Thomas Ouldridge

Keble College - Michaelmas 2009

B2: Condensed Matter Physics and Photonics

Tutorial 1 - Lattices and Scattering

Please leave your work in my Keble pigeon hole by 5pm on Wednesday of 1st week.
Suggested reading: Hook & Hall 1.1-1.5, 11.1-11.2; Kittel 1, 2; Ashcroft/Mermin 4, 5.

---

1 Definition, Geometry and the Reciprocal Lattice

1. Explain the following terms, using one sentence for each: *lattice*, *unit cell* (primitive and conventional), *lattice vector*, *primitive lattice vector*, *basis* and *crystal*.

   Draw the conventional unit cells for each of; *simple cubic*, *body centred cubic* and *face centred cubic* lattices. How many lattice points are there in each conventional unit cell? Identify them.

   Describe the CsCl crystal structure in terms of a lattice and a basis. What does this become if all of the atoms are replaced by Fe? Draw the conventional unit cell of diamond in plan view. List the coordinates of atoms which are in the *conventional* and *primitive* unit cells.

   A 2D lattice has primitive vectors $a\mathbf{i}$ and $1.5a\mathbf{j}$. Show how to construct the Wigner-Seitz unit cell. What special property of the Wigner-Seitz unit cell makes it useful? For the same lattice, construct lattice planes with Miller indices $(1,1), (2,0)$ and $(\overline{1},2)$.

2. Define the set of reciprocal lattice vectors $\{\mathbf{K}\}$ in terms of the set of direct Bravais lattice vectors $\{\mathbf{R}\}$. [Hint: your answer should be an equation involving a scalar product.]

   Let $\mathbf{a_i}$ (i = 1,2,3) be the primitive lattice vectors of the direct lattice. Show that if we define $\mathbf{b_i}$ by:

   $$\mathbf{b_1} = 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1}.(\mathbf{a_2} \times \mathbf{a_3})}, \tag{1}$$

   with similar expressions for $\mathbf{b_2}$ and $\mathbf{b_3}$, $\mathbf{b_i}$ constitute the primitive lattice vectors of the reciprocal lattice.

   Construct the reciprocal lattice and first two Brillouin zones for the 2D lattice in question 1.

   Show that the reciprocal lattice vector $\tau_{hkl} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is normal to the lattice plane with Miller indices (hkl). [Hint: there is no need to make any assumptions about the geometry of the direct lattice. Simply find two vectors which must lie in the (hkl) planes and use them to find the normal, showing it is parallel to τ_{hkl}.]

   Show that the separation of planes with Miller indeces (hkl) is given by $2\pi/|\tau_{hkl}|$.

3. Let us describe the lattice as a sum of delta functions in space, one at each lattice point.

   $$L(\mathbf{r}) = \sum_i \delta^3(\mathbf{r} - \mathbf{r_i}), \tag{2}$$

   where the index i runs over all lattice points. Let $G(\mathbf{k})$ be the Fourier transform of $L(\mathbf{r})$:

   $$G(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int L(\mathbf{r}) \mathrm{e}^{(\mathbf{ik.r})} \mathrm{d}^3\mathbf{r} \tag{3}$$

   When is G($\mathbf{k}$) non-zero? Argue that G($\mathbf{k}$) is the reciprocal lattice (in the same sense that $L(\mathbf{r})$ is the direct lattice).

2 Scattering

4. Incident X-rays or neutrons are scattered, and constructively interfere at certain angles characteristic of the crystal. The expected peaks are given by Bragg's law:

$$\lambda = 2d_{hkl}\sin(\theta)\ , \tag{4}$$

where λ is the wavelength of the incident radiation, d_{hkl} is the spacing of the Miller planes (hkl) and θ is the scattering angle

Derive Bragg's law using

(a) Bragg's geometrical argument

(b) quantum scattering arguments (von Laue's method)

Expanding on your answer to part (b), explain what is meant by the terms *structure factor* and *atomic form factor*. How does the x-ray form factor vary with scattering angle for a typical element?

5. You may wonder why in these analyses we are able to get away with first considering the scattering from each unit cell, as if they were point scatterers, and afterwards including the complications of structure and form factors. Mathematically, the reason is that scattering amplitudes are proportional to Fourier transforms of the crystal structure (this will be discussed more in the class), and that the crystal structure can be expressed as convolutions.

Show that if we define a lattice as in question 3, and the basis as some function $B(\mathbf{r})$, then the convolution $L * B$ is the basis repeated at each lattice point [hint: just do the convolution].

Thus explain why, if scattering amplitudes are proportional to Fourier transforms of the crystal, we can consider the lattice and basis separately, and simply multiply the resultant amplitudes together.

6. Explain how diffraction patterns are determined experimentally. You should discuss the different techniques employed (Laue photograph, rotating crystal, powder method), describe the diffraction pattern obtained in each case and provide a comparison of the relative advantages and disadvantages of x-rays and neutrons in structure determination.

3 Exam-style Questions

Please also attempt questions 4 and 6 from Prof. Boothroyd's problem set. In these questions, and in fact in general, the conventional unit cell of of BCC and FCC lattices is taken as cubic.