phonons in 1D

(based on chapters 9.1-9.3 &   of the book)

✓ **Expected prior knowledge**

Before the start of this lecture, you should be able to:

- Derive Newton's equations of motion for a triatomic chain (previous lecture).
- Write down the dispersion relation of phonon modes in the Debye model.
- Express complex exponentials through trigonometric functions and vice versa.
- Taylor expand trigonometric functions.
- Take derivatives of inverse trigonometric functions.

✏️ **Learning goals**

After this lecture you will be able to:

- Formulate the equations of motion for   phonon modes in 1D atomic chains.
- Derive the dispersion relation from the equations of motion.
- Derive the group velocity, effective mass, and density of states from the dispersion relation.

This lecture:

- Phonons   in chains of infinitely many atoms.
- Main idea: use *periodicity* in space, similar to periodicity in time

Equations of motion

Phonons
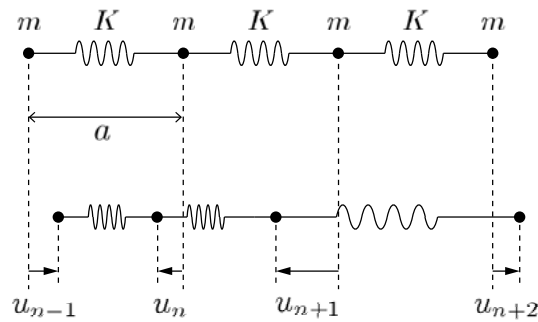
In the Debye model, we assumed that the dispersion relation is strictly linear in k. Now is the time to revisit this assumption. To do that, let us consider a 1D homogeneous chain of atoms. We assume that the atoms in the chain interact only with their nearest neighbors through a harmonic potential, like we derived in the previous lecture. In other words, we model the atoms as point masses connected by identical springs.

We denote the displacement of atom n from equilibrium by u_n. Within this convention, Newton's equation of motion for the n-th atom is given by:

$$m\ddot{u}_n = -\kappa(u_n - u_{n-1}) - \kappa(u_n - u_{n+1}).$$

We use the periodic boundary conditions just like we did in the Sommerfeld model. The boundary conditions imply that in a system of size $L = Na$, we have $u_N = u_0$.

$$u_n = Ae^{i\omega t - ikx_n},$$

Key idea for solving these equations

In order to solve the equations of motion, we need to come up with a reasonable guess. If we take a look at the equations of motion, we see that they are the same for all atoms. To be specific, the structure of the equations is the same no matter what value of n we choose. Since these equations define the solutions, we reason that the solutions should also be independent of the choice of n. As a result, we assume a plane wave solution, also called a *plane wave ansatz*, with the same amplitude for each atom. In the case of phonons, we obtain

$$u_n = Ae^{i\omega t - ikx_n},$$

We already know that the periodic boundary conditions only allow plane waves with k being a multiple of $2\pi/L$. In the case of the electron system, periodic boundary conditions give $\phi_0 = \phi_N$, which results in

$$1 = e^{ik0} = e^{ikNa}.$$

The above equation defines the allowed values of k:

$$k = \frac{2\pi p}{Na}, \quad \text{with} p \in \mathbb{Z}.$$

We use the quantized values of k in our plane wave ansatz: $e^{ikx_n} = e^{ip\frac{2\pi}{Na}na} = e^{i\frac{2\pi np}{N}}$. We notice something interesting if we investigate the case of $p \to p + N$. In this case, the plane wave ansatz becomes $e^{i\frac{2\pi n(p+N)}{N}} = e^{i\frac{2\pi np}{N} + i2\pi n} = e^{i\frac{2\pi np}{N}}$, which is exactly the same solution. Counting the number of inequivalent plane waves, we find exactly N different solutions in total. All that is left is to find the energy of each solution!

The reason why solutions with different values of k are identical is aliasing: because the plane wave is only defined at discrete positions, acquiring a phase factor of 2π between two atoms is equivalent to nothing happening:
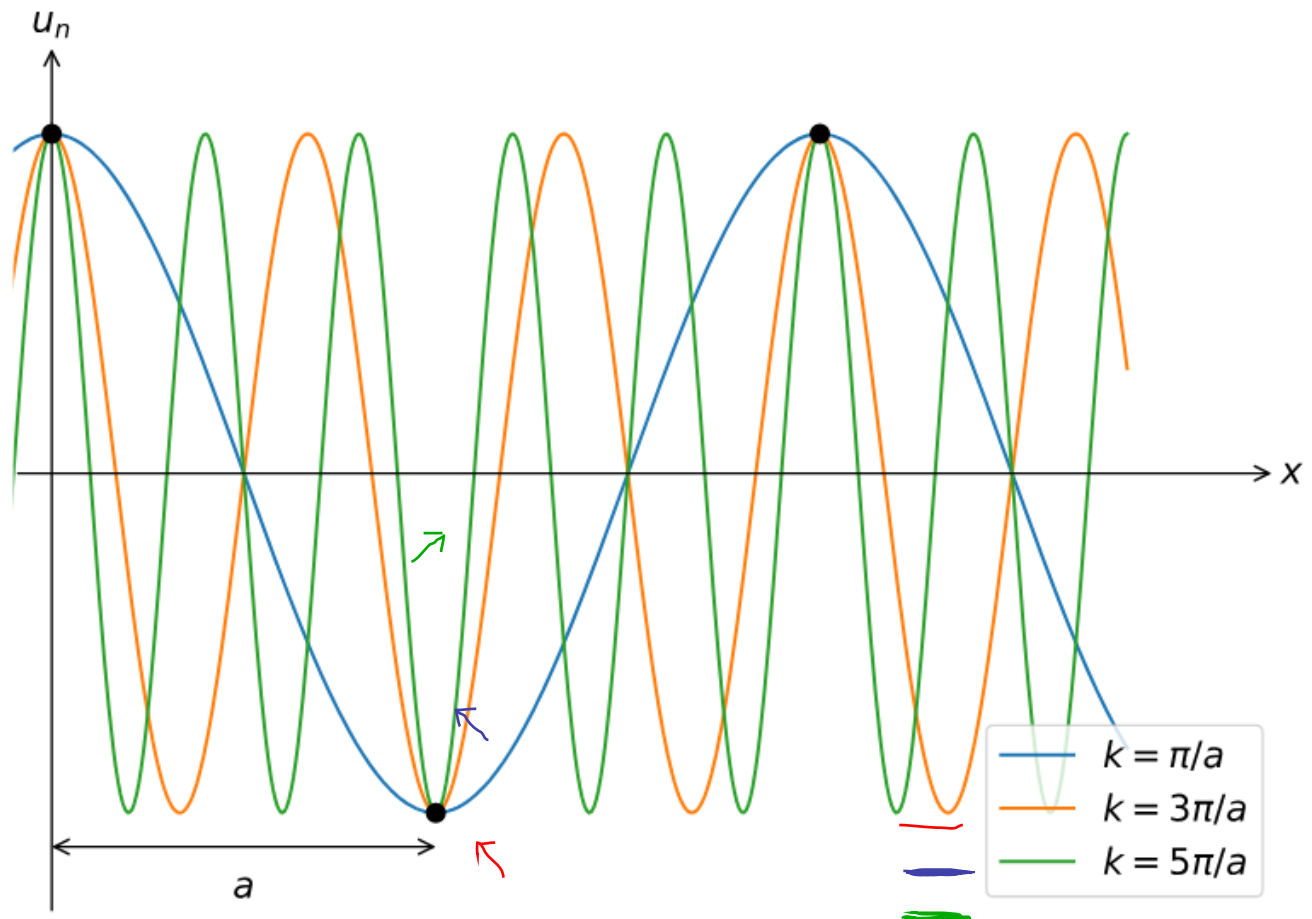
> **?** How many different solutions did we expect to find?   ⌄
>
> We have a system with N degrees of freedom (u_n), and therefore we expect N normal modes (or eigenstates).

Solving the equations of motion

Phonons

We substitute the plane-wave ansatz into the equations of motion:

$$-m\omega^2 A e^{i\omega t - ikx_n} = \kappa A e^{i\omega t}(-2e^{-ikx_n} + e^{-ikx_n + ika} + e^{-ikx_n - ika}).$$
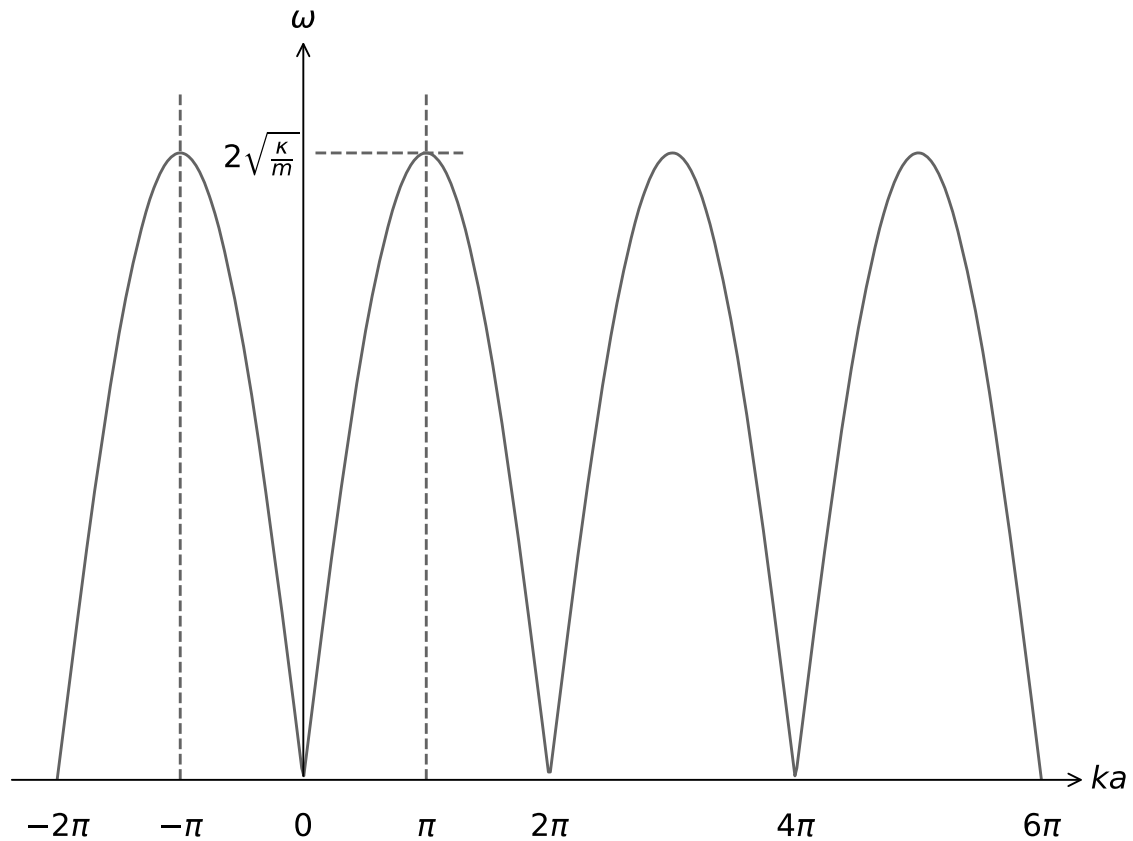
Searching for solutions with $A \neq 0$ we obtain

$$-m\omega^2 = \kappa(-2 + e^{ika} + e^{-ika}) = \kappa[-2 + 2\cos(ka)].$$

Or after a further simplification:

$$\omega = \sqrt{\frac{2\kappa}{m}}\sqrt{1-\cos(ka)} = 2\sqrt{\frac{\kappa}{m}}|\sin(ka/2)|,$$

where we substituted $1-\cos(x) = 2\sin^2(x/2)$.

We arrive at the phonon dispersion relation shown below.

The periodicity of the dispersion relation is a consequence of what we observed before: since plane waves with k-vectors differing by $2\pi/a$ are exactly the same, the repeated periods of the dispersion relation describe the same plane waves.

Comparison to the Debye model

Sound velocity: At small k, $\sin(ka/2) \approx ka/2$. Therefore $\omega \approx \sqrt{\kappa/m}ka = v_s k$, with v_s the sound velocity. We therefore justify the linear dispersion approximation in the Debye model!

Cut-off frequency: The Debye model introduces the cutoff frequency ω_D to limit the number of phonon modes, and does not identify the origin of the cutoff. Now because of the finite number of plane waves, the integration over the k-space has a finite size: $\sum_p \rightarrow \frac{L}{2\pi}\int_{-\pi/a}^{\pi/a}dk$. This automatically gives us a maximal frequency without additional assumptions.
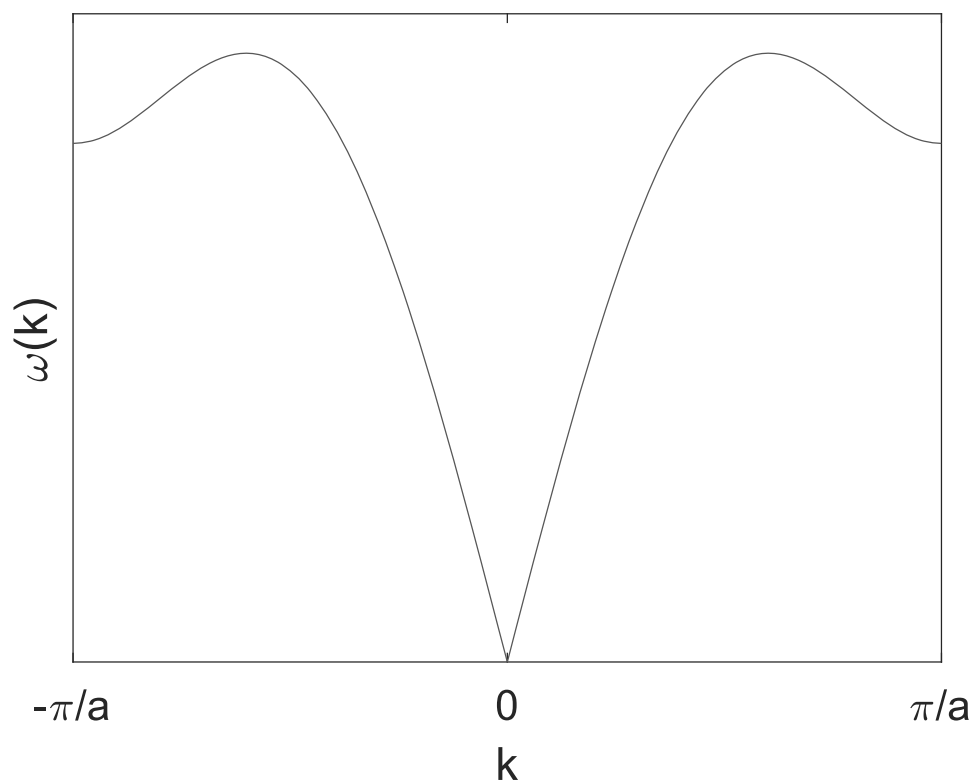
Exercises

Warm-up questions*

1. Sketch the density of states $g(\omega)$ associated with the 1D dispersion relation $\omega(k) = \omega_0 |\sin(ka/2)|$ of the phonon modes of a monatomic chain derived in this lecture. How does $g(\omega \approx 0)$ scale with ω? How does $g(\omega \approx \omega_0)$ scale with ω? Discuss the expected scalings.

Exercise 1*: Analyzing the dispersion of the vibrational modes of a monatomic chain

In the lecture, we derived the dispersion of the vibrational modes of a chain of identical atoms connected by identical springs. Here, we repeat this important derivation. Furthermore, we calculate group velocity and density of states. Finally, we study how to construct the density of states graphically, using a slightly more complex dispersion relation.

1. Write down the equation of motion describing the vibrations of a chain of atoms of mass m connected by spring constants κ. Formulate the Ansatz, and solve for the dispersion relation $\omega(k)$. Sketch the dispersion relation (same as warmup question 1).

2. From the dispersion relation, calculate the group velocity $v_g(k)$ and sketch it.

3. From the group velocity, calculate the density of states $g(\omega)$.

4. Formulate an approximate expression for $g(\omega)$ near the bottom of the energy band. Do the same for $g(\omega)$ near the top of the energy band.

5. In the next lecture, we will find that 1D atomic chains can also yield more complex dispersion relations, such as the $\omega(k)$ sketched in the picture below. For this $\omega(k)$, sketch the group velocity $v_g(k)$ and the density of states $g(\omega)$. How many states are there in this band? Describe in words how you would calculate the density of states, given this dispersion.

Exercise 3: The vibrational heat capacity of a 1D monatomic chain

In the Debye lecture, we formulated integral expressions for the energy stored in the vibrational modes of 1D, 2D, and 3D solids. This enabled us to calculate the phonon contribution to the heat capacity. In this exercise we follow a similar procedure, but now using the density of states of the vibrational modes of a 1D chain of identical atoms connected by identical springs derived in exercise 1.3. We compare the results to the 1D Debye model.

1. Write down an integral expression for the total thermal energy E stored in the vibrational modes of a solid at temperature T.

2. Formulate the integral expression for the heat capacity C.

3. Using the density of states derived in exercise 1.3, compute this heat capacity numerically, using e.g. Python.

4. Also calculate (numerically) the heat capacity that follows from the 1D Debye model. Compare the two and discuss potential differences.