

**Exercise 6.1 Phonons in One Dimension**

In this exercise you will show that a chain of atoms that are harmonically coupled to each other (and may thus oscillate around their equilibrium positions) is equivalent to a collection of harmonic oscillators. When quantized canonically, these are turned into non-interacting bosons. More specifically, consider a chain of atoms with alternating masses, such that atoms at site  $i$  with  $i$  even have mass  $m$  and those at odd sites have mass  $M$ . The potential energy is given by

$$V = v \sum_{i=1}^{N/2} \{ (u_{2i} - u_{2i+1})^2 + (u_{2i} - u_{2i-1})^2 \} \quad (1)$$

- a) Diagonalize the equations of motion to find the eigenmodes of the *classical* system. To achieve this, introduce

$$\tilde{\mathbf{u}}_i = (u_{2i}, u_{2i+1})^T, \quad (2)$$

where  $i$  now labels unit cells instead of atoms ( $\tilde{u}_{i,1}$  ( $\tilde{u}_{i,2}$ ) corresponds to an atom belonging to the even (odd) sublattice), and write

$$\tilde{u}_{j,a}(t) = \sqrt{\frac{2}{N}} \sum_k \sum_\mu C_{a\mu}^k (q_{k\mu}(t) e^{ikj} + q_{k\mu}^*(t) e^{-ikj}), \quad (3)$$

where  $a, \mu \in \{1, 2\}$ . The  $q_{k\mu}(t)$  should be chosen such that the equations of motion are diagonal, i.e. they should acquire the form

$$\frac{d^2}{dt^2} q_{k\mu}(t) + \omega_{k\mu}^2 q_{k\mu}(t) = 0. \quad (4)$$

Plot the dispersion relation defined by the  $\omega_{k\mu}$  in the reduced Brillouin zone to find that there are two different phonon branches (called acoustical and optical branch)!

- b) Following the method introduced in section 3.3 of the lecture notes, quantize the system. You should find two kinds of bosons corresponding to the two branches in the classical dispersion.

**Exercise 6.2 Peierls' Instability in One Dimension**

We consider a one-dimensional chain with nearest-neighbor hopping where the position of the electrons is not fixed. The Hamiltonian is thus given by a (renormalized) hopping and an elastic part:

$$\mathcal{H} = \sum_{i,s} (c_{i+1,s}^\dagger c_{i,s} + h.c.) (-t + \alpha \delta u_i) + \lambda \sum_i \frac{\delta u_i^2}{2} \quad (5)$$

where  $\delta u_i = u_{i+1} - u_i$  and  $u_i$  is the displacement of the atom at site  $i$  from its equilibrium position.  $\lambda > 0$  is a measure of the stiffness of the system and  $\alpha > 0$  is the coupling

constant.

In the following, we consider the half filled case (one electron per site) and make for  $\delta u_i$  the ansatz

$$\delta u_i = u_0 \cos(qr_i) \quad (6)$$

- a) Calculate for  $q = \pi$  the eigenenergies and the eigenstates of the system and the density of states.

**Hint:** Write the electronic part of the Hamiltonian in the Form

$$\mathcal{H} = \sum_{|k| < \pi/2, s} \vec{c}_{ks}^\dagger \mathcal{H}_k \vec{c}_{ks} \quad (7)$$

where  $\vec{c}_{ks}^\dagger = (c_{ks}^\dagger, c_{k+\pi s}^\dagger)$  and  $\mathcal{H}_k$  is a  $2 \times 2$  matrix which can be written in terms of Pauli matrices. The diagonalization is then just a rotation in the space of these matrices. Note that the sum now only runs over a reduced Brillouin zone,  $k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ .

- b) Show that in this one-dimensional system, there is always a finite  $u_0$  that minimizes the total energy.

**Hint:** Show it for large  $\lambda$  and small  $u_0$  by using the elliptic integral of the second kind,

$$E(\varphi, k) = \int_0^\varphi \sqrt{1 - k^2 \sin^2 \alpha} d\alpha \quad (8)$$

and its series expansion

$$E\left(\frac{\pi}{2}, k'\right) = 1 + \frac{1}{2} \left( \log \frac{4}{k'} - \frac{1}{2} \right) k'^2 + O(k'^4) \quad (9)$$

where  $k' = \sqrt{1 - k^2}$ .

- c) Show that the density of electrons per site,  $\rho_i = \sum_s \langle c_{is}^\dagger c_{is} \rangle = 1$  for all  $i$  but the bond density,  $\tilde{\rho}_i = \sum_s \langle c_{is}^\dagger c_{i+1s} + c_{i+1s}^\dagger c_{is} \rangle$  oscillates with position  $i$ . Discuss also the limits  $\lambda \rightarrow 0$  and  $\lambda \rightarrow \infty$  for  $\alpha = t$ .