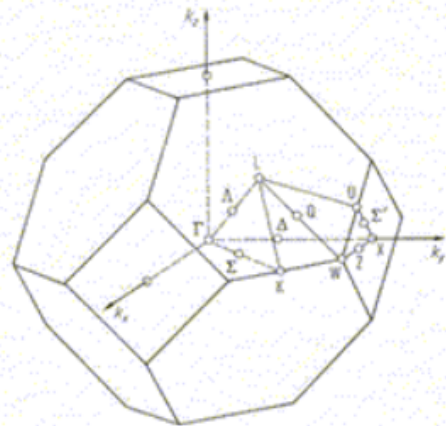
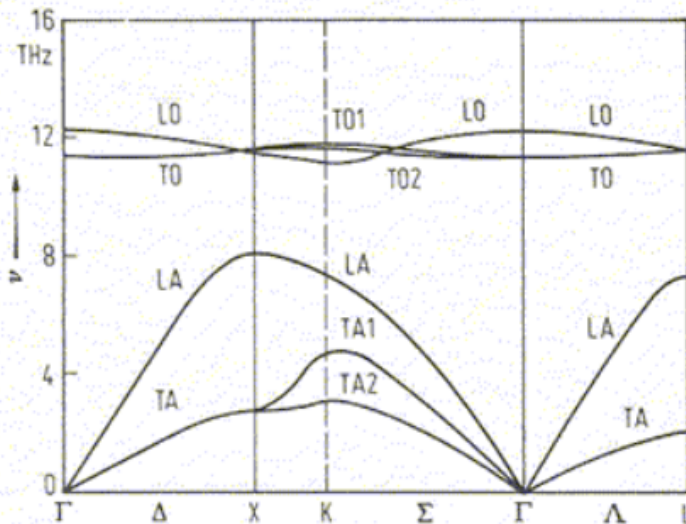


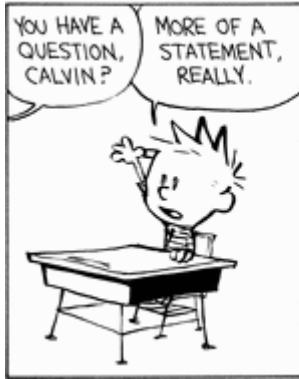
HOMEWORK SET 06
 Theory of Condensed Matter
 UFV/TKL1/99 lecture by Martin Gmitra
 Winter Semester 2021, room KNKTFA(Pa9-PKn)

- [2 points] In one-dimensional chain of identical atoms separated by the distance a there are N_{modes} independent vibration modes calculated within the first Brillouin zone

$$N_{\text{modes}} = \int_{-\pi/a}^{\pi/a} dq \left(\frac{L}{2\pi} \right) = \frac{L}{a} = N_{\text{atoms}}$$
 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 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 unit cell considering spring constants between nearest neighbors only as discussed on lecture.
- In long wave limit, where wave-length $\ell \gg d$ (much larger than 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 acoustic modes in one-dimensional linear chain
 - [1 point] with one atom in the basis
 - [2 points] with two different atoms in the basis
- [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.
- [2 points] Consider one-dimensional chain with one atom in unit cell. Show that when higher-order spring constants K_j acting between other than nearest neighbors can not be ignored, the dispersion relation reads $\omega(q)^2 = \frac{2}{M} \sum_{j=1}^{\infty} K_j (1 - \cos(jqd))$.
- Below is shown phonon dispersion for a fcc crystal along high symmetry lines in Brillouin zone. Assume a lattice constant $a = 2 \text{ \AA}$
 - [1 extra point] how many atoms are in the primitive unit cell of the crystal?
 - [2 extra points] estimate speed of sounds for the Δ , Σ and Λ directions.
 - [1 extra point] What is the shortest phonon wavelength possible in this crystal?
 - [3 extra points] Which of these phonon states would be more than 30% occupied at 300 K?



HOMEWORK SET 06
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2021, room KNKTFA(Pa9-PKn)



I JUST WANT TO SAY THAT EDUCATION IS OUR MOST IMPORTANT INVESTMENT IN THE FUTURE, AND IT'S SCANDALOUS HOW LITTLE OUR EDUCATORS ARE PAID!

