Physics 481: Condensed Matter Physics - Homework 6

---

due date: Thursday, Feb 25, 2011

Problem 1: Model of a nobel gas crystal (20 points)

A simple model of a noble gas crystal consists of a f.c.c. lattice with a Lennard-Jones interaction

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

between the nearest neighbors in the lattice only. Here, r is the nearest neighbor distance, and the parameters are $\epsilon = 0.0104$ eV, $\sigma = 3.40$ Å for argon.

a) How many nearest neighbors does each site have on a f.c.c. lattice? What is the nearest-neighbor distance in terms of the lattice constant a of the conventional cubic unit cell?

b) Find the total cohesive energy $\mathcal{E}$ for a large crystal of N argon atoms (neglecting surface effects) and the lattice constant a of the cubic unit cell. Compare with the experimental values $a \approx 5.3$ Å and $\mathcal{E}/N \approx -0.08$ eV/atom.

c) The crystal is compressed by isotropic pressure. Calculate the work necessary to reduce the lattice constant from a to $a(1-\delta)$ with $\delta \ll 1$.

d) Using the thermodynamic relation $dW = -pdV$, determine how much the lattice constant of the argon crystal changes in 100 atm of pressure (1 atm $=10^5$ N/m^2).

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.

a) Find the vibrational frequencies as a function of wave number q. Study the low q limit and find the sound velocity.

b) Discuss the physical meaning of the two branches. Sketch the way the atoms move in both cases!

c) Discuss the dispersion and the normal modes for $K_1 \gg K_2$.

d) Discuss the limit $K_1 \approx K_2$ and compare with the homogeneous chain where all springs are identical (see class).