Physics 481: Condensed Matter Physics - Test prep Homework 7

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due date: Friday, March 5, 2011

Problem 1: Tetragonal lattice (15 points)

A hypothetical monoatomic substance crystallizes in a centered tetragonal structure. The conventional unit cell can described by primitive vectors $(a, 0, 0), (0, a, 0), (0, 0, c)$ with $c = 3a/2$ and a basis consisting of two atoms at positions $(0, 0, 0)$ and $(a/2, a/2, c/2)$. The lattice constant is $a = 4.2\,\text{Å}$.

a) Calculate the maximum space filling for this lattice.

b) Find the primitive vectors of the reciprocal lattice.

c) A powder specimen of the substance is analyzed by X-ray diffraction using the Debye-Scherrer method. The wavelength of the X-rays is 1.5 Å. Calculate the angles of the first four diffraction rings.

Problem 2: Phonon dispersion in a chain with long-range interactions (Ashcroft-Mermin 22.1 , 15 points)

Consider a one-dimensional chain of identical atoms of mass M. The springs are not only between nearest neighbors but between all pairs of atoms. Thus, the elastic energy reads

$$E_{el} = \frac{1}{2} \sum_n \sum_{m>0} K_m (u_n - u_{n+m})^2$$

where u_n is the displacement of atom n.

a) Find the dispersion relation, i.e., the vibrational frequency ω as a function of wave number q.

b) Assume $K_m = K_0/m^p$ with $p > 1$ a parameter controlling how rapidly the interaction drops of with distance. Study the long-wavelength limit of the dispersion relation for $p > 3$. Determine the sound velocity.

c) Investigate the long-wavelength limit of the dispersion relation for $1 < p < 3$. Show that one gets anomalous sound, i.e., the frequency is not proportional to the wavenumber. (Hint: You may want to approximate the m-sum by an integral.)

Problem 3: Ionic crystals (10 points)

Consider a material consisting of two types of ions with charges +e and −e, respectively. In addition to the Coulomb interaction, they have a short-range repulsive potential of the type A/r^{12}.

a) Assume the substance crystalizes in the NaCl structure. Find the lattice constant by minimizing the cohesive energy. The Madelung constant for the NaCl structure is $\alpha = 1.7476$. (You can restrict the repulsive interaction to the nearest neighbor sites on the lattice.)

b) Do the same for the CsCl structure with a Madelung constant of $\alpha = 1.7627$.

c) Which structure will the material choose?