Homework 3

Due Date: February 25, 2025

3.1 Lattice Symmetries.

(a) Show that any mid-point between two lattice sites $(\boldsymbol{R}_m + \boldsymbol{R}_n)/2$ is an inversion center for a Bravais lattice.

(b) Find all the mirror lines of the square lattice.

(c) (1) Find the six-fold and a three-fold rotation axis for the triangular and honeycomb lattices. For the honeycomb lattice, assume it is made of the same types of atoms in both A and B sublattices like in graphene.

(2) What happens to the six-fold rotation symmetry (of the honeycomb lattice) if the atoms are different for the A and B sublattices, like in hexagonal boron nitride, in which one sublattice is occupied by boron and the other by nitrogen?

(d) (1) Show that five-fold rotation symmetry is inconsistent with lattice translation symmetry in two dimensions.

(2) Give an argument as to why this conclusion holds in three dimensions as well.

3.2 Lattice Sums. As we saw in the X-ray scattering theory, in solid state and condensed matter physics we often face "lattice sums", "$\boldsymbol{q}$-space" sums, and the Poisson summation formula. For lattice vectors $\boldsymbol{R}_n$, find the following sums

(a) $\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}$.

(b) $\sum_n e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}$.

(c) $\left|\sum_n e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}\right|^2$.

(d) Prove the Poisson summation formula,

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a}\sum_{l=-\infty}^{\infty} \tilde{f}(lG) \ , \tag{1}$$

where f is a function of a real variable and we wish to sum the values of f on the sites of a uniform lattice of lattice constant a. $\tilde{f}$ is the Fourier transform of f, $G = 2\pi/a$, and l and n are integers.

3.3 X-rays Diffraction for a Diamond Lattice. Show that scattering from the identical atoms on a diamond lattice produces perfect destructive interference for reciprocal lattice vectors $\boldsymbol{G}_{hkl}$ if $h + k + l$ is twice an odd number (which is not the same thing as an even number!). Here the first basis vector for the reciprocal lattice is chosen to be $\boldsymbol{g}_1 = (2\pi/a)(\hat{y} + \hat{z} - \hat{x})$ and the remaining two are generated by cyclic permutations of the three terms in the second parenthesis. Here a is the lattice constant of the conventional cubic cell.

3.4 Reciprocal Lattice.

(a) Construct the reciprocal lattice of a one dimensional lattice with lattice constant a, and all (not just the first) of the Brillouin zones.

(b) Show that the reciprocal lattice vector $\boldsymbol{G}_m = m_1\boldsymbol{g}_1 + m_2\boldsymbol{g}_2 + m_3\boldsymbol{g}_3$ with

$$\boldsymbol{g}_i = 2\pi \frac{\boldsymbol{a}_j \times \boldsymbol{a}_k}{\Omega_p} , \tag{2}$$

and $(i \to j \to k) = (1 \to 2 \to 3)$ in cyclic order, satisfies the condition $\boldsymbol{G}_m \cdot \boldsymbol{R}_n = 2\pi\nu$ for any translation vector $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, where $\nu = n_1m_1 + n_2m_2 + n_3m_3$, and Ω_p is the primitive cell volume.

(c) Show that the reciprocal lattice of an FCC lattice is a BCC lattice (in reciprocal space), and vice versa. Determine the corresponding lattice constants of the reciprocal lattices, in terms of those of the direct lattices.

(d) Start with a Bravais lattice in any dimension, call this lattice A, and show that the reciprocal lattice of A's reciprocal lattice is the original lattice A.

3.5 More About Lattices.

(a) Consider a square lattice of constant a. The atoms at each site have a magnetic moment. At one temperature the moments are all parallel, in a ferromagnetic array. At another temperature, alternate sites have up and down spin, in an antiferromagnetic array.

  (1) What are the areas of the unit cell, A_0, and the Brillouin zone, A_{BZ}, in the ferromagnetic array?

  (2) What are the areas A_0 and A_{BZ} in the antiferromagetic array? Notice that here the lattice vectors must go between sites with the same spin orientation.

(b) A two-dimensional rectangular crystal has a unit cell with sides $a_1 = 0.468$ nm and $a_2 = 0.342$ nm.

  (1) Draw to scale a diagram of the reciprocal lattice.

  (2) In your drawing, label the reciprocal lattice points for indices in the range $0 \le h \le 3$ and $0 \le k \le 3$.

  (3) Draw the first and second Brillouin zones using the Wigner–Seitz construction.

(c) Find the atomic packing factor (packing fraction) for the SC, FCC, and BCC lattices.