HOMEWORK SET 06
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2024, room KNKTFA

1. [*2 points*] In one-dimensional chain of identical atoms separated by the distance a there are $N_{\rm modes}$ independent vibration modes calculated within the first Brillouin zone $N_{\rm modes} = \int_{-\pi/a}^{\pi/a} dq \left(\frac{L}{2\pi}\right) = \frac{L}{a} = N_{\rm atoms}$, meaning that we have one mode for each atom in the lattice. How many modes we will have in 3D lattice with one atom per unit cell?

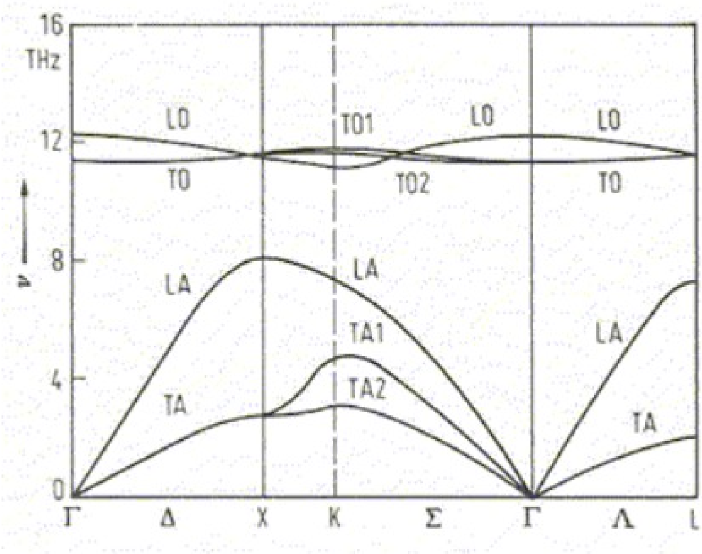
2. [*2 points*] Calculate density of states for the phonon modes as a function of the modes frequency ω for one-dimensional chain with one atom in the unit cell considering spring constants between nearest neighbors only as discussed on lecture.

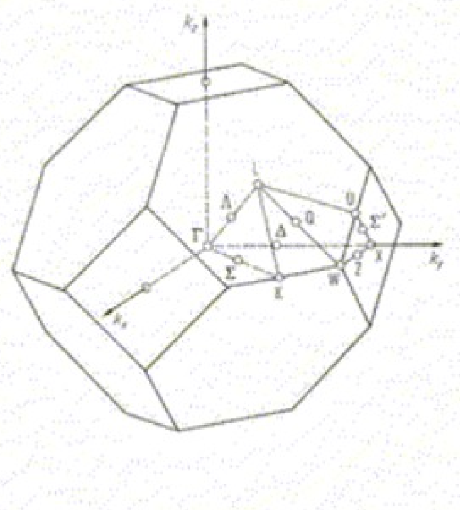
3. In long wave limit, where the wave-length $\ell \gg d$ (much larger then the lattice constant d) the $q = 2\pi/\ell \ll 2\pi/d$ and $qd \ll 1$ the q is small meaning close to the Brillouin zone center. Calculate the sound velocities $v = d\omega/dq$ for the acoustic modes in one-dimensional linear chain
   a) [*1 point*] with one atom in the basis
   b) [*2 points*] with two different atoms in the basis

4. [*1 point*] Sketch density of states for diatomic one-dimensional linear chain and identify the positions of van Hove singularities for both the acoustic and optical branches.

5. [*2 points*] Consider one-dimensional chain with one atom in unit cell. Show that when higher-order spring constants K_j acting between other then nearest neighbors can not be ignored, the dispersion relation reads $\omega(q)^2 = \frac{2}{M}\sum_{j=1}^{\infty} K_j(1-\cos(jqd))$.

6. Below is shown phonon dispersion for a fcc crystal along the high symmetry lines in the first Brillouin zone. Assume a lattice constant $a = 2$ Å
   a) [*1 extra point*] How many atoms are in the primitive unit cell of the crystal?
   b) [*2 extra points*] Estimate speed of sounds for the Δ, Σ and Λ directions.
   c) [*1 extra point*] What is the shortest phonon wavelength possible in this crystal?
   d) [*3 extra points*] Which of these phonon states would be more than 30% occupied at 300 K?





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