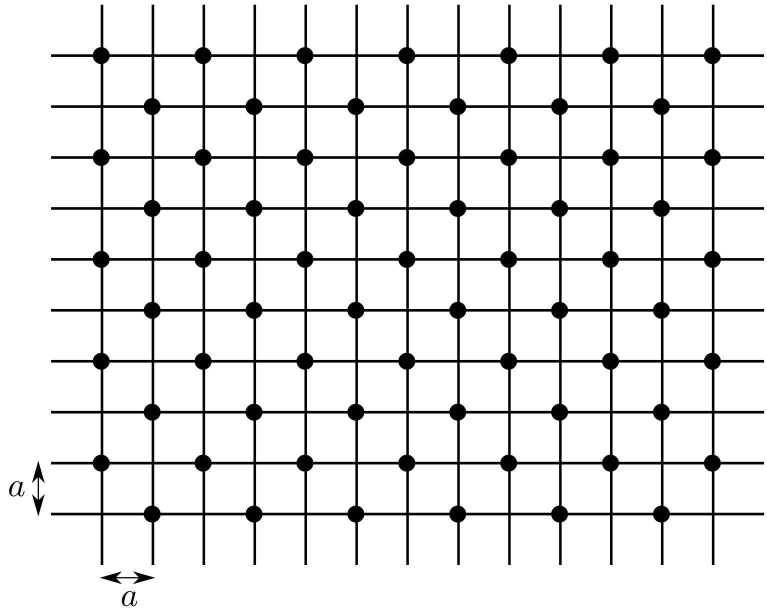
LMU München
WS 2016/2017
Lehrstuhl für Theoretische Nanophysik
PD Dr. F. Heidrich-Meisner
Jan Stolpp, *Questions: jan.stolpp@physik.uni-muenchen.de*

1. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, October 28, 2016.

Exercise 1: Crystal lattice



The figure above shows a two-dimensional lattice of identical atoms.

a. Draw an example of a primitive unit cell into the lattice. Give the basis vectors of the unit cell in dependence of the lattice constant a.

b. Compute the basis vectors of the reciprocal lattice. Sketch the reciprocal lattice and the first Brillouin zone.

Exercise 2: Reciprocal lattice I

The primitive vectors of the reciprocal lattice $\boldsymbol{b}_i$ satisfy the relations:

$$\boldsymbol{b}_i = 2\pi \frac{\boldsymbol{a}_j \times \boldsymbol{a}_k}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)}, \; i, j, k = 1, 2, 3 \text{ and cyclic permutations} \tag{1}$$

$$\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi \delta_{i,j}. \tag{2}$$

a. Show that the reciprocal lattice primitive vectors defined in (1) satisfy

$$\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3) = \frac{(2\pi)^3}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)}. \tag{3}$$

What is the meaning of this quantity?

Hint: Write $\boldsymbol{b}_1$ in terms of the $\boldsymbol{a}_i$ and use the orthogonality relation (2); use the vector identity $(\boldsymbol{A} \times \boldsymbol{B}) \cdot (\boldsymbol{C} \times \boldsymbol{D}) = (\boldsymbol{A} \cdot \boldsymbol{C})(\boldsymbol{B} \cdot \boldsymbol{D}) - (\boldsymbol{A} \cdot \boldsymbol{D})(\boldsymbol{B} \cdot \boldsymbol{C})$.

b. Suppose primitive vectors are constructed from the $\boldsymbol{b}_i$ in the same manner as the $\boldsymbol{b}_i$ are constructed from the $\boldsymbol{a}_i$. Show that these vectors are just the $\boldsymbol{a}_i$ themselves; i.e., show that

$$2\pi \frac{\boldsymbol{b}_2 \times \boldsymbol{b}_3}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a}_1, \text{ etc.} \tag{4}$$

Hint: Write $\boldsymbol{b}_3$ in the numerator in terms of the $\boldsymbol{a}_i$, use the vector identity $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C}) = \boldsymbol{B}(\boldsymbol{A} \cdot \boldsymbol{C}) - \boldsymbol{C}(\boldsymbol{A} \cdot \boldsymbol{B})$.

Exercise 3: Reciprocal lattice II

A possible set of primitive vectors of the simple hexagonal Bravais lattice is:

$$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}, \ \boldsymbol{a}_2 = \frac{a}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}a}{2}\hat{\boldsymbol{y}}, \ \boldsymbol{a}_3 = c\hat{\boldsymbol{z}}. \tag{5}$$

a. Using the primitive vectors given in Eq. (5) and the construction (1) show that the reciprocal lattice of the simple hexagonal Bravais lattice is also simply hexagonal, with lattice constants $\frac{2\pi}{c}$ and $\frac{4\pi}{\sqrt{3}a}$ rotated through 30° about the z-axis with respect to the direct lattice.

b. For which value of $\frac{c}{a}$ does this ratio have the same value in both direct and reciprocal lattices? If $\frac{c}{a}$ is ideal in the direct lattice (i.e. for a hexagonal *close packed* lattice $\left(\frac{c}{a}\right)_{ideal} = \sqrt{\frac{8}{3}}$), what is its value in the reciprocal lattice?

c. The Bravais lattice generated by three primitive vectors of equal length a, making equal angles θ with one another, is known as the *trigonal* Bravais lattice. Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by $-\cos(\theta^*) = \frac{\cos(\theta)}{1+\cos(\theta)}$, and a primitive vector length a^*, given by $a^* = \frac{2\pi}{a}(1 + 2\cos(\theta)\cos(\theta^*))^{-\frac{1}{2}}$.
Hint: It is not required to explicitely set up the basis vectors of the direct lattice.

Exercise 4: Bravais Lattice

Prove that any Bravais lattice has inversion symmetry with respect to any lattice point.
Hint: *Express the lattice translation as linear combinations of primitive vectors with integral coefficients.*