PHY 392K (551900) Solid State Physics I, spring 2020

Homework #4

Due March 31, 2020

Problem 1
Consider a 1D crystal with the lattice constant $\boldsymbol{a}$, and a two-atom basis $\boldsymbol{b_1}$=0, $\boldsymbol{b_2}$=a/3. Say I have a displacement pattern, in which the zeroth cell: $\boldsymbol{u}(0.1a;-0.05\boldsymbol{a})$, meaning that the first atom of the cell is shifted to the right by 0.1 $\boldsymbol{a}$ and the second atom is shifted to the left by 0.05$\boldsymbol{a}$. Can you tell me the distance between the second atom in the fourth cell to the right and the first atom in the fifth cell to the right, if the wave vector corresponding to this pattern is $\pi/\boldsymbol{a}$?

Problem 2
Consider a linear molecule made of four identical atoms of mass $\boldsymbol{m}$ connected by springs with a spring constant $\boldsymbol{\kappa}$. Assume the nearest neighbor interaction and determine the force constant matrix and vibrational frequencies. Treat this as a one dimensional problem.

Problem 3
You have just considered a linear molecule made of four identical atoms. Now make a closed loop out of the same four atoms (you need one more spring) and find the frequencies, still treating this as a linear molecule (1D). Now, define the unit cell with a single atom in it and treat the system using the periodic boundary conditions. Find the frequencies. Compare with the previous “molecular” solution and the open chain of problem 12, explain the differences between the three cases.

Problem 4
Consider an infinite one-dimensional monoatomic chain with atoms of mass $\boldsymbol{m}$ connected by springs with stiffness $\boldsymbol{k}$ and separated by distance $\boldsymbol{a}$. Calculate and sketch the dispersion and corresponding density of states of vibrational modes.

Problem 5
Consider a generalized one dimensional elastic chain with the set of spring constants for the first, second, etc. neighbors $\{\kappa_n\}$, find the sound velocity of this system.

Problem 6
Consider a one-dimensional infinite atomic chain with two atoms per unit cell, with equal masses $\boldsymbol{m}$, and two spring constants $\boldsymbol{\kappa}$ and $\boldsymbol{\gamma}$. Find the dynamical matrix and its eigenvalues. Find the eigenvectors at the Γ point and at the zone boundary.

Problem 7
Consider the same chain as in Problem 6, with atoms at $\boldsymbol{x_1}$ and $\boldsymbol{x_2}$. Construct a matrix $\boldsymbol{B}(\boldsymbol{G})$:

$$B(G) = \begin{pmatrix} e^{iGx_1} & 0 \\ 0 & e^{iGx_2} \end{pmatrix},$$

where $\boldsymbol{G}$ is a Reciprocal lattice vector. Using this matrix for a similarity transformation $B^{+}(\boldsymbol{G})D(\boldsymbol{k})B(\boldsymbol{G})$ of the dynamical matrix $D(\boldsymbol{k})$, show that the eigenvalues of the dynamical matrix are periodic in the reciprocal space.

Problem 8

This calculated phonon structure for NiAl appeared in Phys. Rev. B **68**, 214104 (2003). Ignore the numbers 1, 4, 5 15, 25, in the graph. Focus on either the solid or the dashed lines (not both) until the last items.

a) How many atoms are in the unit cell?
b) Label each branch: L or T, and O or A.
c) Estimate the speed of sound along the ΓX direction.