

Physics 481: Solid State Physics - Homework 6

due date: Thursday, Feb 28, 2008

Problem 1: Phonons in a one-dimensional Lennard-Jones crystal (20 points)

Consider N identical atoms of mass M whose motion is restricted to the x -axis. Nearest neighbor atoms are coupled by a Lennard-Jones potential

$$V(x) = -4\epsilon \left[\left(\frac{\sigma}{x} \right)^6 - \left(\frac{\sigma}{x} \right)^{12} \right]$$

where x is the distance between them (assume periodic boundary conditions).

- Find the equilibrium distance between atoms at zero temperature and the cohesive energy.
- Study small lattice vibrations in this system. To this end, first expand the potential about its minimum. To what order do you have to go?
- Using this expansion, calculate the dispersion (frequency-wavenumber) relation of the phonons. How many branches are there?
- Calculate the speed of sound in terms of the potential parameters ϵ , σ , and M .

Problem 2: Phonon dispersion with alternating spring (Marder problem 13.1, 20 points)

Consider a one-dimensional chain of identical atoms. The springs between them alternate in strength between values K_1 and K_2 .

- Find the vibrational frequencies as a function of wave number q . Study the low q limit and find the sound velocity.
- Discuss the physical meaning of the two branches. Sketch the way the atoms move in both cases!
- Discuss the dispersion and the normal modes for $K_1 \gg K_2$.
- Discuss the limit $K_1 \approx K_2$ and compare with the homogeneous chain where all springs are identical (see class).