

MODERN PHYSICS

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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 ($M_1 = 35.5 \text{ u}$) and Na atoms ($M_2 = 23.0 \text{ u}$). 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.

- 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.
- Use the following wave functions:

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

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

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

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

- 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 phononk-space.

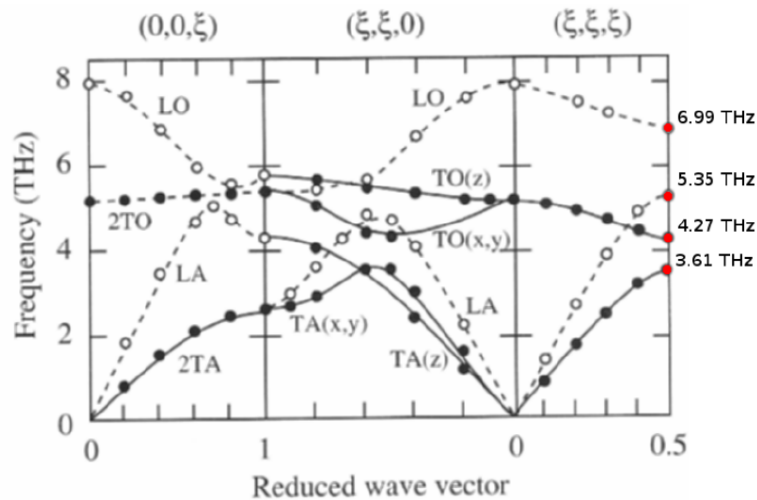


Figure 1: Optical and acoustic phonons

- 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?