
Exercise 2 for Theoretical Solid State Physics in Summer 2021

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Submission: 23.04.2021, 12:00 in the P.O. Box Giesen on D.10 or by e-mail

Discussion: 26.04.2021, 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 $\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$ 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

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

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 $\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$ 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} is the shortest reciprocal vector perpendicular to the planes.

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- (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

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

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

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

- (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} .