PHYSICS 231

Homework 1

Due in class, Monday October 3

Resechduling of lectures

I will be out of town on **Monday October 17** and **Wednesday October 19** and will need to reschedule those lectures.

1. Consider a honeycomb lattice. Show that is it *not* a Bravais lattice but has a basis. What is the Bravais lattice?

2. What is the Bravais lattice formed by all points with Cartesian coordinates (n_1, n_2, n_3), is

   (a) The n_i are either all even or all odd.

   (b) The sum of the n_i is required to be even.

3. Show that the angle between any two of the lines (bonds) joining a site of the diamond lattice to its four neighbors is $\cos^{-1}(-1/3) = 109°28'$.

4. Show that the reciprocal lattice of a bcc lattice is fcc and vice-versa.

5. Show that, in general, the volume of the Brillouin zone is given by

$$v_{Br} = \frac{(2\pi)^3}{v}, \tag{1}$$

   where v is the volume of the unit cell.

6. Prove the following theorem

   > For any family of lattice planes separated by a distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length of $2\pi/d$.

7. From the previous question show that the Laue result that constructive interference occurs when Δk ($\equiv k' - k$) is given by

$$\Delta k = G, \tag{2}$$

   (where G is a reciprocal lattice vector) is equivalent to the Bragg result

$$n\lambda = 2d \sin\theta \tag{3}$$

   in standard notation.

8. The sodium chloride structure can be regarded as an fcc Bravais lattice of cube side a, with a basis consisting of a positively charged ion at the origin and a negatively charged ion at $(a/2)\hat{\mathbf{x}}$. The reciprocal lattice is bcc (as you showed in Qu. (4)) with reciprocal lattice vectors given by

$$\mathbf{G} = \frac{4\pi}{a}\left(\nu_1\hat{\mathbf{x}} + \nu_2\hat{\mathbf{y}} + \nu_3\hat{\mathbf{z}}\right), \tag{4}$$

   where the coefficients, ν_i are either all integers or all integers $+\frac{1}{2}$. If the form factors of the ions are f_+ and f_-, show that form factor of the unit cell is $f_+ + f_-$ if the ν_i are integers and $f_+ - f_-$ if the ν_i are integers $+\frac{1}{2}$. Explain physically why the latter vanishes if $f_+ = f_-$.

9. **Width of diffraction maximum**

To estimate the width of the Bragg peak in diffraction off a *finite* lattice consider a one-dimensional model of N identical scattering centers at points $x_n = na$, where a is the lattice spacing and $n = 1, 2, \cdots, N$. The total scattering amplitude will be proportional to

$$F = \sum_{n=1}^{N} \exp[ina\Delta k]. \tag{5}$$

Evaluate the sum and show that the scattering intensity is proportional to

$$|F|^2 = \frac{\sin^2(\frac{1}{2}Na\Delta k)}{\sin^2(\frac{1}{2}a\Delta k)}. \tag{6}$$

Show that the maximum intensity is proportional to N^2. Also find the width of a diffraction peak, showing that it is proportional to $1/N$, i.e. it is very narrow. The same is true in three dimensions.