

Exercise 1 - Phonons in a monatomic harmonic chain

(2 points)

Consider a one-dimensional chain of $N \gg 1$ (N even) atoms with periodic boundary conditions, where the potential energy is given by

$$U(\{\mathbf{x}\}) = U_0 \sum_{i=-(\frac{N}{2}-1)}^{\frac{N}{2}} (\mathbf{x}_{i+1} - \mathbf{x}_i - \mathbf{a})^2 \quad (1)$$

where $\mathbf{a} = (a, 0, 0)$ and we denote by $\{\mathbf{x}\}$ the set of all coordinates $\{\mathbf{x}_{-(\frac{N}{2}-1)}, \dots, \mathbf{x}_0, \dots, \mathbf{x}_{\frac{N}{2}}\}$.

- (a) Determine the equilibrium positions $\{\mathbf{x}^0\}$ of the atoms.
- (b) Calculate the matrix

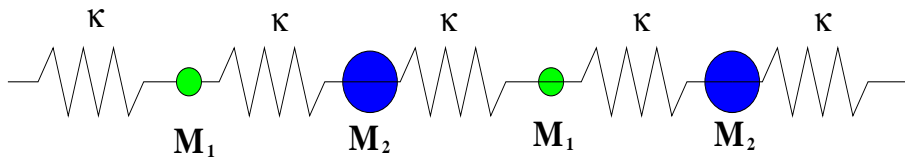
$$D_{\alpha,\beta}(\mathbf{x}_i^0, \mathbf{x}_j^0) = \left. \frac{\partial^2 U}{\partial x_i^\alpha \partial x_j^\beta} \right|_{\mathbf{x}^0}. \quad (2)$$

- (c) Calculate the dynamical matrix and determine the eigenfrequencies of the system from the eigenvalues of the dynamical matrix.
- (d) Plot the dispersion relation of the phonons inside the first Brillouin zone.

Exercise 2 - Phonons in a diatomic harmonic chain

(2 points)

Calculate the dispersion for acoustical and optical phonons in a diatomic chain as shown in the figure below,



Show that the dispersion can be written as

$$\omega^2(q) = \kappa \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm \kappa \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4}{M_1 M_2} \sin^2\left(\frac{qa}{2}\right)} \quad (3)$$

where κ is the force constant and M_1 and M_2 are the two masses. Plot the dispersion of the phonons inside the first Brillouin zone.

Hint: Write down the equations of motion for the coordinates u , show that the dynamical matrix is a 2×2 matrix, and calculate its eigenvalues.

Exercise 3 - Lattice specific heat in 3D solid

(2 points)

1. Show that the specific heat for acoustic phonons in the Debye model can be written as

$$\frac{C_v}{Nk_B} = 9 \cdot \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{y^4 e^y}{(e^y - 1)^2} dy, \quad (4)$$

where N is the total number of atoms, and $\Theta = \hbar\omega_D/k_B$ is the Debye temperature given in terms of the Debye frequency cutoff ω_D .

2. Make a plot of C_v/Nk_B and discuss its T dependence in the low and high temperature limits.

Solutions due on: 13 May, 2011