Exercise 1 - Phonons in a monatomic harmonic chain (2 points)

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

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

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

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

(b) Calculate the matrix

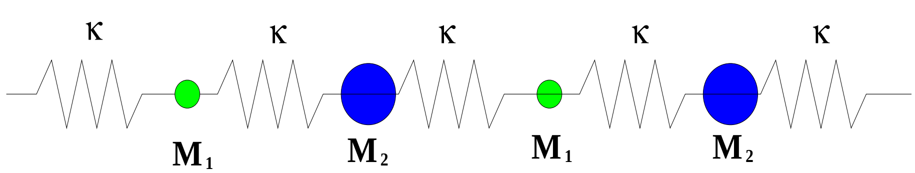
$$D_{\alpha,\beta}(\mathbf{x}_i^0, \mathbf{x}_j^0) = \left.\frac{\partial^2 U}{\partial x_i^\alpha x_j^\beta}\right|_{\mathbf{x}^0}. \tag{2}$$

(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

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

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
$$\frac{C_v}{Nk_B} = 9 \cdot \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{y^4 e^y}{(e^y - 1)^2} dy, \tag{4}$$
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 the 22nd of April, 2013