Homework 2

Phys 155, Winter 2008, UCSC

Due Jan 24

Each problem is 5 points. For problems from H&H, please note that solutions are included in the textbook. However, use those solutions simply as a guide, if necessary. If you do, your answers should show clear evidence (your own words, logic, details, diagrams, etc.) for your own understanding.

1. Consider the structural factor $S(\vec{q}) = \sum_m f_m(\vec{q}) \exp(-i\vec{q}\cdot\vec{r}_m)$ where $\vec{r}_m$ is the position of atoms in the basis relative to a lattice point, and m sums over all atoms in the basis. [$\vec{r}_m$ can be taken as 0 if there is only one atom per basis. In another example, for a body-centered-cubic (bcc) crystal described by a simple cubic (sc) conventional unit cell, $\vec{r}_m$ can be taken to be 0 and $(\vec{a} + \vec{b} + \vec{c})/2$.]

   (a) Consider an fcc lattice with one atom per unit cell. Instead of dealing with a primitive unit cell, it is more convenient to deal with a conventional unit cell that is simple cubic, and so let us do that. Remember that once we use the simple cubic description, we have a four atom basis. Notice that in this case these four atoms are really the same in every possible way, so are f_m's for all four atoms. Compute $S(\vec{q})$ for this basis and show that $S(\vec{q}) \neq 0$ only if $\vec{q}$ is a point of a bcc lattice. Explain why this means that the reciprocal of an fcc is a bcc. In class, we learned that the product of the unit cell volume of a Bravais lattice and the unit cell volume of its reciprocal lattice is $(2\pi)^3$ [in 3 dimensions]. Show that this particular example satisfies this general property [as it should], by considering the volumes of the *primitive* (not conventional) unit cells of real and reciprocal lattices.

   (b) Do the same thing as (a), but starting from a conventional unit cell description of a bcc lattice with one atom per unit cell. I.e., show that $S(\vec{q}) \neq 0$ only if $\vec{q}$ is a point in an fcc lattice, and that the product of volumes of the primitive unit cells in real and reciprocal lattices satisfies the general property.

   [You may view this as a more convenient and more illuminating way of proving the fcc-bcc reciprocal relationship. See H&H 11.2.3 for a more brute force method. This kind of consideration also sheds light on how one can think about diffraction patterns obtained on a multiple-atom-basis crystal with some atomic scattering factors f_m not so different from one another.]

2. Let us show why the Bragg diffraction can be formulated as either $2d\sin\theta = n\lambda$ or $\vec{q} = \vec{G}$. Recall that $\vec{q} = \vec{k}_f - \vec{k}_i$, $|\vec{k}_i| = |\vec{k}_f| = 2\pi/\lambda$ (we consider an elastic Bragg scattering), $\vec{G}$ is a reciprocal lattice vector. d and θ were defined in slide 9 of Lecture 3, or equivalently in Figure 1.16 of H&H.

   (a) Show that for any given lattice plane, reciprocal lattice vectors perpendicular to it are expressed as $n\vec{g}$ (n = integer), where $|\vec{g}| = 2\pi/d$, where d is the spacing between adjacent lattice planes. [Hint: Construct unit vectors of the lattice by starting from unit vectors of the lattice plane and then adding one more unit vector, connecting two adjacent lattice planes. See slide 15 of Lecture 2, if you need help. Then, using the definition of the reciprocal lattice (slide 5 of Lecture 3 – applicable to any dimensions actually), show that $\vec{g}$ can be identified as the reciprocal unit vector normal to the lattice plane.]

(b) Show that for an arbitrary, but non-zero, reciprocal lattice vector $\vec{G}$ there exists a lattice plane perpendicular to it. Show that the set of all reciprocal lattice vectors parallel to $\vec{G}$ can be expressed as $n\vec{g}$ (n = integer) and that the spacing between the lattice planes is given by $d = 2\pi/|\vec{g}|$. [Hint: Note that $\vec{g}$ can be taken as a unit vector of the reciprocal lattice.]

(c) By (a,b), we just proved that there is a one-to-one mapping between a set of lattice planes and one dimensional sub-lattice $n\vec{g}$ (n=integer) of the reciprocal lattice. Using this equivalence, show that the two expressions $2d\sin\theta = n\lambda$ and $\vec{q} = \vec{G}$ are completely equivalent. Note that the last expression should be visualized as a triangle where two sides are given by $\vec{k}_{in}$ and $\vec{k}_{out}$ and the third side is given by $\vec{G}$ [cf. Figure 11.4 of H&H, albeit with different notations.]

[Note for a more ambitious student: For a given but arbitrary set of unit vectors $\vec{a}, \vec{b}, \vec{c}$, note that $\vec{g}$ in (a,b) should be expressed as $\vec{g} = l\vec{a}^* + m\vec{b}^* + n\vec{c}^*$. (lmn) is none other than Miller indices for that choice of unit vectors.]

3. H&H, 2.1