PHYS40352 Solid State Physics Examples 1

1. In lectures it was shown that the two-dimensional centered rectangular lattice (also known as the *rhombic lattice*) is distinct from the rectangular P-lattice. Why would a centered *square* lattice not be any different from the simple square lattice?

2. A beam of neutrons of energy 0.015 eV is incident on a crystal of caesium chloride, which has a conventional unit cell side of 4.11 Å. At what angles will Bragg reflections from the (1 1 0) planes occur?

   Note: You will need to calculate the de Broglie wavelength of these non-relativistic neutrons.

3. Show that

   $$\boldsymbol{a}_1 = [\bar{1}\,1\,1]a/2, \quad \boldsymbol{a}_2 = [1\,\bar{1}\,1]a/2, \quad \boldsymbol{a}_3 = [1\,1\,\bar{1}]a/2$$

   are *primitive vectors* of the cubic I-lattice (BCC).

   Note: You need to show that you can reach the lattice points at the corners of the cell and at the centre of the cell by means of linear combinations $n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, where n_1, n_2, n_3 are all integers.

4. Do a similar job for the cubic F-lattice (FCC), using the vectors

   $$\boldsymbol{a}_1 = [0\,1\,1]a/2, \quad \boldsymbol{a}_2 = [1\,0\,1]a/2, \quad \boldsymbol{a}_3 = [1\,1\,0]a/2.$$

5. Use the formulas

   $$\boldsymbol{b}_1 = \frac{2\pi\,\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot [\boldsymbol{a}_2 \times \boldsymbol{a}_3]}, \quad \boldsymbol{b}_2 = \frac{2\pi\,\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot [\boldsymbol{a}_2 \times \boldsymbol{a}_3]}, \quad \boldsymbol{b}_3 = \frac{2\pi\,\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot [\boldsymbol{a}_2 \times \boldsymbol{a}_3]}$$

   and the vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ from Problem 3 to show that the reciprocal of the cubic I-lattice is the cubic F-lattice. Similarly show that the reciprocal of the cubic F-lattice is the cubic I-lattice. In each case, relate the conventional cubic lattice constant of the reciprocal lattice to that of the direct lattice, which is a.

6. If you have time, show that the reciprocal of the reciprocal of *any* given lattice is just the original lattice.

   Note: One valid (but algebraically awkward) approach is to apply the formulas of Problem 5 twice. Another way is to consider the equation $\exp[i\boldsymbol{G} \cdot \boldsymbol{R}] = 1$, which defines the reciprocal lattice vectors $\boldsymbol{G}$; if you think carefully enough, you may be able to avoid doing *any* vector calculation.

7. Monochromatic X-rays are incident in the [0 0 1] direction upon a single crystal of a material with a cubic structure whose conventional cubic lattice constant $a = 3.61$ Å. What X-ray wavelength is needed for first-order reflection from the (1 1 1) planes?

   Given that the crystal is copper (FCC structure), would the (1 1 1) reflection actually be observed? One approach would be to regard the FCC structure as a cubic P-lattice with a basis consisting of four identical atoms per lattice point; you would then need to calculate the structure factor. Alternatively, you could make use of the work you did for Problem 5. If you have time, try both methods.

8. Calculate the atomic form factor,

   $$f(\boldsymbol{G}) = \int n(\boldsymbol{r})\, e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}\, d^3\boldsymbol{r},$$

   for an atom consisting of Z electrons uniformly distributed throughout a sphere of radius r_0. Use spherical polar coordinates to do the integral and write the result in terms of the magnitude of the scattering vector,

   $$G = |\boldsymbol{k}' - \boldsymbol{k}| = 4\pi\,\frac{\sin\theta_B}{\lambda}\,.$$