University of Zurich[UZH]

Solid State Physics
Exercise Sheet 5
Phonons

HS19
Prof. Dr. Marta Gibert

Assistant: Gabriele De Luca

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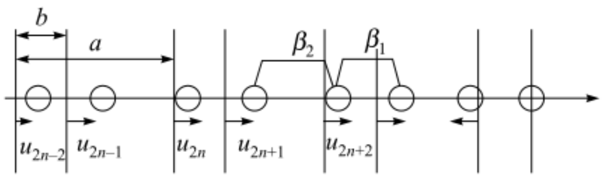
Exercise 1 *General phonon dispersion*

Consider a linear lattice with constant a having as a basis two identical atoms of mass m situated in a line and spaced at equilibrium by b ($b < a/2$). Consider only the nearest neighbors interactions (with spring constant β_1 and β_2 as shown in the figure. The u_is sketch the displacement from the equilibrium position).

1. Calculate the dispersion relation $\omega(k)$.
2. Determine the amplitude ratio between the different oscillation modes in the center of the Brillouin zone ($k = 0$). Make a sketch of the motion of the atoms in the linear chain.
3. Find the expression of the sound velocity and draw the dispersion curve assuming $\beta_1/\beta_2 = b/(a\text{-}b)$. Consider both the general and the limit cases ($b = a/2$ and $b << a$).



Exercise 2 *Second nearest neighbors interaction*

Consider a linear lattice with parameter a formed by identical atoms of mass m. Each atom is submitted to a force (spring) constant β_1 by nearest neighbors and to β_2 from its second nearest neighbors.

1. Find the equation of motion governing the displacement of atom n.
2. Calculate the dispersion relation $\omega(k)$ using a plane wave solution.
3. Find the expression of the sound velocity and the β_1-β_2 relation at which the dispersion curve peaks inside the first Brillouin zone.
4. Consider the hypothesis $\beta_2 > 0$ (second nearest neighbor attractive) and $\beta_2 < 0$ (second nearest neighbor repulsive) and discuss the possible scenarios.

Exercise 3 *Soft modes*

A linear chain consists of polarizable molecules which are separated by lattice spacing a. In this case the force constant is directly given by the electrostatic force. The molecules are fixed to their position, but they have an internal degree of freedom described by the equation of motion

$$\frac{\partial^2 p}{\partial t^2} = -\omega_0 p + E\alpha\omega_0^2 \tag{1}$$

where p is the electric dipole moment of the molecule (assumed to be parallel to the chain), E the local electric field due to all other molecules and α the polarizability.

1. Find the dispersion relation $\omega(k)$ for small polarization amplitude (small α).
   (Hint: the electric field at site n due to site m is $E_{nm} = \frac{2p_m}{d_{nm}^3}$ with $p_m = p_0 e^{ikam} e^{-i\omega t}$)
2. Discuss qualitatively the dependence of $\omega(0)$ on the polarizability α.

Questions

1. Given the crystallographic structure of NaCl, diamond, graphite and TiO_2, how many phonon dispersion branches do you expect, for each structure, in the first Brillouin zone?