Physics 481: Condensed Matter Physics - Homework 2

due date: Friday, Jan 28, 2011

Problem 1: Packing fractions in two and three dimensions (20 points)

To find the degree of space filling for a given lattice, first find the distance $d_{\min}$ between nearest neighbors. Then put circles (in two dimensions) or spheres (in three dimensions) of diameter $d_{\min}$ on each lattice site, and ask what portion of space is occupied by the circles or spheres. This number is the *packing fraction*.

a) Calculate the packing fractions for the square and hexagonal lattices in two dimensions.

b) Calculate the packing fractions for the following three-dimensional lattices: simple cubic, body-centered cubic, face-centered cubic, hexagonal close-packed, and diamond.

Problem 2: Reciprocal lattice in three dimensions (8 points)

Consider a Bravais lattice with primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$. The primitive vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$ of the reciprocal lattice are defined via the condition $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$.

a) Verify that the vectors

$$2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},\ 2\pi\frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},\ 2\pi\frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

are the primitive vectors of the reciprocal lattice!

b) If V is the volume of the primitive cell of the direct lattice, show that the volume of the primitive cell of the reciprocal lattice is $8\pi^3/V$.

Problem 3: Face-centered and body-centered cubic lattices (12 points)

The face-centered cubic (fcc) lattice can be defined by the primitive vectors

$$\frac{a}{2}(1,1,0),\ \frac{a}{2}(1,0,1),\ \frac{a}{2}(0,1,1)$$

where a is the lattice spacing of the conventional cubic unit cell. For the body-centered cubic (bcc) lattice, a set of primitive vectors is

$$\frac{a}{2}(1,1,-1),\ \frac{a}{2}(-1,1,1),\ \frac{a}{2}(1,-1,1).$$

a) Calculate the volumes of the primitive cells and compare them with the volume of the conventional cubic unit cell. What does this tell you about the number of particles in the cubic cell?

b) Show that the reciprocal lattice of a fcc lattice is a bcc lattice and vice versa.