Quantum Analogs
Chapter 4
Student Manual

Modeling a
One Dimensional Solid

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4. Modeling a one-dimensional solid

There are two different ways to explain how a band structure in a periodic potential of a solid develops. One approach starts with a free moving electron in a constant potential that has a parabolic dispersion relation E(k). Introducing periodic scattering centers with small reflection probability results in the opening of band gaps. The other approach is to start from an atom with its discrete states. The next steps in this approach are the splitting of the eigenstates states in a two-atom molecule and further splitting in a chain with *n* atoms. With the acoustic analog, you can study both approaches experimentally. We will do this in the next two sections. In later sections, we will model the electronic structure in more complex solids with superstructures (Section 4.3) and defects (Section 4.4).

4.1 From a free electron to an electron in a periodic potential

To model a free electron in one dimension, we are using propagating sound in a tube. Since we cannot work with infinitely long tubes, we restrict ourselves to a finite tube with hard walls on both ends. This is actually the same setup we used in Chapter 1 to model the "particle in a box". Due to the finite length *L* of the tube we get resonances with the frequencies *f* :

$$f_n = n\frac{c}{2L} \qquad (4.1)$$

(*c* is the speed of sound and *n* is an integer number $n=1,2,...\infty$). The longer the tube, the denser the resonances become. In an infinitely long tube, the resonances would be infinitely dense. In solid-state physics, the so-called "density of states" is used in this context. Now let's do an experiment.

Equipment Required:

TeachSpin Quantum Analog System: Controller, V-Channel & Aluminum Cylinders, Irises
Two-Channel Oscilloscope
Two adapter cables (BNC - 3.5 mm plug)
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running

Setup:

First, set the *ATTENUATOR* knob on the Controller at 0.2 (out of 10) turns

Using the tube-pieces, make a tube with the end-piece containing the speaker on one end and the end-piece with the microphone on the other. Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Using the adapter cable, connect the output of the sound card to one arm of the splitter. With a BNC cable, convey the soundcard signal from the splitter to Channel 1 of your oscilloscope. Plug the lead from the speaker end of your experimental tube to *SPEAKER OUTPUT* on the controller. The sound card signal is now going to both the speaker and Channel 1.

Connect the microphone on your experimental tube to *MICROPHONE INPUT* on the controller. Put a BNC splitter on the controller connector labeled *AC-MONITOR*. From the splitter, use an adapter cable to send the microphone signal to the microphone input on the computer soundcard and a BNC cable to send the same signal to Channel 2 of the oscilloscope. Channel 2 will show the actual signal coming from the microphone.

The computer plots the instantaneous frequency generated by the sound card on the x-axis and the amplitude of the microphone input signal on the y-axis. Configure the computer so that "microphone" or "line-in" is chosen as the input

You will need to adjust the magnitude of both the speaker and microphone signals to keep the microphone input to the computer from saturating. (*It is the user's responsibility to ensure that the adapter cables are NOT used with signals greater than 5 Volts peak-to-peak*.)

Refer to the Appendix titled 'Recognizing and Correcting Saturation' for instructions.

Experiment:

Measure the resonances in tubes of different length and analyze the distance between the resonances $\Delta f = f_{n+1} - f_n$ as function of tube length. Convince yourself that the resonances become more and more dense with increasing tube length. (As you use longer tubes, you will to increase the *ATTENUATOR* setting in order to get good data.)

The quantum numbers used in solid-state physics are different from those used in atomic and molecular physics. In the measurements you have made, you will have noticed that there are equidistant resonances, which can be characterized by numbering them in the order of their frequency. From theory, we know that they belong to standing waves in the tube with wavelength

$$\lambda = \frac{2L}{n} \qquad (4.2)$$

The wavelength can also be expressed by another quantity called "wave number" k (in three dimensions it is the "wave-vector", $\vec{k}$).

$$k = \frac{2\pi}{\lambda} = n\frac{\pi}{L} \qquad (4.3)$$

In the case of infinitely dense eigenstates, it is not useful to number the states by an integer number. It is better to use the wave-number k (or wave-vector $\vec{k}$ in higher dimensions) to label the eigenstates. In atomic physics we have characterized the quantum mechanical system by energies $E(n,l,m)$ as function of integer quantum numbers, in solid-state physics the quantum mechanical system is characterized by the energy $E(k)$ as function of wave number. This relation is called "dispersion relation". We will do this analogously in the acoustic experiments.

In the tube with finite length, we have discrete eigenstates, so that it is easy to determine the wave number by the index n of the resonance using eqn. 4.3. This now allows us to measure the dispersion relation for a sound wave in an empty tube.

Experiment:

Measure the frequencies of the resonances in a tube of length L = 600 mm and plot the frequency as function of wave number k.

What do you notice?

What is analogous, what is different?

Sound waves show a linear dispersion with a slope proportional to sound velocity.

$$f(k) = \frac{c}{2\pi}k \qquad (4.4)$$

Electrons, however, have a parabolic dispersion

$$E(k) = \frac{\eta^2}{2m}k^2 . \qquad (4.5)$$

Modifications of this so called free-electron like dispersion are observed, when electrons have a wavelength that is comparable to twice the lattice constant, *a*, of the solid. In this case, the electrons are scattered effectively by the periodic lattice.

In the acoustic analog, we introduce periodic scattering centers separated by a distance, *a*, that is comparable to half the wavelength of sound. A typical wavelength, at reasonable frequency, (3.4 kHz) is λ = 10cm (≈4 inch). Therefore, we can model a lattice by periodic scattering centers at a separation distance of about *a* = 5cm (≈2 inch).

Experiment:

Take an overview spectrum (0-12 kHz) of a tube made from 12 tube-pieces each 5 cm long.

Now, insert 11 irises with an inner diameter of 16 mm between the pieces and measure a spectrum again.

What do you observe?

Due to the introduction of the periodic scattering sites, a band structure has developed. It shows bands and band-gaps. Because we have a tube with a finite length, the bands consist of discrete resonances. The band-gaps indicate frequency ranges in which no sound can propagate through the periodic structure.

Experiment:

Remove the end-piece with the microphone and put your ear in its place.

Choose a frequency within a band. Then choose a frequency within a band gap. Listen to the difference in loudness.

Now we want to study how the spectrum is influenced by a variety of parameters (Diameter of the irises *d*, number of pieces *j* and length of a tube-piece *a*).

Experiment:

Replace the end-piece and measure spectra with irises of 13 mm and 10 mm diameter.

Now we will measure spectra for a different number of unit cells. In solid-state physics, a "unit cell" is the part of space that is repeated periodically to build up the solid. In our case, it is the combination of a tube-piece and an iris. We have not put a 12th iris in front of the microphone, since the end-piece reflects the sound perfectly, anyway. You may convince yourself that the use of a 12th iris at one of the end-pieces makes no significant difference in the spectra. Small changes are due to the amount of air within the hole of the iris. For future experiments, you may decide for yourself whether to put an iris at an end-piece.

Experiment:

Put in the 16 mm irises again and measure spectra for different numbers of tube-piece / iris .

Describe the way the spectrum changes. Are there any mathematical patterns?

Now let's study how the spectrum depends on the length of a tube-piece *a*, which corresponds to the lattice constant in solid-state physics.

Experiment:

Take a spectrum with 8 pieces 50mm long and irises of 16mm diameter. Than replace the 50 mm long pieces by 75 mm long pieces. What difference in the spectra do you observe? Can you find a mathematical pattern?

Background information:

Band gaps open up when the "Bragg condition" is fulfilled. Probably you know the Bragg condition from x-ray and neutron scattering at crystals, which are both examples of wave reflection at a periodic lattice. The Bragg conditions is fulfilled, when

$$n\lambda = 2a \tag{4.6}$$

(*a* is the distance of reflecting planes). In our one-dimensional case the reflecting irises represent the reflecting planes of a solid. Reflection in the solid is so effective at this wavelength since the reflected waves from each plane add up constructively with perfectly fitting phase. This is the reason why waves cannot propagate easily at this wavelength.

A very convenient way to describe the scattering phenomena at periodic structures is to use the so-called "reciprocal space". The reciprocal space is the space of the wave vectors $\vec{k}$. In our one-dimensional case we have a one-dimensional reciprocal space with the wave-numbers k. If a wave is reflected at a periodic structure and the Bragg condition is fulfilled and the wave number $\vec{k}$ has changed to $\vec{k}'$, then the difference $\vec{k}' - \vec{k} = \vec{G}$ is called a "reciprocal lattice vector" $\vec{G}$. In our one-dimensional case the wave has been reflected and *k* has changed to *–k* with a *k* that fulfils the Bragg condition.

$$k = n\frac{\pi}{a} \tag{4.7}$$

In consequence, the reciprocal lattice vectors for the one-dimensional case are given by

$$G = n\frac{2\pi}{a} \tag{4.8}$$

with an integer number *n* that can be positive or negative or zero. In general, the reciprocal lattice vectors are forming a periodic lattice in the reciprocal space, which is called the "reciprocal lattice". In this reciprocal lattice you can define unit cells of the reciprocal space that are called "Brillouin zones". For the one-dimensional case the reciprocal lattice points and the Brillouin zones (BZ) are displayed in Fig. 4.1.

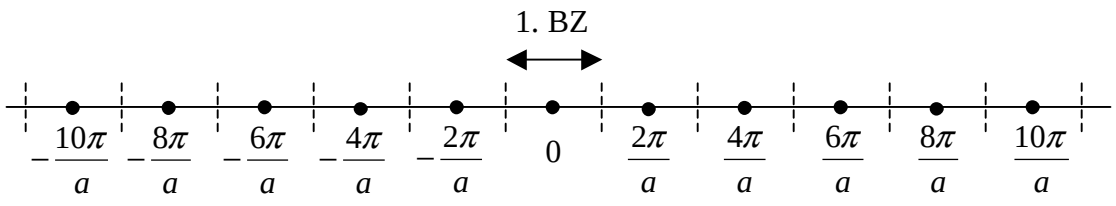

Fig. 4.1: Reciprocal lattice points (black dots), and Brillouin zones boundaries marked by dashed lines.

Due to the finite length of the tube we have discrete k-points in the reciprocal at which an eigenstate (resonance) is observed. They are given by eqn 4.3. If we compare the smallest reciprocal lattice vector

$$G = \frac{2\pi}{a} \tag{4.9}$$

with the distance of the discrete k-points in the tube of finite length L

$$k = \frac{\pi}{L} \tag{4.10}$$

we can see that there are $2L/a$ discrete k-points in each Brillouin zone. Since $L=j\cdot a$ we can conclude that the number of discrete k-points in a Brillouin zone is twice the number of unit cells. At k=0 and zero frequency (energy) there is no resonance (eigenstate) for a finite system.

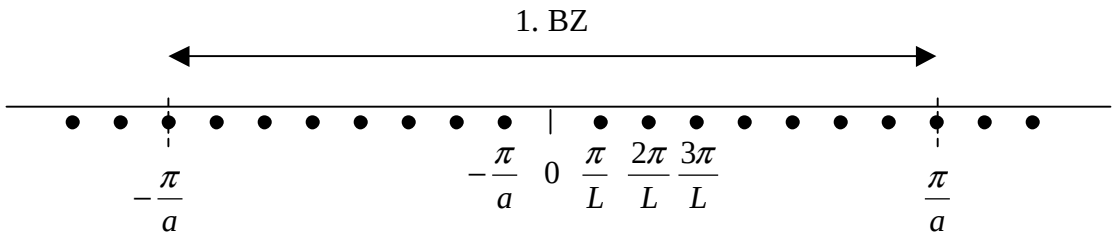

Fig. 4.2: Discrete k-points in reciprocal space (black dots), and first Brillouin zone marked by dashed lines. The example represents a setup with 8 unit cells.

Let us now explore the dispersion relation in reciprocal space.

Analyze the data:

Plot the frequency as function of wave number for resonances in a setup made from 8 pieces 50 mm long and 7 irises of 16 mm diameter.

Determine the wave number as given in eqn. 4.3.

Where, in reciprocal space, do the band gaps open up?

When counting the resonances, please note that the little peak at 370 Hz is **not** a resonance. It is a peak in the transmission function of the speaker/microphone combination.

Background Information

From Bloch's theorem, we know that wave functions in a periodic structure can be written as the product of a function $u_k(x)$ that has the periodicity of the lattice and exp(ikx) with the periodicity given by the wave number.

$$\psi(x) = u_k(x)e^{ikx} \tag{4.11}$$

A function of this form can be written in the form

$$\psi(x) = \sum_G C_{(k-G)}e^{i(k-G)x} . \tag{4.12}$$

From this form of notation, we see that the wave function cannot be assigned to a single point in the reciprocal space. The wave function is a sum with contributions from a single k-point in each Brillouin zone. All of these k-points are connected by reciprocal lattice vectors. In solid-state physics, therefore, the dispersion $E(k)$ is usually plotted only in the first Brillouin zone. This is called the "reduced zone scheme" in contrast to the "extended zone scheme".

Analyze the data:

Plot the dispersion relation $E(k)$ in the reduced zone scheme

Analyze the data:

Analyze the spectra for a setup made from 10 unit cells with 50 mm tubes and 16 mm irises and for a setup made from 12 unit cells with 50 mm tubes and 16 mm irises.

Plot the dispersion relation into the reduced zone scheme. Note that at higher frequencies, the first and the last resonance in a band cannot be identified easily.

You should keep in mind that each band has j resonances when it is build up from j unit cells. Only the first band has j-1 resonances because the lowest state of that band has zero frequency and is not visible. This is important when you determine the wave number from the resonance number n.

Analyze the data:

Analyze the spectra for a setup made from 8 unit cells with 75 mm tubes and 16 mm irises and compare it to a setup made from 8 unit cells with 50 mm tubes and 16 mm irises.

Plot the dispersion relation into the reduced zone scheme.

Analyze the data:

Analyze the spectra for a setup made from 8 unit cells with 50 mm tubes and 16 mm, 13mm and 10 mm irises, respectively.

Plot the dispersion relations into the reduced zone scheme.

How does the dispersion depend on the iris diameter?

In condensed matter physics, the density of states (DOS) is often discussed. If the dispersion relation is known in the complete Brillouin zone, the DOS can be calculated from these data. To illustrate how the DOS of a one-dimensional system looks, we will now analyse the data with respect to this quantity.

Analyze the data:

Let's take the spectrum for a setup made from 8 unit cells with 50 mm tubes and 16 mm irises and use it to determine the DOS. Since this is a system with a small number of unit cells, we cannot simply count the number of states within an energy interval. We will therefore calculate the density by one over the frequency distance between two states.

$$\rho(f) \approx \frac{1}{f_{i+1} - f_i} \qquad (4.12)$$

In a one-dimensional band structure, there are singularities in the density of states expected at the band edges (van Hove singularity), since the slope of the bands approaches zero at zone boundaries and symmetry planes. Due to the finite number of unit cells, the density of states is finite in our experiment, but a significant upturn of DOS at the band edges is clearly visible.

4.2 Atom – Molecule – Chain

In the previous section, we have seen how band-gaps develop in a free moving wave when periodic scattering sites are introduced. The other approach to solid-state physics starts with the eigenstates of a single atom. When two atoms are combined into a molecule, a splitting of the eigenstates into bonding and anti-bonding states is observed. Finally, bands develop from these levels, when many atoms are arranged into a chain. In theory, this approach is called the tight binding model. Now we want to study this approach experimentally starting with an atom, which we will model with a 50 mm long cylinder with the speaker on one end and the microphone on the other.

Experiment:

Take an overview spectrum (0-22 kHz) in a single 50 mm long tube-piece.

The peaks at 370 Hz, 2000 Hz and 4900 Hz are not resonances in the tube. They are due to the frequency response of the speaker and microphone combination, which is not frequency independent. Below 16 kHz there are 4 resonances in the 50 mm long cylinder, which can be described as standing waves with 1, 2, 3 and 4 node-planes perpendicular to the cylinder axis, respectively. At frequencies above 16 kHz, resonances are observed that have radial nodes (cylindrical node surfaces). The inner diameter of the tube, which is 25.4 mm (1 inch), determines the frequency of the first radial mode. In the following, we want to concentrate on the resonances below 16 kHz (longitudinal modes). For these states, the magnetic quantum number *m* is zero (σ-states).

Experiment:

Measure a spectrum in a longer tube-piece (75 mm). You will see that the resonances of the longitudinal modes shift down in energy, but the first radial mode stays above 16 kHz.

The next step is to model a molecule by combining two pieces of 50 mm long tube with an iris of 10 mm diameter (Ø10mm) between them. We are choosing to use the smallest iris because we want to model a weak coupling of the atoms.

Experiment:

Take a spectrum (0-12 kHz for example) in a combination of two 50 mm long tube-pieces with an iris Ø10 mm between them. What do you observe?

Note that the lowest bonding state has the frequency zero. The first antibonding state is observed at about 1100 Hz. For the other peaks the splitting in bonding / antibonding states is visible clearly. Remember that the small peaks at 370Hz and 2000Hz are due to the frequency response of speaker and microphone.

Experiment:

Repeat the experiment with Ø13 mm and Ø16 mm irises. What is different?

Experiment:

Take spectra with an increasing number of unit cells and observe how bands develop.

Analyze data

Compare the frequency difference between bonding and antibonding states with the width of the corresponding band in a setup with large number of unit cells.

4.3 Superstructures and unit cells with more than one atom

In this section, we will study the band structure of a periodic lattice that has a more complicated periodicity. A superstructure is a periodic perturbation of a periodic lattice. The periodic perturbation has a translation vector that is an integer multiple of the original lattice vector. This can be, for example, a modification of every second unit cell. A superstructure results in a new periodicity with a larger lattice vector, smaller Brillouin zone and a smaller reciprocal lattice vector. There are many fields in condensed matter physics where superstructures play an important role. For example, in surface science many surface structures show a superstructure with respect to the bulk lattice. Another well-known example for a superstructure in a bulk lattice is a Peierls distortion. We will study the effect on band structure by introducing a periodic perturbation into our one-dimensional lattice.

Experiment:

Make a setup of 12 tube-pieces 50 mm long and 13 mm irises and measure a spectrum. Then, replace every other iris by a 16 mm iris and measure the spectrum again. What do you observe? Plot the band structure for both cases.

Experiment:

Make a setup of 5 unit cells with each unit cell made of a 50 mm tube, a 16 mm iris, a 75 mm tube, and 16 mm iris. Measure a spectrum and plot the band structure.

Experiment:

We want to understand this band structure better by using the tight binding model and compare therefore the energy levels with the resonances found in the single “atoms”. Take spectra in a 50 mm tube and in a 75 mm tube. Compare the “atomic” levels with the band structure. What can you conclude? You may also compare to a spectrum measured in a single unit cell.

Experiment:

You may now build different superstructures by yourself and try to understand the change in band structure due to the new periodicity.

4.4 Defect states

In this section we will see how defects change the band structure. Defects destroy the periodicity of the lattice. They are localized perturbations. If the defect density is small, the band structure is more or less conserved and additional states are introduced due to the defects. The most important example for such defects states in condensed matter physics is certainly the doping of semiconductors. The introduction of defect-states creates the acceptor and donator levels that are responsible for the unique properties of these materials.

Experiment:

Make a setup of 12 tube-pieces 50 mm long and 16 mm irises and measure a spectrum.

Then, replace one tube-piece by a 75 mm long piece and measure the spectrum again. What do you observe?

Plot the band structure for both cases.

Note that the defect-state that is observed in the first band-gap has a localized wavefunction. Since it is localized, it cannot be assigned to a sharp wave-number. The state is therefore plotted as a horizontal line into the band structure in order to indicate that it has no well-defined wave-vector. You may have noticed that the peaks within the upper bands have shifted a little bit and no longer show the high regularity they did without defect. This is due to the fact that the lattice has lost its periodicity and, strictly speaking, it is no longer allowed to use the wave-number as a good quantum number. However, from the plot of the band structure you see that the defect does not change the band structure significantly. We can treat it as a small perturbation and use the reciprocal space with the Brillouin zone as we did in the periodic lattice.

Experiment:

Put the defect at other positions within the one-dimensional lattice and measure the spectra produced. Does the frequency of the defect-resonance depend on the position?

Experiment:

Use other tube lengths as a defect. You can try 25 mm, 37.5 mm and 62.5 mm for example.

In some cases you find the defect state close to a band edge. Such a situation is used in doped semiconductors. Donor-levels are defect states that are occupied by electrons and have a position just below the conduction band. The electrons can be excited easily into the conduction band and move there freely. This is very similar our case with a 62.5 mm tube as a defect. Acceptor-levels are unoccupied defect states just above the valence band. Electrons can be excited easily from the valence band into the defect states and the remaining holes in the valence band are responsible for the conductivity.

Further experiments:

You may build other setups with different types of defects. Be aware that, within a band gap, the propagation of a wave is suppressed strongly by reflection at the lattice. If the defects are too far from each other, or from speaker and microphone, they cannot be observed. You may try using shorter setups that have a small number of unit cells. In this case, it is easier to observe all defect-states with sufficient amplitude.