

# Applied Physics 195 / Physics 195 — Assignment #6

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Date: October 25th, 2015

Due: **5pm SHARP (4:50pm + 10 min grace period)**, November 6th, 2015; slide your work under through the door at Maxwell-Dworkin Room 131.

## Problem 1 (80 pt): X-ray diffraction by a lattice with a basis

Let's recap on the derivation of the Laue condition (Lecture #9). Strength of light diffraction by a crystal is proportional to  $|\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle|^2$ , where  $n(\vec{r})$  is the periodic electron density distribution across the crystal.<sup>1</sup> As  $n(\vec{r} + \vec{R}) = n(\vec{r})$  for any direct lattice vector  $\vec{R}$ ,  $n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$  where  $\vec{G}$  represents reciprocal lattice vectors with  $n_{\vec{G}}$  being Fourier components. Then the overlap integral is

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = \int_{\text{crystal}} e^{-i\vec{k}' \cdot \vec{r}} n(\vec{r}) e^{i\vec{k} \cdot \vec{r}} d^3\vec{r} = \sum_{\vec{G}} n_{\vec{G}} \int_{\text{crystal}} e^{i[\vec{G} - (\vec{k}' - \vec{k})] \cdot \vec{r}} d^3\vec{r}. \quad (1)$$

This vanishes unless  $\vec{k}' - \vec{k}$  is equal to a certain  $\vec{G}$ . Thus the Laue condition,  $\vec{k}' - \vec{k} = \vec{G}$ , is necessary for diffraction to occur. In contrast, it is in general not sufficient for diffraction to occur; even if  $\vec{k}' - \vec{k} = \vec{G}$  for a certain  $\vec{G}$ , the resulting overlap integral

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = V n_{\vec{G}} = \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n(\vec{r}) d^3\vec{r} \quad (2)$$

will vanish if  $n_{\vec{G}} = 0$  ( $V$ : crystal volume). The situation of  $n_{\vec{G}} = 0$  occurs, for example, if a monatomic crystal with BCC lattice is described using SC conventional unit cell with a basis (two identical atoms). The spatial frequency of  $n(\vec{r})$  coming from all atoms can be twice larger—along certain crystal directions—than the spatial frequency described by  $\vec{G}$  vectors derived from the SC lattice that misses out body-centered atoms; therefore,  $n_{\vec{G}} = 0$  for a certain set of  $\vec{G}$  vectors. For another example, for a diatomic crystal of CsCl structure, whose description is now natural with the SC lattice a basis (two different atoms), if the two basis atoms have similar electron density distributions,  $n_{\vec{G}}$  can be close to zero for certain  $\vec{G}$  vectors for the same reason as above.

More generally,  $n_{\vec{G}}$  will vary with the positions and electron density distributions of basis atoms. To show this explicitly, we first decompose  $n(\vec{r})$  into  $n(\vec{r}) = \sum_{i=1}^u n_i(\vec{r} - \vec{d}_i)$  ( $u$ : number of basis atoms per unit cell;  $n_i$ : periodic electron density distribution across the crystal due to the  $i$ -th basis atoms;  $\vec{d}_i$ : position of the  $i$ -th basis atom in each unit cell). By plugging this into Eq. (2), we obtain

$$\begin{aligned} \langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle &= V n_{\vec{G}} = \sum_{i=1}^u \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r} - \vec{d}_i) d^3\vec{r} = \sum_{i=1}^u \left[ e^{-i\vec{G} \cdot \vec{d}_i} \times \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r}) d^3\vec{r} \right] \\ &= \sum_{i=1}^u f_i e^{-i\vec{G} \cdot \vec{d}_i}, \end{aligned} \quad (3)$$

where

$$f_i \equiv \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r}) d^3\vec{r}, \quad (4)$$

is the property of the  $i$ -th basis atom and is roughly proportional to  $Z_i$ , the atomic number. For  $\vec{G} = l\vec{b}_1 + h\vec{b}_2 + k\vec{b}_3$  ( $l, h, k$ : integers) and  $\vec{d}_i = x_i\vec{a}_1 + y_i\vec{a}_2 + z_i\vec{a}_3$  ( $x, y, z$ : real),

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = V n_{\vec{G}} = \sum_{i=1}^u f_i \exp[-i2\pi(lx_i + hy_i + kz_i)]. \quad (5)$$

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<sup>1</sup>Lecture #9 uses  $V(\vec{r})$ —effective periodic potential for light scattering—in lieu of  $n(\vec{r})$ .  $V(\vec{r}) \sim n(\vec{r})$  for light scattering.

This explicitly shows the impact of the electron density distribution and position of each basis atom on the diffraction strength.

(a) Let a monatomic BCC crystal be described using the SC conventional unit cell with two basis atoms. Show that diffraction does not occur for  $(l, h, k) = (1, 0, 0)$  but occurs for  $(l, h, k) = (1, 0, 0) \times 2$ ; can you explain this from the Bragg point of view, considering relevant lattice planes? Show that diffraction occurs for both  $(l, h, k) = (1, 1, 0)$  and  $(l, h, k) = (1, 1, 0) \times 2$ ; can you again explain this from the Bragg point of view? Show in general that no diffraction occurs if  $l + h + k$  is an odd integer.

(b) Consider a monatomic FCC crystal described using the SC conventional unit cell with four basis atoms. Show that no diffraction occurs unless all of  $l$ ,  $h$ , and  $k$  are even integers, or all of them are odd integers.

(c) A monatomic crystal of diamond structure is described using the SC conventional unit cell with eight basis atoms. State the condition for  $l$ ,  $h$ , and  $k$  for diffraction to occur.

(d) Let a NaCl crystal be described with the SC conventional unit cell containing 8 basis atoms (4 sodium and 4 chloride atoms). Evaluate Eq. (5), while denoting the atomic form factor ( $f_i$ ) for sodium as  $f_{Na}$  and that for chloride as  $f_{Cl}$ . You may use the approximation  $f_{Cl}/f_{Na} \sim 17/11$ . Show that diffraction occurs only when all of  $l$ ,  $h$ , and  $k$  are even integers, or all of them are odd integers. Which of these two diffraction groups exhibits stronger diffraction?

**Problem 2 (50 pt): Electronic  $s$ -band of body-centered cubic crystal**

Show that under the tight-binding approximation the dispersion relation of the electronic  $s$ -band of the body-centered cubic crystal (one atom per primitive unit cell) is given by

$$\epsilon(\vec{k}) = \epsilon_0 - 8t \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2}, \tag{6}$$

where  $\epsilon_0$  is the atomic  $s$ -level energy and  $t > 0$  is the strength of electron hopping between the  $s$  levels of two nearest neighbor atoms. Now, if we consider the electron hopping (hopping strength:  $t' > 0$ ) between the  $s$  levels of two next-to-nearest atoms as well, show that the electronic  $s$ -band dispersion relation is modified to

$$\epsilon(\vec{k}) = \epsilon_0 - 8t \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} - 2t' [\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]. \tag{7}$$

**Problem 3 (80 pt): Electronic band structure with a 2D crystal — I**

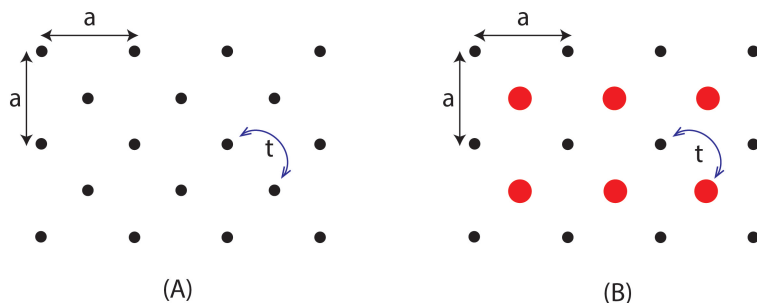


Figure 1:

Consider the 2D crystal (one valence electron per atom) of Fig. 1(A), where solid black circles are periodically arranged atoms. We will delocalize atomic ground states (energy  $\epsilon_0$ ) under tight binding approximation. The electron hopping strength between ground states of any two nearest neighbor atoms is  $t > 0$ .

- (a) Calculate the dispersion relation  $\epsilon(\vec{k})$  of the electronic band.
- (b) Draw the reciprocal lattice, 1st Brillouin zone, and single-electron energy contour map. Identify the  $\vec{k}$ -space region filled with electrons. Argue that this crystal is a metal. Evaluate the Fermi energy  $\epsilon_F$ . Finally, calculate the cohesive energy (electronic contribution).

**Problem 4 (80 pt): Electronic band structures with a 2D crystal — II**

In the 2D crystal (one valence electron per atom) of Fig. 1(B), the smaller solid black circles and the larger solid red circles represent two different types of atoms. This crystal can be described using a lattice with a basis. We will delocalize atomic ground states (with energy  $\epsilon_A$  and  $\epsilon_B$  for the two different types of atoms) under tight binding approximation. The strength of electron hopping between ground states of any two nearest neighbor atoms (which are necessarily the two different atom types) is  $t > 0$ .

- (a) Show that there are two electronic bands, and calculate the dispersion relation  $\epsilon(\vec{k})$  for both bands.
- (b) Draw the reciprocal lattice, 1st Brillouin zone, and single-electron energy contour map (for both bands). Identify the electron-filled region in the  $\vec{k}$  space. What is the size of the band gap? Argue that this crystal is an insulator (at  $T = 0$  at least).