# Modern Physics

Instructor: Prof. Bernd Pilawa (bernd.pilawa@kit.edu)

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Exercise 12

## § Solids §

## Problem 1: Phonons in a linear diatomic chain and the NaCl lattice

Consider a crystal of NaCl which has a fcc structure. In the [111] direction the perpendicular planes contain alternately only Cl ($M_1 = 35.5\,\mathrm{u}$) and Na atoms ($M_2 = 23.0\,\mathrm{u}$). Hence, the lattice vibrations can be modeled by a linear diatomic chain. Assume each plane interacts only with its nearest-neighbors and that the force constants are identical.

a) Write down the equations of motion for the $1D$- diatomic chain denoting $u_s$ and $v_s$ as the displacements of masses $M_1$ and $M_2$ in the unit cell $s$ and $D$ as the force constant.

b) Use the following wave functions:

$$\begin{aligned} u_s &= u e^{i(ksa-\omega t)} \\ v_s &= v e^{i(ksa-\omega t)} \end{aligned} \tag{1.1}$$

to derive a system of homogeneous linear equations in the amplitudes $u$ and $v$. $a$ is the separation between nearest identical planes.

c) The solutions are only non-trivial if the determinant of the coefficients of the system of equations vanishes. Solve the thus resulting equation for $\omega^2$ given by:

$$\omega^2 = D\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm D\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\left(\frac{ka}{2}\right)}. \tag{1.2}$$

d) Derive an expression for the ratio of the frequencies of the optical to the acoustical phonon branch at the edge of the Brillouin zone ($k = \frac{\pi}{a}$). Compare this ratio for NaCl with the ones derived from longitudinal and transversal dispersion curves each (edge of the Brillouin zone in the [111] direction) shown in phononkspace.

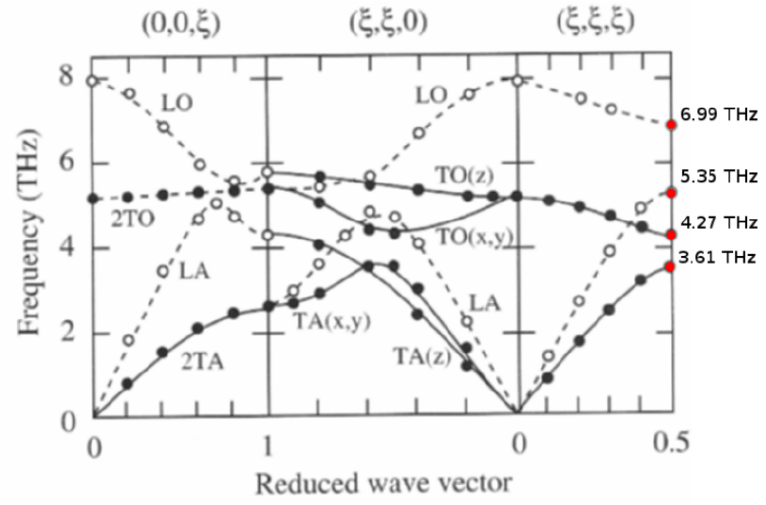


**Figure 1:** Optical and acoustic phonons

e) Calculate the average force constants for the longitudinal and the transversal branches from the same data points.

f) The maximum phonon frequency in the diagram is about 8 THz. What is the minimum energy required in neutron scattering experiments to allow excitation of all the shown phonon branches?

*Hint*: Compare with Kittel's 'Introduction to Solid State Physics' 8th ed., p.95 (Data from Phys. Rev. **178** 1496 (1969)).

## Problem 2: Binding Types

Crystalline solids can be categorized according to the bonds formed by their valence electrons. What binding types do you expect to form in the case of:

a) Chlorine?

b) Potassium?

c) Potassiumchloride?