Assignment 4

Diatomic Chains, Dispersion Relations
Please no AI-generated solutions. Would be your loss!

Question 1

The dispersion relationship for a $1D$ diatomic chain is:

$$\omega^2 = \gamma\left(\frac{1}{m_a}+\frac{1}{m_b}\right) \pm \gamma\sqrt{\left(\frac{1}{m_a}+\frac{1}{m_b}\right)^2 - \left(\frac{4}{m_a m_b}\right)\sin^2\left(\frac{ka}{2}\right)}, \tag{1}$$

where γ is the interaction between neighbouring masses m_a and m_b and the wavevector is k.

(a) Find the group velocity $d\omega/dk$ for the acoustic and optical branches. It's okay to use a integrater software.

(b) Sketch a possible graph for the density of states $g(\omega)$ versus ω, identifying the location of the singularities in the graph. I am not expecting you to plot the entire $g(\omega)$ accurately (even though it is possible).

Question 2

In the Debye Model, the energy (for a single polarization) and N atoms is given by:

$$U = \frac{3Vk_B^4T^4}{2\pi^2\hbar^3v^3}\int_0^{x_D} dx\frac{x^3}{(e^x-1)}, \tag{2}$$

where V is the volume of the solid, v is the speed of sound in the medium, $x = \hbar\omega/k_BT$, and $x_D = \hbar\omega_D/k_BT = \theta_D/T$. In the low temperature limit, x_D in the upper limit can be replaced by infinity. What does the temperature dependence of $C_V = \frac{\partial U}{\partial T}|_V$ look like at these ultra-low temperatures?

Question 3

In class, we derived the following equations of motion for the displacements in a diatomic, $1D$ chain:

$$\begin{pmatrix} -\omega^2 + \dfrac{2\gamma}{m_a} & -\dfrac{\gamma}{\sqrt{m_a m_b}}\left(1 + e^{-ika}\right) \\ -\dfrac{\gamma}{\sqrt{m_a m_b}}\left(1 + e^{ika}\right) & -\omega^2 + \dfrac{2\gamma}{m_b} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = 0, \tag{3}$$

where the displacements are:

$$S_{n,a} = \frac{u_a}{\sqrt{m_a}}\, e^{ikna}, \qquad S_{n,b} = \frac{u_b}{\sqrt{m_b}}\, e^{ikna}, \tag{4}$$

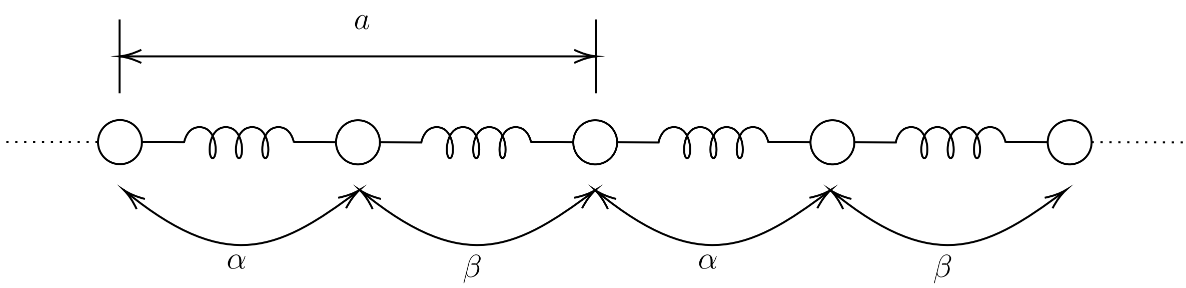
while we have suppressed the time dependence.

(a) What is the ratio $S_{n,a}/S_{n,b}$ for the acoustic branch at $k = 0$?

(b) What is the ratio $S_{n,a}/S_{n,b}$ for the optical branch at $k = 0$?

Show that the amplitudes for the two kinds of atoms are in phase (acoustic) and 180° out of phase (optical).

Question 4



Consider a $1D$ chain of atoms which has an alternating interaction strength (say α and β) between adjacent atoms. All atoms have the same mass M. We have to treat this system, effectively as a diatomic system with two atoms a and b per unit cell. The equations of motion are:

$$-\omega^2 u_a + D_a^a u_a + D_a^b u_b = 0, \tag{5}$$
$$-\omega^2 u_b + D_b^a u_a + D_b^b u_b = 0, \tag{6}$$
$$\tag{7}$$

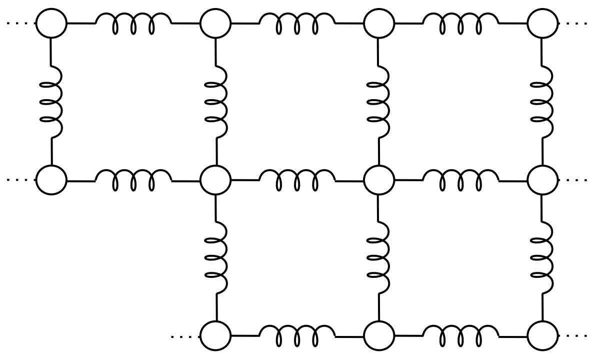
where $D_a^b = \sum_m \Phi_{n,a}^{m,b} e^{i\vec{k}\cdot(\vec{r}_m - \vec{r}_n)}$.

(a) Find the constants Φ in term of α and β. Start by writing the potential energy in terms of α and β.

(b) Find the dynamical matrix elements D.

(c) Find and plot the dispersion relation $\omega(k)$ for this alternating coupling strength atomic chain.

Question 5



(a) Find the density of states $g(\omega)$ for a two-dimensional network of atoms, as shown above. Assume a dispersion relationship $\omega = vk$.

(b) Find the Debye frequency ω_D.

(c) Find the total energy associated with these oscillations in the $2D$ crystal.

(d) Find C_V. Express your answer in terms of T and $\theta_D = k_B T/\hbar$. Use the low temperature approximation.

Note:

$$\int_0^\infty dx \frac{x^2}{e^x - 1} = 2\zeta(3) = 2.404,$$

where $\zeta(n)$ is the Riemann zeta function:

$$\zeta(n) = \sum_n^\infty k^{-n}.$$