

1 Integral with Fermi-sphere constraints

2 Density of states

3 Reciprocal lattice

a. $\exp(i\vec{G} \cdot \vec{T}) = 1$

Solution: Let's begin with the definition of the reciprocal basis vectors b_i

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)} \epsilon_{ijk}, \quad (1)$$

where ϵ_{ijk} is the Levy-Civita symbol, and \mathbf{a}_i are the direct basis vectors. Let's move forward and define this two vectors,

$$\mathbf{T} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \quad n_i \in \mathbb{Z}, \quad (2)$$

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3 \quad m_i \in \mathbb{Z}. \quad (3)$$

From eq. 1 it is easy to notice that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$, we will use this fact on the next step. Now, let's compute the following dot product

$$\begin{aligned} \mathbf{G} \cdot \mathbf{T} &= (n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3) \cdot (m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3), \\ &= n_1 \mathbf{a}_1 \cdot (m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3) \\ &\quad + n_2 \mathbf{a}_2 \cdot (m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3) \\ &\quad + n_3 \mathbf{a}_3 \cdot (m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3), \\ &= n_1 m_1 \mathbf{a}_1 \cdot \mathbf{b}_1 + n_2 m_2 \mathbf{a}_2 \cdot \mathbf{b}_2 + n_3 m_3 \mathbf{a}_3 \cdot \mathbf{b}_3, \\ &= 2\pi(n_1 m_1 + n_2 m_2 + n_3 m_3), \\ &= 2\pi\gamma, \quad \gamma \in \mathbb{Z}. \end{aligned} \quad (4)$$

Where in the last step we used the fact that $n_i, m_j \in \mathbb{Z}$. Now it's trivial to prove what we wanted to prove.

$$\exp(i\mathbf{G} \cdot \mathbf{T}) = \exp(2\pi i\gamma) = 1. \quad \blacksquare \quad (5)$$

b. Reciprocal of a cubic lattice

Solution: For this exercise I will use the following vector identity

$$(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}). \quad (6)$$

Now from equation 1 I will compute $\mathbf{b}_i \cdot \mathbf{b}_\alpha$, for the case when $i \neq \alpha$.

$$\begin{aligned} \mathbf{b}_i \cdot \mathbf{b}_\alpha &= \left(2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)} \epsilon_{ijk} \right) \cdot \left(2\pi \frac{\mathbf{a}_\beta \times \mathbf{a}_\gamma}{\mathbf{a}_\alpha \cdot (\mathbf{a}_\beta \times \mathbf{a}_\gamma)} \epsilon_{\alpha\beta\gamma} \right) \\ &= C(\mathbf{a}_j \times \mathbf{a}_k) \cdot (\mathbf{a}_\beta \times \mathbf{a}_\gamma), \\ &= C((\mathbf{a}_j \cdot \mathbf{a}_\beta)(\mathbf{a}_k \cdot \mathbf{a}_\gamma) - (\mathbf{a}_j \cdot \mathbf{a}_\gamma)(\mathbf{a}_k \cdot \mathbf{a}_\beta)). \end{aligned} \quad (7)$$

At this point we need to be really smart (maybe normal-smart), first to notice that C absorbed all the non-vector quantities, because for reasons that will become clear soon, we don't care about

them. And second, to know that the \mathbf{a}_i basis has three vectors but on eq. 7 we have 4 vectors. So we must have one vector repeated, once with italic index and once with greek index (by definition it can't have both latin or greek indexes), we can have two repeated vectors because this would lead to $\mathbf{b}_\alpha = \mathbf{b}_i$. Therefore one of the latin indexed vectors is not repeated on the greek indexed part. Using this and the fact that $\mathbf{a}_i \cdot \mathbf{a}_j = a^2 \delta_{ij}$ we can unravel the mystery. Let's suppose without loss of generality that j is the index such that $j \neq \beta, \gamma$ and see how this influences our calculations

$$\begin{aligned} \mathbf{b}_i \cdot \mathbf{b}_\alpha &= C((\cancel{\mathbf{a}_j \cdot \mathbf{a}_\beta})^0 (\mathbf{a}_k \cdot \mathbf{a}_\gamma) - (\cancel{\mathbf{a}_j \cdot \mathbf{a}_\gamma})^0 (\mathbf{a}_k \cdot \mathbf{a}_\beta)), \\ &= 0. \end{aligned} \quad (8)$$

Therefore $\mathbf{b}_i \cdot \mathbf{b}_\alpha = 0$ if $i \neq \alpha$, and we can conclude that the reciprocal lattice is also cubic. ■

c. Brillouin zone

Solution: The Brillouin zone can be found as the Wigner-Seitz cell of every lattice point. To find it we can trace lines to first neighbors and the medians to those lines. The area enclosed inside the medians will be the Brillouin zone. The lattice will look like this

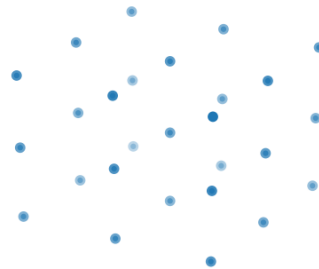


Figure 1: Reciprocal lattice in k space

The Brillouin zone will be then as shown in the following figures

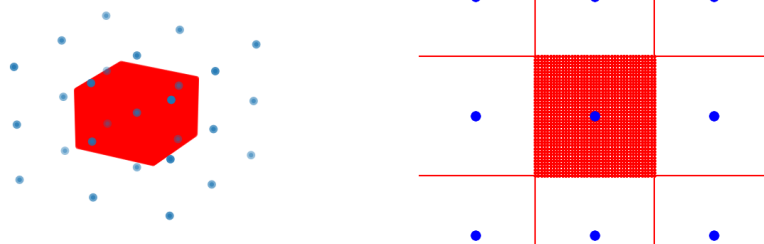


Figure 2: Brillouin zone on 3D (left side) and contour plot for $z = 0$ (right).

Finally, how would I find it numerically.

Honestly I would Google algorithms to find Voronoi-Diagrams because there must be pretty intelligent algorithms to do that. But if that's not a possibility I would do the following

1. Generate a finer mesh.
2. Travel along the points of this mesh.
3. For each point detect what lattice points are near.
4. Measure the distance to all of them.
5. Assign that mesh point to the closest lattice point.