ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Solid State Theory
Exercise 7

FS 10
Prof. M. Sigrist

Exercise 7.1 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

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

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

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

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). Next write

$$\tilde{u}_{j,a}(t) = \sqrt{\frac{2}{N}} \sum_k \sum_\mu C^k_{a\mu} \left(q_{k\mu}(t) e^{ikj} + q^*_{k\mu}(t) e^{-ikj} \right), \tag{3}$$

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

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

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 7.2 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:

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

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 δu_i the ansatz

$$\delta u_i = u_0 \cos(q r_i) \tag{6}$$

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

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

where $\vec{c}^{\dagger}_{ks} = (c^{\dagger}_{ks}, c^{\dagger}_{k+\pi s})$ and $\mathcal{H}_k$ is a 2×2 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 λ and small u_0 by using the elliptic integral of the second kind,

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

and its series expansion

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

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

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