Physics 240A: Homework Problem Set 2

Due 10/17/07.

1. Two Descriptions of the Same Lattice. 10 points.
A body-centered cubic (bcc) crystalline material has the direct lattice vectors

$$\vec{R}_1 = (1,1,-1)\frac{a}{2}, \vec{R}_2 = (1,-1,1)\frac{a}{2}, \vec{R}_1 = (-1,1,1)\frac{a}{2}.$$

(a) Find the reciprocal lattice vectors. Show work.
(b) This crystal can be described equally well as this bct Bravais lattice

$$\vec{R}_1 = (1,0,0)a, \vec{R}_2 = (0,1,0)a, \vec{R}_1 = (1,1,1)\frac{a}{2}.$$

Show, using clear descriptive reasoning or a clean mathematical proof, that these lattices are equivalent (i.e. they give the same set of lattice points).

2. Fourier Components. 10 points.
A simple 1D lattice problem: find the Fourier components of

$$f(x) = Asin(2\pi x/a) + Bcos(4\pi x/a) + Csin(10\pi x/a)cos(12\pi x/a).$$

The lattice constant is denoted by a.

3. Structure Factor. 10 points.
Determine the structure factor for these three lattices: diamond, ZnS, NaCl. [The last two are known by these names: zincblende, rocksalt, respectively.] Show work (of course).

4. Structure Factor for the HCP Lattice. 20 points.
The *hexagonal close-packed* (hcp) structure for an elemental material (Be, Zn, Gd are examples) consists of a hexagonal Bravais lattice (described in text) and a basis of two atoms in the primitive cell, at $(0,0,0)$ and at $\frac{2}{3}\vec{R}_1 + \frac{1}{3}\vec{R}_2 + \frac{1}{2}\vec{R}_3$.
(a) Calculate the fundamental reciprocal vectors $\vec{G}_1, \vec{G}_2, \vec{G}_3$; show work.
(b) Express the positions of the atoms in the HCP primitive cell in terms of the direct lattice vectors (in preparation for the next part).
(b) For a general reciprocal lattice vector $\vec{G} = h\vec{G}_1 + k\vec{G}_2 + \ell\vec{G}_3$, calculate the structure factor and identify regularities, extinctions, etc. Interpret what you find.