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Condensed Matter Theory 1 — Exercise 1

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https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2023/11/02*

1. Reciprocal lattice of the trigonal lattice

The trigonal lattice is a Bravais lattice generated by three primitive vectors of equal length a enclosing equal angles θ with one another, see Figure 1 (left). Show that the reciprocal lattice of a trigonal lattice is also trigonal one with primitive vectors of equal length $b = \frac{2\pi}{a}\cot\frac{\theta}{2}/\sqrt{1+2\cos\theta}$ and the trigonal angle $\cos\theta^* = -\cos\theta/(1+\cos\theta)$. Discuss the limit $\theta \to \pi/2$.

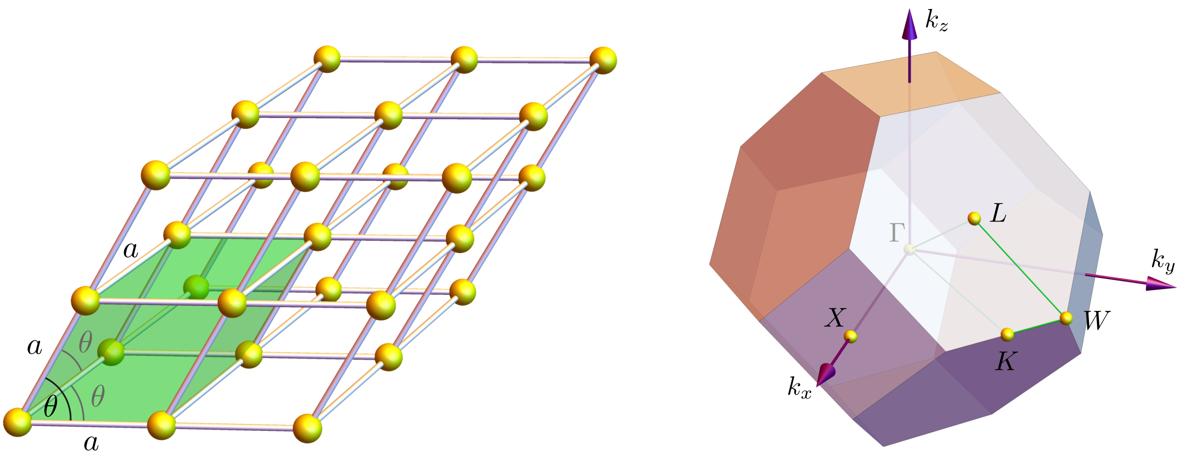

Figure 1: Left: Trigonal Bravais lattice. Right: The first Brillouin zone of the fcc Bravais lattice.

2. Brillouin zone of the fcc Bravais lattice

The first Brillouin zone of the fcc Bravais lattice is the truncated octahedron shown in Figure 1 (right).

a) The edge length of the cubic unit cell of the fcc lattice is equal to a. Find the distances ΓX, ΓK, ΓL, KW, and WL between points of the first Brillouin zone.

b) Convince yourself that the volume of the first Brillouin zone Ω_{BZ} calculated by means of geometrical methods (using the results of **a)**) coincides with the volume calculated by means of the formula $\Omega_{\text{BZ}} = (2\pi)^3/\mathcal{V}_{\text{PUC}}$ with $\mathcal{V}_{\text{PUC}}$ being the volume of the primitive unit cell of the fcc Bravais lattice.

3. Miller indices

The Miller indices $h, k, l \in \mathbb{Z}$ of a lattice plane (h, k, l) are the coordinates of the shortest reciprocal vector $\vec{K}_0 = h\vec{b}^1 + k\vec{b}^2 + l\vec{b}^3$ perpendicular to this plane. Here $\{\vec{b}^1, \vec{b}^2, \vec{b}^3\}$ are the primitive basis vectors of the reciprocal lattice. The distance between the lattice planes is $d = 2\pi/|\vec{K}_0|$.

a) Show that the distance between the lattice planes (h, k, l) of the trigonal lattice (Figure 1 (right)) is

$$d = a\left\{h^2 + \frac{\left[l\cot\frac{\theta}{2} - (h+k)\cot\theta\right]^2}{1+2\cos\theta} + \frac{(h\cos\theta - k)^2}{\sin^2\theta}\right\}^{-1/2}. \tag{1}$$

b) Derive the corresponding formulae for the distance between the lattice planes (h, k, l) of a simple cubic lattice with lattice constant a and a hexagonal lattice with the lattice constants a and c.

4. Geometrical structure factor

a) Consider diffraction by a monatomic lattice with a two-point basis, i.e., identical atoms are placed at points $\vec{R}_{\vec{n}}$ and $\vec{R}_{\vec{n}} + \vec{d}$. Each atom scatters with a potential $u(\mathbf{r})$. The scattering intensity is proportional to $|V_{\vec{k}}|^2$, where $V_{\vec{k}}$ is the Fourier transform of the total scattering potential that is produced by all atoms. With the help of the formula $\mathcal{V}_{\text{PUC}} \sum_{\vec{R}_{\vec{n}}} e^{i\vec{q}\vec{R}_{\vec{n}}} = \sum_{\vec{G}_{\vec{m}}} (2\pi)^3 \delta(\vec{q} - \vec{G}_{\vec{m}})$, where $\mathcal{V}_{\text{PUC}}$ is the volume of the primitive unit cell and $\vec{G}_{\vec{m}}$ are reciprocal lattice vectors, show that

$$V_{\vec{k}} = \sum_{\vec{G}_{\vec{n}}} \frac{(2\pi)^3}{\mathcal{V}_{\text{PUC}}} \delta(\vec{k} - \vec{G}_{\vec{n}}) u_{\vec{G}_{\vec{n}}} S_{\vec{G}_{\vec{n}}} \tag{2}$$

where $u_{\vec{G}_{\vec{n}}}$ is the Fourier component of the atomic potential and $S_{\vec{G}_{\vec{n}}} = 1 + e^{-i\vec{G}_{\vec{n}}\vec{d}}$ is the geometrical structure factor.

b) In principle, the body-centered cubic (bcc) lattice is a Bravais lattice. Sometimes, however, it is convenient to regard the bcc lattice as a simple cubic (sc) lattice with a two-point basis. Evaluate the geometrical structure factor for this case and determine the Bragg reflections that are forbidden, i.e., for which $S_{\vec{G}_{\vec{n}}}$ vanishes. Keeping only the points on the reciprocal lattice with a finite structure factor, confirm that you obtain a face-centered cubic (fcc) lattice which is indeed the reciprocal lattice of the bcc lattice.