PHY 555: Solid-State Physics I

Homework #4

Due: 07/11/2025

Homework is due by the end of the due date specified above. ***Late homework will be subject to 3 points off per day past the deadline, please contact me if you anticipate an issue making the deadline.*** *It should be turned in via blackboard. For the conceptual and analytical parts, turn in a scan or picture of your answers (please ensure that they are legible) or an electronic copy if done with, e.g., LaTeX. For the computational part, turn in your source code and a short description of your results (including plots). The description can be separate (e.g., in LaTeX or word), or combined (e.g., in a jupyter notebook). Let me know if you are not sure about the format.*

Conceptual

1. ***(5 points)*** Explain the adiabatic Born-Oppenheimer approximation used in calculating nuclear dynamics.

2. ***(10 points)*** Assume you have a 1D lattice with 2 atoms per unit cell, one very massive (like for example Pb) and one very light (like H). Atoms can only move in 1D How many optical branches will you expect to have? How accurate is the use of the Born-Oppenheimer approximation in this system?

Analytical/Numerical

3. ***(20 points)*** The classic formula for the velocity of sound in a solid is $v_s = \sqrt{B/\rho}$ where B is the (isotropic or mean) bulk modulus and ρ is the atomic mass density.

   (**a**) Evaluate v_s for a free electron gas using the electron bulk modulus and density. Recall that the definition of bulk modulus is $B = -V\frac{dP}{dV}$. Hence you will need to compute the dependence of the Pressure (P) of the free electron gas with volume (V).

   (**b**) Are these sound waves the same as ordinary sound waves?

   (**c**) Evaluate this v_s for a gas of He-3 atoms, for neutrons, muons and protons, asuming in each case a concentration of n fermions/cm^3.

   (**d**) What is the K_F for each group of fermions above?

4. ***(20 points)*** Consider a graphene crystal. Ignore the degree of freedom along the direction perpendicular to the carbon atomic plane (i.e. this is an structuly 2D crystal).

   (**a**) How many acoustic phonon branches and optical phonon branches are there for this 2D crystal? Why?

   (**b**) Using the Debye model for the phonon density of states, obtain the temperature dependence of its phonon heat capacity at low T.

   (**c**) What is the minimum number of van Hove singularities for each optical phonon branch of such a 2D crystal? (see Cohen and Louie Section 4.5)

Computational

(**d**) ***(40 points)*** Consider the lattice described in Problem 2. Compute the phonon band structure and plot it in the first Brilloin zone. Assume that the lattice constant of the unit cell is a=7 Å. also assume that the atoms alternate in the lattice and their spring constant is $K = 10 \times 10^2 N/m$.

i. Write a program that plots the energy dispersion $\omega(q)$ in the first Brillouin zone given inputs a, K, m, M

ii. For inputs: a=7 Å, $b = 0.01$ Bohr, $K = 10 \times 10^2 N/m$, Plot the dispersion (energy versus k in the first Brillouin Zone). Use the masses of Pb (82 uma) and H (1 uma). Make sure all the units are consistent.

iii. The density of states (DOS) gives the number of states at a given energy (summed over q), i.e.,

$$D(E) = \sum_{m,q} \delta(\omega - \omega_{m,q}) \tag{1}$$

A common approach to plot the DOS is to smear the delta function into a Gaussian with a finite width. Plot the DOS for using this approach.

iv. Replace Pb by Oxygen. What are the most relevant changes to the phonon band structure?