Institute for Theoretical Physics
University of Cologne

Prof. Dr. Simon Trebst
Peter Bröcker

Solid State Theory

Problem set 2

Winter Term 2016

Website: http://www.thp.uni-koeln.de/trebst/Lectures/2016-SolidState.shtml
Due date: Discussed in class on **Thursday, November 24th**.

If you turn in your solutions by Wednesday noon (November 23rd), they will be graded. Please submit your solutions to Henry Legg at hlegg@uni-koeln.de.

1. Diatomic chain

In this exercise, we consider the physics of an infinitely long diatomic chain depicted in Fig. 1.

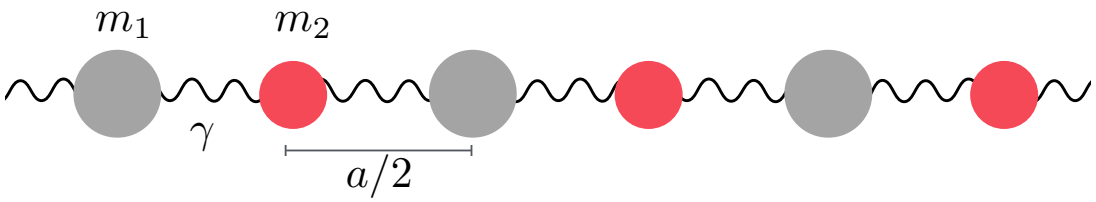

Figure 1: A diatomic chain with two types of atom of masses m_1 and m_2 that are connected by a spring with constant γ. At rest, each atom is separated from its neighbor by a distance $a/2$.

1. We start by discussing qualitative properties of the chain's physics. Draw a short region of the chain and highlight the unit cell for the two cases (a) $m_1 = m_2$ and (b) $m_1 \neq m_2$, respectively. How many branches will the phonon dispersion have in these two cases?
2. Calculate the volume of the unit cell and the volume of the 1. Brillouin zone.
3. The Hamiltonian of the chain is given as

$$H = \sum_{i=-\infty}^{\infty} \frac{p_{i,1}^2}{2m} + \frac{p_{i,2}^2}{2m} + V(\{x_{i,j}\}), \tag{1}$$

where the sum runs over all unit cells i and includes contributions from all types of atoms j. The potential V in the most general case depends on all atoms in all unit cells $V(\{x_{i,j}\})$. Making use of the sketch depicted in Fig. 1 and the definition of the dynamical matrix

from the lecture, explain why the potential can be approximated as

$$V\left(\{x_{i,j}\}\right) = \sum_{i=-\infty}^{\infty} \frac{\gamma}{2}\left[(\delta x_{i,1} - \delta x_{i,2})^2 + (\delta x_{i,2} - \delta x_{i+1,1})^2\right], \tag{2}$$

with δx denoting the displacement of an atom from its equilibrium position.

4. Now use the ansatz

$$\delta x_{j,i} = \sqrt{a} \int_{-\pi/2}^{\pi/2} \frac{\pi}{2\pi} \frac{1}{\sqrt{m_i}} e^{\mathrm{i}kx_{j,1}^{(0)}} q_i(k) \tag{3}$$

$$p_{j,i} = \sqrt{a} \int_{-\pi/2}^{\pi/2} \frac{\pi}{2\pi} \sqrt{m_i} e^{\mathrm{i}kx_{j,1}^{(0)}} p_i(k) \tag{4}$$

to rewrite the Hamiltonian in the form

$$H = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \frac{1}{2} \left[\sum_m p_m(k) p_m(-k) + 2\gamma \sum_{m,n} q_m(k) \tilde{V}_{m,n} q_n(-k)\right]. \tag{5}$$

Why can we savely use the displacement as our variable instead of the full coordinate? *Hint:* You will need to use an identity for Fourier sums that we studied on the previous exercise sheet to fully simplify the expression obtained from plugging in the Ansatz.

5. Continue to first determine the eigenvalues $d_i(k)$ of the matrix $2\gamma\tilde{V}$ and use them in a second step to find the dispersion relations $\omega_i(k) = \sqrt{d_i(k)}$.
6. How do the dispersions relations change as $m_1 \to m_2$? Explain how this ties in with your answer for question 1.

2. Phonons in Python

For this exercise, we provide a simple Python notebook that you can study and play around with to explore the physics of phonons. In particular, it allows you visualize the different oscillation modes and how the overall kinetic and potential energies are interchanged during the movement. It is loosely based on a paper by Freeman J. Dyson in which he studies the general case of a chain of oscillators where both the mass *and* the spring constants are allowed to be different for each site and bond, respectively.

In this notebook, the mode used for display is selected by the variable *idx* that is set in the fifth input cell from the top. Its values range from 0, which is the ground state to $N-1$, the state highest in energy. You can further explore what happens when the masses and spring constants are changed. This can be achieved by changing how the mass and spring constant arrays in the second input cell are initialized. After running the following cells, the matrix will be updated according to your choices and rediagonalized so that you can have a look at how your choice affects the oscillation modes.