Exercise 2 for Theoretical Solid State Physics in Summer 2023

Prof. Dr. Andreas Klümper
Dr. Vladislav Popkov

Submission: 19.04.2023, 12:00 in the P.O. Box Popkov on D.10
Discussion: 19.04.2023, 14:15

1. **Reciprocal lattice (2 Points)**
   Show that the reciprocal lattice of the reciprocal lattice is again the original lattice.

2. **Face centered tetragonal structure (8 Points)**
   Let $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$ be the basis of a Bravais lattice and $\left\{\vec{b}_1, \vec{b}_2, \vec{b}_3\right\}$ the basis of the corresponding reciprocal lattice. A lattice plane can be defined by three integers m_1, m_2, m_3, the so-called Miller indices. The Miller indices indicate in which three points

   $$\vec{x}_j = \frac{\vec{a}_j}{m_j}, \qquad j = 1, 2, 3$$

   the plane intersects the lattice axes determined by the primitive vectors $\vec{a}_j$. If one of the m_j equals zero, the intersection is at infinity and the corresponding plane is oriented parallel to the axis.

   (a) Show that the vector

   $$\vec{k} = \sum_{j=1}^{3} m_j \vec{b}_j$$

   is perpendicular to the plane fixed by m_1, m_2, m_3.

   (b) Show that the plane in (a) has the perpendicular distance $\frac{2\pi}{||\vec{k}||}$ to the origin.

3. **Symmetries of unit cells (3 Points)**
   All lattice planes of a Bravais lattice can be characterized by normal vectors, which according to task 2 can be expanded in the basis $\left\{\vec{b}_1, \vec{b}_2, \vec{b}_3\right\}$ of the reciprocal lattice. For a perpendicular distance d of the planes the reciprocal lattice vector $\vec{k} = \sum_{j=1}^{3} m_j \vec{b}_j$ is of length $\frac{2\pi}{d}$. Since the m_j have no common divisor, $\vec{k}$ ist the shortest reciprocal vector perpendicular to the planes.

(a) Show that the density of lattice points per unit area in the lattice planes is $\frac{d}{V}$, where V is the volume of the unit cell spanned by $\vec{a}_1, \vec{a}_2, \vec{a}_3$.

(b) Show that the reciprocal lattice of the face-centered cubic lattice with lattice constant a is a body-centered cubic lattice with constant $\frac{4\pi}{a}$. By definition the lattice constant a is the edge length of the cube which envelops the unit cell of the face-centered cubic lattice with primitive vectors

$$\vec{a}_1 = \frac{a}{2}\left(\vec{e}_y + \vec{e}_z\right), \qquad \vec{a}_2 = \frac{a}{2}\left(\vec{e}_x + \vec{e}_z\right), \qquad \vec{a}_3 = \frac{a}{2}\left(\vec{e}_x + \vec{e}_y\right).$$

The corresponding primitive vectors for the body-centered cubic lattice with lattice constant a' are

$$\vec{a}'_1 = \frac{a'}{2}\left(-\vec{e}_x + \vec{e}_y + \vec{e}_z\right), \qquad \vec{a}'_2 = \frac{a'}{2}\left(\vec{e}_x - \vec{e}_y + \vec{e}_z\right), \qquad \vec{a}'_3 = \frac{a'}{2}\left(\vec{e}_x + \vec{e}_y - \vec{e}_z\right).$$

(c) Find the Miller indices (m_1, m_2, m_3) of that plane of the face-centered cubic lattice which has the highest density of lattice points. Here it may be helpful to use the connection between the density and the reciprocal lattice vector $\vec{k}$.