Physics 481: Condensed Matter Physics - Midsemester test

Friday, March 4, 2011

Problem 1: Structure determination (70 points)

Debye-Scherrer X-ray diffraction is used to study a powder specimen of a monoatomic substance that is known to crystallize in a cubic Bravais lattice structure with primitive vectors $\vec{a}_1 = (a, 0, 0)$, $\vec{a}_2 = (0, a, 0)$ and $\vec{a}_3 = (0, 0, a)$. The wavelength of the X-rays is 1.4 Å.

a) Find the primitive vectors of the reciprocal lattice. (15 points)

b) Find the four shortest possible lengths of reciprocal vectors. (20 points)

c) The first diffraction ring is at an angle of $\vartheta = 17.9°$ from the incident direction. Determine the lattice constant a. (20 points)

d) Find the angles of the next three diffraction rings. (15 points)

Problem 2: One-dimensional Morse solid (80 points points)

Consider N identical atoms of mass M whose motion is restricted to the x-axis. Nearest neighbor atoms are coupled by the so-called Morse potential

$$V_M(r) = D\left(1 - e^{-\alpha(r-r_0)}\right)^2 - D$$

where r is the distance between them and D, α, and r_0 are positive constants.

a) Calculate $V_M(0)$, $V_M(\infty)$ and qualitatively sketch the Morse potential. (10 points)

b) Find the equilibrium distance between the atoms at zero temperature and the cohesive energy. (10 points)

c) Determine the harmonic approximation to the total potential energy $V = \sum_j V_M(x_{j+1} - x_j)$ by expanding to quadratic order in the displacements u_j from the rest positions. (15 points)

d) Write down the classical equations of motion for the displacements in harmonic approximation. (15 points)

e) Calculate the dispersion (frequency-wavenumber) relation of the phonons, assuming periodic boundary conditions. (20 points)

f) Calculate the speed of sound in terms of the potential parameters D, α, r_0 as well as the mass M. (10 points)

Problem 3: Phonons of a square lattice (50 points)

Consider a two-dimensional solid of identical atoms of mass M on a square lattice of lattice constant a. In this problem, we investigate vibrations perpendicular to the lattice plane. The equations of motion for the displacements $u_{j,l}$ read

$$M\ddot{u}_{j,l} = K(u_{j+1,l} - u_{j,l}) + K(u_{j-1,l} - u_{j,l}) + K(u_{j,l+1} - u_{j,l}) + K(u_{j,l-1} - u_{j,l})$$

Here, j and l index the atom position in the x and y directions, respectively.

a) Determine the dispersion relation (ω as a function of $\vec{q}$) of the phonons for a wave with a wave vector $\vec{q} = (q_x, q_y)$. (30 points)

b) Calculate the speed of sound in terms of K and M. Does it depend on the direction of $\vec{q}$? (20 points).

BONUS: The chain of problem 2 is stretched by a small external tension force T. Calculate the change in length ΔL. (15 BONUS points)