

C1: One-dimensional phonon modes

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1 Introduction

The basic theory of phonons is covered in the textbooks, which should be studied carefully before the exercise. In these, all important mathematical results are derived in detail, however those most relevant to the exercise will still be repeated here below.

In this computer exercise, we will focus on understanding the concept of phonons. Therefore a program has been developed which takes care of all calculations, where the user only needs to supply proper numeric values and press buttons with the mouse to make things happen. Nevertheless, it is of fundamental importance to understand the model implemented, in order to correctly interpret the results. Therefore some time during the exercise will be devoted to the basic theory of phonons. Especially, we will look at the two underlying approximations used in the theory, which is the adiabatic approximation and the harmonic approximation.

The computer model uses a finite representation of the ideal one-dimensional linear chain, with possibilities for two different types of boundary conditions: periodic, to make the chain effectively infinite, or fixed ends for a finite chain. Mass and force constant may be changed, and the program displays both the dispersion curve and the particular eigenmode selected. It is even possible to show an animation of the motion of the atoms in each eigenmode.

There is also the possibility to have a diatomic chain, with alternating atoms of two different masses. The force constants are still assumed to be the same for all atoms. Finally, one can introduce an impurity atom in the chain. This is interesting, since we have no simple way of treating this case analytically, but are referred to numerical simulations.

During the exercise we will study the basic features of the one-dimensional phonon model, including important issues such as symmetry, and see how the impurity is able to create localized eigenmodes, which are very important in scattering theory.

2 Preparation questions and report

In the next section we will cover the basic theory of phonons relevant to the exercise, in principle focusing entirely on the one-dimensional case. In that section there are a number of questions. The answers to these, together with the results obtained during the practical work, will constitute the report. Study these questions before the exercise; at the start of the exercise the supervisor will check your answers. The answers do not have to be correct, but you must show that you have thought about the problems.

Some of the questions, especially the first ones, you should have the answer to only after the exercise – that is the point of it! Nevertheless, it is important to think them through anyway, for three reasons. First, it is very interesting to see what your perception of phonons is, based on what you have learned during the lectures. Second, once you identify what you do *not* know, it will be much easier to take in the richer understanding about phonons, which hopefully this exercise can provide. Third, the exercise will waste less time, and so we will be able to spend more time on the important issues. As for most of the other questions, the answers are readily available in the lecture notes.

In principle you should be able to compile the entire material for the report during the exercise itself, and later just type it out nicely (hand-written reports are accepted only if you have a very nice handwriting), and submit it. As usual the report should be submitted no later than two weeks from the day of the exercise to be graded.

The report does not have to contain anything already covered in this guide, i.e. there is no need to repeat the theory, or description of the model. Simple answers to each question will qualify you for the degree 2. To get the higher grade 3, the report must show a degree of understanding of both questions asked and their answers, and also show a certain amount of individual insight into the treated problems.

Please feel free also to include in your report some words about how you experienced the exercise itself. Such comments will surely not affect your grade, as long as any criticism or positive remarks are constructive and motivated. You may supply suggestions for improvements, you may have felt that some parts were irrelevant, or that the exercises and preparation questions were too difficult or simple, relative to your background knowledge of phonons, or something completely different.

Have fun and good luck!

3 Basic phonon theory

3.1 Fundamental questions

Before we begin, there are a couple of fundamental questions, without which everything else we do is rather pointless. Try to formulate your own ideas and thoughts about these concepts, even if you are not supposed to know the full answers to these questions until after the exercise.

Question 1: What is a phonon?

Question 2: How are phonons created?

Question 3: Why are phonons important?

At the bottom of any successful theory lies a set of constituting assumptions and, often, approximations. Our phonon theory relies on two different approximations; the *adiabatic approximation* and the *harmonic approximation*.

3.2 The adiabatic approximation

When discussing the properties of solids different approaches can be used. Here we consider two of them.

In the first one, only the electronic degrees of freedom are considered, and they give rise to a multitude of important effects. Such calculations are almost always performed assuming that the underlying ion lattice has no influence on the motion of the electrons and many important features of solids can be explained, even in details, from studying only the electrons.¹

However, experiments show that when for instance a solid is subjected to a heat gradient or outside force like hitting it, the electrons can make up only part of the measured specific heat or certain heat and sound transport properties. From these and other indications that the ions also play an important role in the properties of solids (other than just making up the crystal lattice), we are led to undertake a detailed study of *phonons* – or lattice vibrations. So in the second approach, we set up a theory for the phonons where the electronic degrees of freedom does not appear directly, even though they play a crucial role, which we will now discuss.

¹ This approach will not be further considered in this exercise.

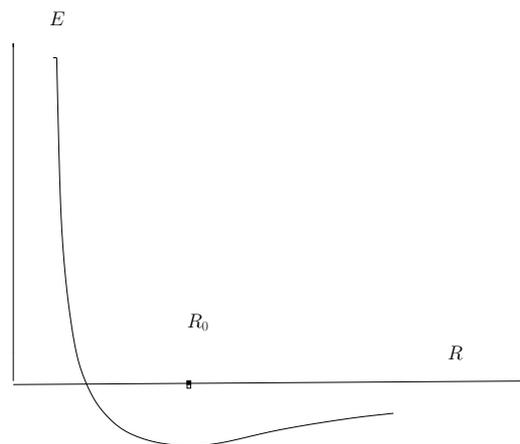


Figure 1: Typical binding energy of a diatomic molecule

If you solve the Schrödinger equation for a two atom system as a function of a fixed distance R between the nuclei, you will find that the total ground state energy of the system behaves as shown in Fig. 3.2. The energy is minimal for a certain distance R_0 , and the atoms will be bound together. In other words, the electrons create the “spring force between the ions (see e.g. Fig. 3). The same analysis can be generalized to more atoms which forms a lattice, but to do the calculations thoroughly and obtain numerical values for the spring constants requires heavy numerical tools as e.g. *Density Functional Theory (DFT)*.

That the electronic degrees of freedom can be treated effective as spring constants in the model relies heavily on the *adiabatic approximation*.

Question 4: The adiabatic approximation states that the ionic motion does not disturb the electronic degrees of freedom (and vice versa). What is the underlying physical reason for this?

The adiabatic approximation allows us to treat the electrons effectively when looking at the ionic degrees of freedom. It should nevertheless be noted, that in some cases one has to connect the two systems, electrons and phonons, more exactly, typically using perturbation theory of some sort. This is however a complicated task well beyond the scope of this introductory course, and so from here on we are concerned with a system which consists solely of ions (using this term in the broadest sense), and the electrons only play the role of making the system electrically neutral and creating the attractive force between the ions.

The idea behind the adiabatic approximation can be difficult to grasp. As an every day example of an *adiabatic approximation* we consider the situation where we place a hand in a bucket of water. As long as we move the hand slowly, the water surface is almost flat, i.e. at every instant the water molecules can rearrange themselves so that the water is in its ground state (the flat surface). Note that the influence of the water on the movement of the hand cannot be neglected, because it gives a friction force.

If the hand is moved faster, the surface is not flat and waves and vortices appear. The water is no longer in the ground state. This is because the speed of the hand and the water are comparable.

3.3 The harmonic approximation

In the previous section we argued that the energy of the total system has a minimum energy as a function of the positions of all the ions in the crystal, $V(\{\mathbf{R}_i\})$.

Now we consider a situation where the ions are *not* in their equilibrium positions \mathbf{R}_{i0} , but slightly aside it, at \mathbf{R}_i . Since we expect, or rather demand, that the displacements $\mathbf{u}_i \equiv \mathbf{R}_i - \mathbf{R}_{i0}$ are small compared to the interatomic distances, it is natural to make a Taylor series expansion of the energy in the displacements. As our second approximation,

we drop all terms above the quadratic, which gives us

$$V(\{|\mathbf{R}_i - \mathbf{R}_j|\}) = \frac{1}{2} \sum_{ij} (\mathbf{u}_i - \mathbf{u}_j) \cdot \left[\nabla_{\mathbf{R}_{ij}} \nabla_{\mathbf{R}_{ij}} V(\{|\mathbf{R}_{ij}|\}) \Big|_{\mathbf{R}_i = \mathbf{R}_{i0}} \right] \cdot (\mathbf{u}_i - \mathbf{u}_j), \quad (3.1)$$

where $\mathbf{R}_{ij} \equiv \mathbf{R}_i - \mathbf{R}_j$ and $\{|\mathbf{R}_i - \mathbf{R}_j|\}$ denotes the set of all distances $|\mathbf{R}_i - \mathbf{R}_j|$.

Question 5: We also drop the zero and first order terms. Why? And why can we drop higher order terms?

Keeping only the second order term in the Taylor expansion is called the *harmonic approximation*.

3.4 Monatomic one-dimensional linear chain

We now jump to our case of interest: a one-dimensional infinite ideal linear chain of atoms of a single kind. Thus the positions of the atoms in the chain are simply $R_{i0} = ia$ where a is the lattice constant and i an integer. Inserting this into what is left of the expansion, Eq. (3.1), and defining the *force constant*

$$C_{ij} \equiv \left[\frac{\partial^2 V(R_{ij})}{\partial R_{ij}^2} \right]_{R_i = R_{i0}} \quad (3.2)$$

we get the rather simple expression

$$\begin{aligned} V(\{|R_i - R_j|\}) &= \frac{1}{2} \sum_{ij} C_{ij} (u_i - u_j)^2 = \\ &= \frac{1}{2} \sum_i \sum_p C_p (u_i - u_{i+p})^2, \end{aligned} \quad (3.3)$$

where p is a positive integer.

Thus the force on the s -th atom, becomes

$$F_s = -\frac{\partial V}{\partial u_s} = \sum_p C_p (u_{s+p} + u_{s-p} - 2u_s). \quad (3.4)$$

Question 6: Verify Eq. (3.4).

From Newton's second law, the equations of motion for the displacements $u_s(t)$ thus become

$$M \frac{d^2 u_s}{dt^2} = \sum_p C_p (u_{s+p} + u_{s-p} - 2u_s), \quad (3.5)$$

where M is the mass of the atom. Note that this expression corresponds to the equation of motion for a set of coupled springs with spring constant C , which further emphasizes

the relation between phonons and lattice vibrations.

For the simple case of a monoatomic chain an analytic result for the equations of motion, Eq. (3.4), can be obtained by making an Ansatz with a particular form of $u_s(t)$. Since we anticipate travelling waves, to which we attribute a frequency ω , the time-dependence can be taken as $e^{-i\omega t}$. We may therefore write

$$u_s(t) = u_0 e^{-i\omega t} e^{isKa}, \quad (3.6)$$

where u_0 is a time- and space-independent constant. K is the wavenumber, determining the propagation direction of the wave (in 3 dimensions K is a vector) and its wavelength $\lambda = 2\pi/K$.

Next we make the approximation to drop all terms in Eq. (3.5) except those corresponding to *nearest-neighbor interaction*. We also assume that all interactions have the same strength, with force constant C . Thus the equation of motion, after also substituting for u_s the Ansatz (3.6) and canceling the common factor $u_0 e^{iKa}$, becomes an equation for ω ,

$$-\omega^2 M = C (e^{iKa} + e^{-iKa} - 2), \quad (3.7)$$

which can be written as (show this!)

$$\omega^2 = \frac{4C}{M} \sin^2\left(\frac{Ka}{2}\right). \quad (3.8)$$

Eq. (3.8) is called the *dispersion relation*, and is plotted in Fig. 2.

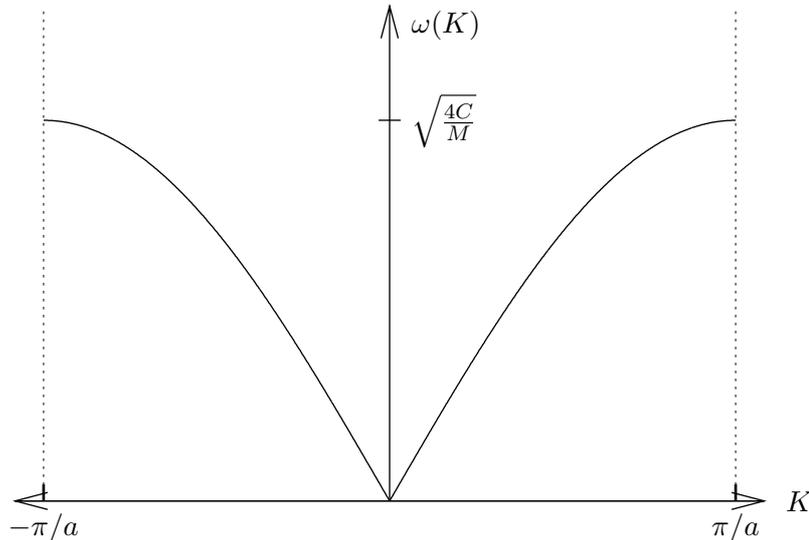


Figure 2: Dispersion relation for the infinite monoatomic linear chain.

The allowed values of K are determined by the boundary conditions. For the simplest model, our infinite chain, we have infinitely many solutions to the problem. It is however easy to see that it is enough to consider values of K within the first Brillouin zone, $-\pi/a \leq K < \pi/a$.

Question 7: How is this easy to see, and why don't we choose the interval $0 \leq K < 2\pi/a$ instead? Why is the point $K = \pi/a$ not included (open interval)?

The derivative

$$v_g = \frac{\partial \omega}{\partial K} = \sqrt{\frac{Ca^2}{M}} \cos\left(\frac{Ka}{2}\right) \quad (3.9)$$

is the *group velocity* of the wave packet. This velocity, unlike the phase velocity ω/K which is of little interest here, is the velocity of energy propagation, or put differently, the sound velocity. The group velocity is K -dependent and therefore wavelength dependent, so waves with different wavelengths will travel at different speeds, hence the name *dispersion*: an initial wave package consisting of several wavelengths, like natural sound, will be distorted while traversing the sample. Simply put, it will sound differently when emerging on the other side than it did when entering.

Note that the group velocity is constant (linear relation between ω and K) for small K . At the zone boundary, the velocity drops to zero, which corresponds to standing waves.

Question 8: Use Eq. (3.8) to estimate very roughly the temperature needed to excite a single phonon with angular frequency corresponding to this expression. Discuss the implications this result has regarding the importance of phonons at typical experimental temperatures. *Hint: Estimate the Coulomb force between two singly charged ions separated by typical inter-atomic distances in solids and compare this with the energy of a spring to find the force constant.*

Keep in mind that the phonon frequency ω is *not* temperature dependent, which is clearly seen from Eq. (3.8). There is still a dependence on temperature, in the sense that with higher temperature, *more* phonons are created, as mentioned already earlier.

3.5 Diatomic linear chain

Obviously the linear monatomic chain is an extreme oversimplification of real solids. It would be interesting to come somewhat closer to reality, as we expect the theory of phonons to contain more aspects than the most basic ones we are able to derive based upon the model of the previous section. However, to make a more realistic, three-dimensional model including interactions and so on is a huge step, which requires very elaborate calculations. Instead we try the next simplest thing, the diatomic infinite linear chain, in hope that some interesting physics will emerge.

In the lecture notes such a model is presented in some detail. For this exercise it was however chosen to work with a slightly different – and somewhat simpler – model. Therefore the derivations are not very complicated (but the important physics will come out the same), and they will be demonstrated below, without going too deep into details.

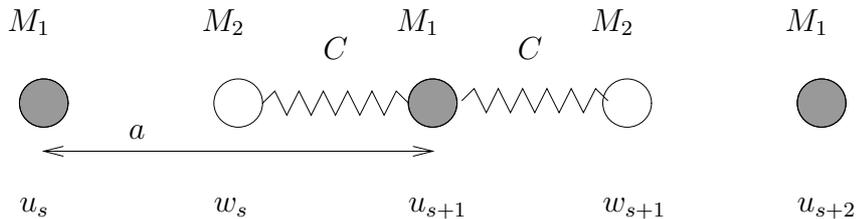


Figure 3: The infinite diatomic chain, with alternating masses but with the same force constant everywhere.

Our model is the same infinite linear chain of atoms, but we now replace every second atom with an atom of a different kind. We still keep the force constant between all atoms equal. This is obviously not very realistic, but neither is the model as such, and the results will still display the physical effects we are aiming to study. So we have the system as given by Fig. 3.

Again using the approximation of only nearest neighbor interactions and following the proceedings of the previous section, we obtain the potential energy

$$V = \frac{1}{2} \sum_s C (u_s - w_s)^2 + \frac{1}{2} \sum_s C (w_s - u_{s+1})^2, \quad (3.10)$$

using notation defined in Fig. 3 with u_s and w_s the time dependent position coordinates for the s -th atom of respective kind. Note that there is no term with $C(u_s - w_{s-1})^2$, as this would mean double counting the interactions.

Next we calculate the forces on the atoms using Newton's second equation:

$$\begin{aligned} M_1 \frac{\partial^2 u_s}{\partial t^2} &= -\frac{\partial V}{\partial u_s}, \\ M_2 \frac{\partial^2 w_s}{\partial t^2} &= -\frac{\partial V}{\partial w_s}. \end{aligned} \quad (3.11)$$

Inserting a similar Ansatz as Eq. (3.6), but with different constants u_0 and w_0 for the two subsystems of different masses, into Eq. (3.10) we end up, after canceling the common factor $e^{-i\omega t} e^{isKa}$, with the secular problem

$$\begin{aligned} M_1 \omega^2 u_0 &= C(u_0 - w_0) - C(w_0 e^{-iKa} - u_0) \\ M_2 \omega^2 w_0 &= -C(u_0 - w_0) + C(w_0 - u_0 e^{iKa}) \end{aligned} \quad (3.12)$$

for the frequency ω .

This is straightforward to solve (set the determinant equal zero and solve for ω), and the dispersion relation becomes

$$\omega^2 = \frac{C}{M_1 M_2} \left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos(Ka)} \right). \quad (3.13)$$

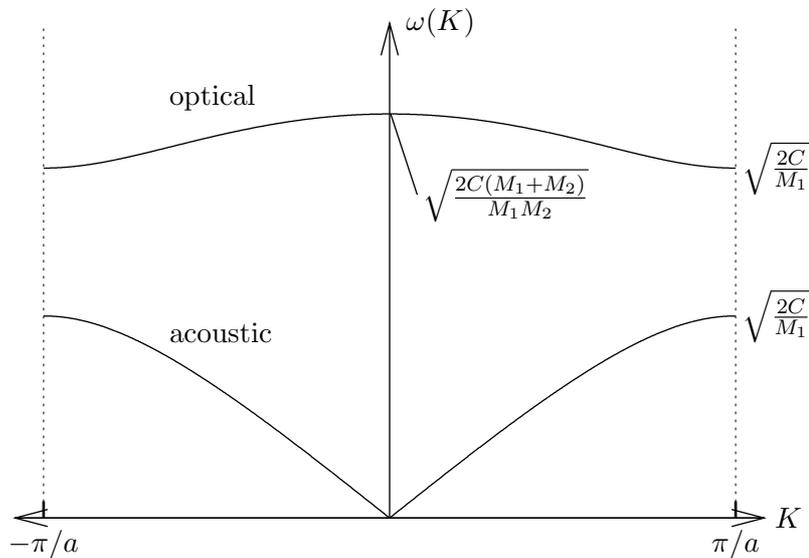


Figure 4: Dispersion relation of the infinite diatomic linear chain, with optical and acoustical branches.

This is plotted in Fig. 4. We note several important differences compared to the dispersion relation (3.8). First of all we should check that in the limiting case $M_1 = M_2$ we get back the results of the monatomic chain, which is left as an exercise.

Question 9: Show that Eq. (3.13) gives back Eq. (3.8) when $M_1 = M_2$.

The biggest difference from the monatomic case is that the dispersion now splits into two parts, known as the *optical* and *acoustic branches*. We will discuss this in more detail during the exercise. Also note that there is a *gap*, an interval of frequencies where it is impossible to create phonons.

Other limiting cases such as $M_1 \gg M_2$ and expansions of the dispersion relation near the zone boundary and near $K=0$ are very instructive and recommended as home exercises. It is further very interesting to calculate the eigenvectors of the secular problem and study the difference between the two branches, but we will discuss this – in a more illustrative way – as part of the exercise.

For more discussions on the physics of this and the monatomic dispersion curve, in particular dispersion relations for real materials in three dimensions, the ambitious student is referred to standard texts on solid state physics, such as the book by Ashcroft and Mermin.

4 Matrix representation

To solve the phonon problem described in the previous sections numerically, and to be able to introduce impurities into the chain, we use a finite representation, with N atoms, of the problem. By this, we are able to convert the equations of motion into a matrix eigenvalue problem.

Since we now use a finite set of atoms, we also need to specify *boundary conditions*. These may be either of two: periodic or fixed. If we use periodic boundary conditions, it means we assume that atom number $N + 1$ is identical to atom number 1. In practice, this means we actually put the atoms not in an infinite chain but on a ring. The consequences are nevertheless the same: we are able to produce traveling wave solutions.

Using fixed boundary conditions means we fix the first and last atom, so that they cannot move. This is analogous to taking a rope, and instead of making a ring, like with the periodic boundary condition, tying the ends to two walls. Obviously we cannot produce travelling waves in this case, but instead the eigenmodes will be standing waves.

To transform Eq. (3.5) into a matrix eigenvalue problem is straightforward, and gives

$$C \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 & -1 \\ -1 & 2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 & 0 \\ \vdots & & & & \ddots & & \vdots \\ 0 & 0 & 0 & 0 & \dots & 2 & -1 \\ -1 & 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix} = M\omega^2 \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix} \quad (4.1)$$

where we have assumed a harmonic time-dependence, i.e. the displacement of the s -th atom is $u_s(t) = u_s e^{-i\omega t}$. So when solving the matrix equation the eigenvector \mathbf{u} gives the displacements u_s at some initial time for a corresponding eigenvalue ω^2 .

To find the corresponding K vector, the program perform a discrete Fourier transformation, which gives the dispersion relation $\omega(K)$.

Note how the periodic boundary conditions are introduced, in the upper right and lower left corner, which makes the matrix wrap around itself. For fixed boundary conditions, we instead set the entire first and last rows and columns to zero.

Question 10: Using N sites with periodic boundary conditions, how many eigensolutions do we get? If we instead use fixed ends, how many do we then get?

With the finite representation, it is very simple to model the case of two atoms per basis, or introduce impurities in the chain. We may write the right-hand-side of (4.1) as

$$-\omega^2 \begin{pmatrix} M & 0 & 0 & \dots & 0 & 0 \\ 0 & M & 0 & \dots & 0 & 0 \\ 0 & 0 & M & \dots & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \dots & M & 0 \\ 0 & 0 & 0 & \dots & 0 & M \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix}, \quad (4.2)$$

and so by instead using a "mass matrix" of the type

$$\begin{pmatrix} M_1 & 0 & 0 & \dots & 0 & 0 \\ 0 & M_2 & 0 & \dots & 0 & 0 \\ 0 & 0 & M_1 & \dots & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \dots & M_1 & 0 \\ 0 & 0 & 0 & \dots & 0 & M_2 \end{pmatrix} \quad (4.3)$$

we have created a representation of the problem with two atoms in the basis. Similarly, for a monoatomic chain with an impurity with mass M' at position 3, we would use

$$\begin{pmatrix} M & 0 & 0 & \dots & 0 & 0 \\ 0 & M & 0 & \dots & 0 & 0 \\ 0 & 0 & M' & \dots & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \dots & M & 0 \\ 0 & 0 & 0 & \dots & 0 & M \end{pmatrix}. \quad (4.4)$$

This method allows for any combination of atoms of different masses to be constructed, and the corresponding eigensolutions to be found. During the exercise we will study the eigenmodes of both monoatomic and diatomic chains, with and without impurities.

For simplicity we still always use the same force constant between all atoms. This is of course not very realistic, but it makes it easier to discuss the results and compare with the theoretical expressions. In principal, however, once the problem is cast into the matrix representation, there is no longer any need to keep only nearest-neighbor interactions, the force constants can be allowed to vary freely, and any number of impurities with different masses can easily be accommodated. To interpret the results of such calculations then becomes an interesting but difficult task.

Question 11: During the exercise, we will introduce impurities in the ideal chain, atoms with different mass inserted into the chain. What may these impurities represent in real samples?

5 Exercises

This section contains a set of exercises to be performed during the computer exercise. Answers to the questions should be included in the report, along with your own reflections and conclusions, based on what transpires while completing the exercises.

To run the phonon code, we use the powerful mathematical program Matlab, which is an excellent program for numerical work in general and matrix manipulations in particular. During this exercise you will however not learn anything about Matlab, nor are you required to have any skills in programming or running that type of programs.

Start Matlab according to instructions from the supervisor. Within the program, change into the directory holding the phonon code; again check with the supervisor to verify the location of the files. Then, you just need to give the command which starts the phonon code, namely: phonon.

Once the graphical environment has started, play around with it for couple of minutes, and make sure you understand the role of each control. If you leave the mouse hanging over a button or slider, a help text will appear with additional information. Whenever the masses of "red" and "blue" atoms are equal, the program assumes we only have one type of atoms.

Note that the program uses dimensionless units, which is usually absolutely necessary in all numerical work in modern physics. This is because the magnitudes of the commonly appearing constants and units, for instance the electron charge and mass, not to mention Planck's constant, are so very small, that round-off errors soon become unacceptably large, due to the finite precision of the computer.

5.1 Monatomic chain with different boundary conditions

Using the default values already entered into the program (one type of atoms only, no impurity and periodic boundary conditions), compare the numerical results with the analytical dispersion law Eq. (3.8). The analytical curve is shown as a solid yellow line behind the matrix eigensolution, which are shown as red circles.

Exercise 1: Before changing N , try to guess how small you expect we can make N before the eigenvalues, due to the fact that we use not an infinite chain but a finite matrix representation of it, start to differ from the analytic curve? Then decrease N to the value you guessed and study the dispersion law. Explain why you get the result you do.

Using around 50 atoms, select mode number 48. Analytically, we know that the eigensolutions should be travelling waves, thus have a cosine shape. However, what we see looks like a *modulated* wave. That is because the yellow line which connects the points is *not* a representation of the analytical eigenmodes. Instead, the red circles show the displacements of each atom frozen at a certain moment in time. These are the elements in the eigenvector \mathbf{u} for a given ω -mode. The yellow line merely serves as a guide to the eye.

Exercise 2: Start the animation, and try to adjust the speed and range of atoms so that you can observe how a wave travels through the sample. The wave propagates as a contraction and elongation of the chain, and it is in fact this contraction, moving through the chain with a certain speed and frequency (the pattern keeps repeating over and over), that is the *phonon*!

Exercise 3: Change the boundary conditions to fixed ends, and observe in the animation and eigenmode plot how this freezes the end atoms. As discussed in the preparation questions, we expect only $N - 2$ modes now. Verify that this is indeed the case. All the remaining modes are changed compared with the periodic case, but especially two modes

are missing. Explain why these two particular modes vanish.

5.2 Impurity atom in a monatomic chain

Exercise 4: Start with periodic boundary conditions, and introduce an impurity atom. Carefully study and describe the effect on the dispersion relation depending on if the impurity is heavier or lighter than the other atoms.

Note how the *localized mode*, which you should have discovered, decays in space over a certain interval, i.e. the mode is localized. When looking at the localized mode, the program is somewhat misleading, and it is important to understand the underlying calculation.

The program solves the the eigenvalue equation, Eq. (4.1), with a mass tensor of the form in Eq. (4.4). For each ω^2 with a corresponding \mathbf{u} -vector, it performs a discrete Fourier transformation, but in case of an impurity in the chain the result is no longer a single plane wave, but instead a superposition of several plane waves, e^{ika} , i.e. a wave packet. The largest of these k -values is the one assigned to the mode in the dispersion relation. The analytic result shown in the dispersion relation is the result for no impurities in the chain.

The more localized the phonon is, the more k -values it contains. This is the same as Heisenberg's uncertainty relation in quantum mechanics: $\Delta x \Delta k \sim 1$. When $\Delta x = \infty$ as it is for a plane wave, we get $\Delta k = 0$, but now $\Delta x < \infty$, and so we must have $\Delta k > 0$.

In fact, it turns out that by Fourier decomposing the localized mode, we find that it contains only K within the first Brillouin zone. The more localized it becomes (the smaller the impurity mass M' is), the broader range of K will it contain, ultimately filling the entire interval from $-\pi/a$ to π/a . For $M' \approx M$, the localized mode contains wave vectors close to the zone boundary, which is consistent with the observation that as $M' \rightarrow M$, the localized mode converges into the continuous dispersion curve, at precisely $K = -\pi/a$.

What is the importance of such a localized mode? To answer this, let us consider a simplistic model for electric conductivity in a solid. By applying a voltage V to the ends of the solid, we create a constant electric field. $E = V/L$ inside the solid, where L is the length of the solid. Hence the electrons will be subjected to a constant force $F = -eE$, and thus be accelerated. If the voltage is strong enough, they may reach very high speeds. However, experiments show that the electrons travel at constant speed, and that this speed is very low.

From this we conclude that the electrons must be held back, braked, by some process, and it is natural to make an analogy with *diffusion*. The electrons bounce back and forth, but with a net drift velocity towards the positive terminal. So the electrons collide with something, change direction, are accelerated by the electric field, collide again, and so on. What possible objects of collision may be considered? It could be the positive ions in the lattice. However, when solving the electronic equations of motion, we assume a perfect periodic potential. Thus the ion lattice is already taken into account. It could be other electrons, but proper calculations show that electron-electron scattering is a very weak process, and cannot account for large effects like the one we are seeking.

Instead, the scattering objects are *impurities*, which may be represented for instance by dislocations (an ion slightly out of place), foreign atoms (such as dopants in semiconductors), and even different isotopes of the same atom; in short, anything which breaks the perfect periodicity of the lattice. Obviously, also phonons themselves will cause breaking of the symmetry, as the ions are vibrating instead of sitting still in a perfect lattice.

For a simple but clear picture of how impurities act as sources of scattering for electrons, we simply have to note the strong similarities between the theory of phonons above and the theory of Bloch electrons. In both cases, without impurities the solutions are travelling plane waves of infinite extension. The effect of an impurity is to create localized modes which act as scattering centers, since the localization forces the mode to abandon its sharp value of the crystal momentum $\hbar k$.

Due to energy and momentum conservation, an electron with a specified wave vector k can only scatter against electrons or phonons with certain wave vectors. This means that a localized mode, electronic or phonon, because it "contains" many different values of K , can scatter electrons with a wide range of wave vectors, making it a particularly efficient source of scattering.

Impurity scattering is in many cases, in particular at low temperatures where no phonons exist, the dominant scattering process. At higher temperatures, there is a growing contribution from phonon scattering, both "normal" and localized phonon modes.

Exercise 5: Switch to fixed ends boundary conditions. Again vary the impurity mass, and describe the differences in behavior to the periodic case.

Symmetries of all kinds are very often of great importance in all fields of physics. To see what symmetries we have in our present case, we shall see if there is any difference when using even or odd number of atoms, and if there is a difference between the two boundary conditions.

Exercise 6: Go back to periodic boundary conditions. By studying eigenmodes with K both positive and negative (but of the same magnitude), explain what symmetry you see. What important physical concept is behind this symmetry? Is there any difference in using an even or odd N ? *It is easiest to use rather small N , around 20, and look at modes with small $|K|$.*

Exercise 7: Switch to fixed ends boundary conditions. Do you see any symmetry in this case? If you put the impurity in the middle of the chain, is there now any symmetry? Explain this, and why there is a difference when using even or odd N .

5.3 Diatomic chain

Now we make a chain of two alternating kinds of atoms with different masses. We immediately see that the dispersion curve splits into two parts, known as the *optical* (upper) and *acoustical branches* (see Fig. 4).

Exercise 8: By studying the animated vibrations, explain the fundamental difference

between the two branches (select long wavelength modes to see the effects more clearly). From these results, can you find a possible explanation for the names "optical" and "acoustic" branches, and also why the optical branch has higher energy (larger ω)? *It is easiest to use $M_1 \approx M_2$ and study modes with fairly small K .*

6 References

Ibach, H., Lüth, H., *Solid State Physics*, Springer, 2003.

Ashcroft, N.W. and Mermin, N.D., *Solid State Physics*, Saunders College Publishing 1976