Solid State Physics

Homework 2: Phonons

5% of final grade, divided into 50 pts

Key concepts: dispersion, displacement waves, vibrational modes vs phonons, Bose-Einstein distribution, density of states, heat capacity, group velocity. This homework will involve more Mathematica (or other program, your call) than prior assignments.

1. **1D Atomic Chains. (15 pts)**

   (a) Double check that you can get Mathematica/MatLab to be well-behaved: Begin with a monoatomic 1D chain of atoms with mass M_1 and spring constant C. Calculate and plot the dispersion relation $w(\vec{q})$ for the acoustic and optical branches.

   (b) In class, we briefly considered the dispersion for a diatomic chain of alternating atoms of mass M_1 and M_2 with spring constant C. Now calculate and plot the dispersion relations $w(\vec{q})$ for the acoustic and optical branches.

   (c) What is the ratio of u_o/v_o for the maximum frequency optical mode? See Eq 4.25 for some guidance in Kittel version 8. What is the physical interpretation of this result?

   (d) What happens to the gap between acoustic and optical modes as the mass ratio diverges away from or converges to 1? Plot and comment on the results.

   (e) Plot the group velocity (v_g vs ω) and DOS ($D(\omega)$ vs ω). Careful that your program doesn't explode. Does your result make sense?

   (f) Solve the dispersion for a three atom basis with M_1, M_2 M_2 with spring constant $C_{1,2}$, $C_{2,3}$, $C_{3,1}$ and plot the dispersion. What is the physical interpretation of this result? If all masses become the same but the spring constants remain different, what happens?

   Hints: (a) Please don't try to do this entirely by hand. (b) Before trying to plot a function, make sure that it has a real value. Mathematica will plot nothing if one of your values is complex. (c) Mathematica may not set the y-axis range correctly, PlotRange will help here.

2. **Square Lattice. (10 pts)**

   Let's consider the vibrations of a planar square lattice with a basis of atom X at (0, 0).
   Let $u_{l,m}$ denote the displacement magnitude of an atom at lattice point l, m **normal** to the plane of the lattice. The mass of each atom is m and C is the force constant for nearest neighbor interactions. Assume that the equation of motion can be approximated for small displacements as:
   $m(d^2u_{l,m}/dt^2) = C[(u_{l+1,m} + u_{l-1,m} - 2u_{l,m}) + (u_{l,m+1} + u_{l,m-1} - 2u_{l,m})$

   (a) Assume solutions of the form: $u_{l,m} = u_o e^{i(lq_x a + mq_y a - wt)}$ where a is the magnitude of the lattice vectors. Determine an expression for $\omega(q_x, q_y)$.

   (b) Use Mathematica to plot $\omega(q_x, q_y)$ using the Plot3D function with q_x and q_y ranges: -π/a to π/a. (or whatever the MatLab equivalent is)

   (c) We don't normally visualize these plots in 3D, instead we look at sections through them. Sketch by hand a single diagram of *omega* vs q from Γ to X ($\vec{g}_1/2$) to Y ($\vec{g}_2/2$) and back to Γ.

3. **Real Phonon Dispersions. (10 pts)**

   (a) How many vibrational modes do the 1D (1, 2, and 3 atom basis) and 2D solid (1 atom basis) considered above have? Assume the interatomic distance d is the same between each pair of atoms and solid has length L in every relevant direction. At 0K, how many phonons are in the system?

(b) Plot the phonon occupation for each mode as a function of frequency at 3K, 30K, 300K and 3000K. Use a log axis for the occupation, linear for the frequency. Let the maximum frequencies be 10 and 5 THz for the longitudinal and transverse branches, respectively. This is not the time to ignore units.

(c) Plot the vibrational amplitude and vibrational energy density as a function of frequency for the above temperatures for the longitudinal and transverse modes. Assume physically reasonable values as needed.

(d) Why are there three branches of the phonon dispersion for fcc Cu and Al (Figure **??**?

(e) Compare and contrast the dispersions for Cu and Al.

(f) Compare and contrast the dispersions for Si and Ge (Figure **??**).

(g) Why does the dispersion Si have 6 branches and Mg_2SiO_4 have so many more?

4. **Low temperature phonon transport (15 pts)**
Late one night in the lab, you're running measurements on single crystals of diamond and PbO at low temperature (5 K). You get some peculiar results and ultimately conclude that the thermal conductivity of diamond at these temperatures has to be **lower** than that of PbO! Thinking that it might be an electronic effect, you measure the electrical conductivity and find both samples are electrically insulating. So much for that theory. Now it's getting really late and you decide to email your advisor your results and call it a night. The next morning, you crawl out of bed and find an angry email from your advisor saying your results is ridiculous and if you don't shape up, you'll be out of a job. After a tense hour of coding, you realize that your advisor is a jerk and in fact, it's all simple phonon physics. Draft a letter to your advisor that highlights your argument and quantitatively shows that he owes you a beer.

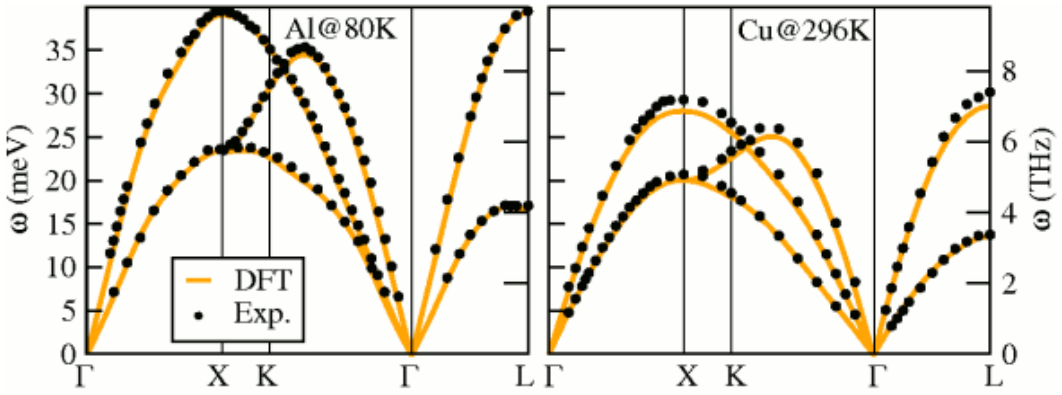

Figure 1: Phonon dispersions for Al and Cu.

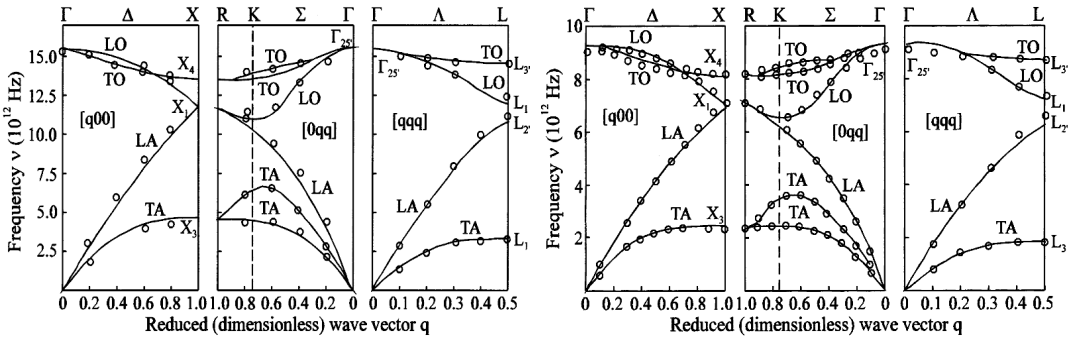

Figure 2: Phonon dispersions for Si (left) and Ge (right).

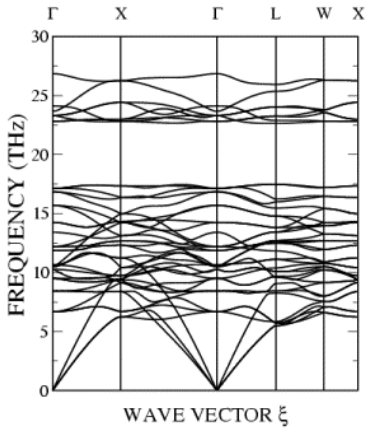

Figure 3: Phonon dispersion for Mg_2SiO_4.