u_n) + \gamma_1(v_{n-1} - u_n)$$
$$m_2 \ddot{v}_n = \gamma_1(u_{n+1} - v_n) + \gamma_2(u_n - v_n)$$

but I said I would leave the details of the normal mode calculations to you. For your calculations, you may assume that $m_1 = m_2 = m$ for simplicity.

(a) Use the ansatz

$$u_n = Ae^{-i(kna - \omega t)} \qquad v_n = Be^{-i(kna - \omega t)}$$

to find a system of equation for the amplitudes A and B.

(b) Show that your system has a solution only if

$$\omega_{\pm} = \sqrt{\frac{\gamma_1 + \gamma_2}{m} \pm \frac{1}{m}\sqrt{(\gamma_1 + \gamma_2)^2 - 4\gamma_1\gamma_2 \sin^2\left(\frac{ka}{2}\right)}}$$

(*hint:* turn your system into a matrix equation)

(c) Plot the first Brillouin zone of the dispersion relation above for $\gamma_2 = 1.5\gamma_1$.

(d) In your own words, comment on the physical significance/origins of the name given to each branch of the dispersion relation you plotted above.

(e) Find an expression for the speed of sound for small k.