

Lecture 3

The Hamiltonian analysis of lattice vibrations. Phononic Bandgap.

Program:

1. Lattice vibrations in 1D “diatomic” lattice:
2. The emergence of acoustic and optical modes
3. Lattice vibrations in a monoatomic 1D lattice: relevance to elastic properties

Questions you should be able to answer by the end of today’s lecture:

1. How is the spring constant related to the elastic moduli?
2. How is the elastic moduli measured in a material?
3. What is the difference between optical and acoustic modes of the dispersion relation and in what types of crystals do they emerge?

References:

1. Kittel, Chapter 4, page 99.
2. Ashcroft and Mermin, Chapter 22, page 422.

Connection with elasticity theory: Spring Constants and Young's Modulus.

How can we connect the atomistic view of oscillating bonds between atoms with elastic response of a material as a whole? What is the relationship between the Young's modulus and the bond strength?

The harmonic analysis described above assumed elastic energy that is proportional to the displacement squared:

$$V(u) = \frac{K}{2} u^2$$

The resulting restoring force (acting on the atoms in the lattice) is:

$$F = -\frac{dV(u)}{du} = -Ku$$

K represents the bond stiffness. In order to compress a solid of cross section A with N bonds within the cross section by the displacement u we need to apply a force:

$$F_{\text{applied}} = -F_{\text{restoring}} = N \cdot Ku$$

Then the force per unit area or **stress** is:

$$\sigma = \frac{F}{A} = \frac{N}{A} Ku$$

If the area occupied by a unit cell is on average a , where a is the equilibrium bond length, then:

$$\sigma = \frac{N}{Na^2} Ku = \frac{K}{a} \frac{u}{a} = E\varepsilon; \quad E = \frac{K}{a}, \quad \varepsilon = \frac{u}{a}$$

Here ε is the bond displacement per bond length or **strain** and E is Young's modulus or bond stiffness per bond length. This relates (in an oversimplified way) the spring constant (or bond stiffness) to the Elastic moduli E , which is the macroscopically measured quantity.

Bond type	S_0 (Nm ⁻¹)	E (GPa) (with $r_0 = 2.5 \times 10^{-10}$ m)
Covalent, e.g. C-C	50-180	200-1000
Metallic, e.g. Cu-Cu	15-75	60-300
Ionic, e.g. Na-Cl	8-24	32-96
H-bond, e.g. H ₂ O-H ₂ O	2-3	8-12
Van der Waals, e.g. Polymers	0.5-1	2-4

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How do we measure Young's modulus?

Remember in long wavelength ($ka \ll 1$) limit we found that group velocity (or velocity of sound)

$v_g = \sqrt{\frac{K}{m}} \cdot a$. This means if we measure velocity of sound we can find K and hence Young's

modulus E : $K = Ea \Rightarrow v_g = \sqrt{\frac{Ea^3}{m}} = \sqrt{\frac{E}{\rho}} \Rightarrow E = \rho v_g^2$

In real experiments: One typically attaches a piezoelectric crystal to one end and measures the time it takes the sound excitation to reach the other end.

**Longitudinal vibrations of a one-dimensional diatomic lattice.
(For example: cubic crystals with diatomic basis).**

Degrees of freedom:

When a crystal has two atoms or more per primitive basis, such as Rocksalt structure of NaCl (FCC with two atom basis), Diamond structure (FCC with two atom basis) of Si, Ge, diamond carbon or α -Sn each vibrational mode develops two branches known as acoustic and optical. In general, if there are N atoms in the primitive cell, there are 3N branches to the dispersion relations: 3 acoustical branches and 3N-3 optical branches.

In order to gain intuition about the nature of acoustic and optical vibrational modes, for simplicity, we will focus on 1D lattice to the one discussed above:

- I. The system:** Let's consider a 1D lattice of pairs of atoms connected by a bond of different strength than the bonds connecting the two-atom units to each other.

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II. The Hamiltonian

The energy for this system:

$$E = \sum_s \frac{mv_{1s}^2}{2} + \sum_s \frac{mv_{2s}^2}{2} + \sum_s \frac{K}{2} (x_{2s} - x_{1s} - a)^2 + \sum_s \frac{G}{2} (x_{1s+1} - x_{2s} - (a-d))^2$$

Similarly to our example from the last lecture, it is natural to consider the energy as a function of the displacements u_{1s} and u_{2s} rather than in terms of coordinates x_{1s} and x_{2s} .

Then the Hamiltonian for this lattice is:

$$H = \sum_s \frac{p_{1s}^2}{2m} + \sum_s \frac{p_{2s}^2}{2m} + \sum_s \frac{K}{2} (u_{2s} - u_{1s})^2 + \sum_s \frac{G}{2} (u_{1s+1} - u_{2s})^2$$

III. Equations of motion

Let's consider the part of the Hamiltonian that is dependent on all "s" components:

$$H_s = \frac{p_{1s}^2}{2m} + \frac{p_{2s}^2}{2m} + \frac{K}{2} (u_{2s} - u_{1s})^2 + \frac{G}{2} (u_{1s+1} - u_{2s})^2 + \frac{G}{2} (u_{1s} - u_{2s-1})^2$$

Then the Hamilton's Equations yield the following equations of motion:

$$\left\{ \begin{array}{l} \frac{du_{1s}}{dt} = \frac{\partial H_s}{\partial p_{1s}} = \frac{p_{1s}}{m} \\ \frac{du_{2s}}{dt} = \frac{\partial H_s}{\partial p_{2s}} = \frac{p_{2s}}{m} \\ \frac{dp_{1s}}{dt} = -\frac{\partial H_s}{\partial u_{1s}} = K(u_{2s} - u_{1s}) + G(u_{2s-1} - u_{1s}) \\ \frac{dp_{2s}}{dt} = -\frac{\partial H_s}{\partial u_{2s}} = K(u_{1s} - u_{2s}) + G(u_{1s+1} - u_{2s}) \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \frac{d^2 u_{1s}}{dt^2} = \frac{K}{m}(u_{2s} - u_{1s}) + \frac{G}{m}(u_{2s-1} - u_{1s}) \\ \frac{d^2 u_{2s}}{dt^2} = \frac{K}{m}(u_{1s} - u_{2s}) + \frac{G}{m}(u_{1s+1} - u_{2s}) \end{array} \right.$$

IV. Solutions

By analogy with the example from last lecture we look for solutions in the form:

$$u_{1s} = u_1 e^{iksa} e^{-i\omega t}, \quad u_{2s} = u_2 e^{iksa} e^{-i\omega t}$$

V. Dispersion relations

Substituting the solutions into the equations of motion, we obtain the following linear equations:

$$\left(\omega^2 - \frac{(K+G)}{m} \right) u_1 + \left(\frac{K}{m} + \frac{G}{m} e^{-ika} \right) u_2 = 0$$

$$\left(\frac{K}{m} + \frac{G}{m} e^{ika} \right) u_1 + \left(\omega^2 - \frac{(K+G)}{m} \right) u_2 = 0$$

This homogenous linear system of equations has a solution only if the determinant of the coefficient matrix is zero:

$$\begin{vmatrix} \left(\omega^2 - \frac{(K+G)}{m} \right) & \left(\frac{K}{m} + \frac{G}{m} e^{-ika} \right) \\ \left(\frac{K}{m} + \frac{G}{m} e^{ika} \right) & \left(\omega^2 - \frac{(K+G)}{m} \right) \end{vmatrix} = 0$$

From the determinant equation we get a quadratic equation with the following solutions:

$$\omega^2 = \frac{K+G}{m} \pm \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}$$

$$\frac{u_1}{u_2} = \mp \frac{K + G e^{-ika}}{\sqrt{K^2 + G^2 + 2KG \cos ka}} = \mp \frac{K + G e^{-ika}}{|K + G e^{-ika}|}$$

For each k there are two solutions, which are called the two branches of the dispersion curves.

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Let us examine the following limiting cases of the dispersion relations:

Case I: Long wavelength $ka \ll 1$

$$\text{Optical Branch: } \omega^2 = \frac{K+G}{m} + \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}, u_1 = -u_2$$

$$\text{Acoustic branch: } \omega^2 = \frac{K+G}{m} - \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}, u_1 = u_2$$

Using Taylor series expansion near $ka=0$, we obtain:

$$\omega^2 \cong 2 \left(\frac{K+G}{m} \right), u_1 = -u_2$$

$$\omega^2 \cong \frac{K+G}{m} - \frac{1}{m} \sqrt{K^2 + G^2 + 2KG - KGk^2 a^2} \cong \frac{K+G}{m} \left(1 - \sqrt{1 - \frac{KG}{(K+G)^2} k^2 a^2} \right) \cong \frac{KG}{2m(K+G)} k^2 a^2, u_1 = u_2$$

Figure removed due to copyright restrictions. Fig. 22.11: Ashcroft, Neil W., and N. David Mermin. *Solid State Physics*. Cengage, 1976.

Case II: Edges of the Brillouin zone $ka = \pi$

Optical Branch: $\omega^2 \left(k = \frac{\pi}{a} \right) = \frac{2K}{m}, u_1 = -u_2$

Acoustic Branch: $\omega^2 \left(k = \frac{\pi}{a} \right) = \frac{2G}{m}, u_1 = u_2$

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Case III: $K \gg G$

The bond between the atoms within the unit is much stronger than the bond between units.

Optical branch: $\omega^2 = \frac{K+G}{m} + \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}, u_1 = -u_2$

Acoustic branch: $\omega^2 = \frac{K+G}{m} - \frac{1}{m} \sqrt{K^2 + G^2 + 2KG \cos ka}, u_1 = u_2$

Optical branch: $\omega^2 \cong \frac{K}{m} + \frac{K}{m} = \frac{2K}{m}, u_1 = -u_2$

Acoustic branch:

$$\omega^2 \cong \frac{K+G}{m} - \frac{K+G}{m} \sqrt{1 - \frac{4KG}{(K+G)^2} \sin^2 \frac{ka}{2}} \cong \frac{K}{m} \cdot \frac{2KG}{K^2} \left| \sin^2 \frac{ka}{2} \right| \cong \frac{2G}{m} \left| \sin \frac{ka}{2} \right|, u_1 = u_2$$

The optical branch now has a frequency, which is k independent and is approximately equal to that of the frequency of vibration of a diatomic molecule. This leads to an additional insight into the physical interpretation of the optical branch and the distinction between it and the acoustic branch. Essentially, this branch is a band of frequencies, which results from the broadening associated with the coupling between the individual oscillators. The motion thus originates from the diatomic motion. In the acoustic mode the ions in a cell are moving in the same direction and thus the motion is essentially a collective motion.

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