1 Exercise 1 - Reciprocal lattice

a. Reciprocal lattice of FCC

Solution: Let's first define the primitive vectors for the FCC and BCC lattices. First the FCC structure

$$\hat{a}_1 = \frac{a}{2}\left(\hat{y} + \hat{z}\right), \tag{1}$$

$$\hat{a}_2 = \frac{a}{2}\left(\hat{z} + \hat{x}\right), \tag{2}$$

$$\hat{a}_3 = \frac{a}{2}\left(\hat{x} + \hat{y}\right). \tag{3}$$

Then, we define the primitive vectors for the BCC lattice

$$\hat{c}_1 = \frac{a}{2}\left(\hat{y} + \hat{z} - \hat{x}\right), \tag{4}$$

$$\hat{c}_2 = \frac{a}{2}\left(\hat{z} + \hat{x} - \hat{y}\right), \tag{5}$$

$$\hat{c}_3 = \frac{a}{2}\left(\hat{x} + \hat{y} - \hat{z}\right). \tag{6}$$

Here we used different names, $\hat{a}_i$, and $\hat{c}_i$ for convenience. Later we will need to be able to recognize vectors from one basis or another. Another important thing is to remember that $\hat{x}, \hat{y}, \hat{z}$ are orthonormal vectors.

First, we will obtain the reciprocal basis for the FCC structure. For this it will be helpful to calculate the box product separately.

$$\hat{a}_i \cdot (\hat{a}_2 \times \hat{a}_3),$$

using eqs. 1-3

$$\begin{aligned}
\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) &= \frac{a^2}{4}\hat{a}_1 \cdot \left(\left(\hat{z} + \hat{x}\right) \times \left(\hat{x} + \hat{y}\right)\right), \\
&= \frac{a^2}{4}\hat{a}_1 \cdot \left(\hat{y} + \hat{z} - \hat{x}\right), \\
&= \frac{a^3}{8}\left(\hat{y} + \hat{z}\right) \cdot \left(\hat{y} + \hat{z} - \hat{x}\right), \\
&= \frac{a^3}{8}\left(\cancelto{1}{\hat{y} \cdot \hat{y}} + \cancelto{1}{\hat{z} \cdot \hat{z}}\right), \\
&= \frac{a^3}{4}.
\end{aligned} \tag{7}$$

We can proceed with out calculations of the reciprocal vectors,

$$\begin{aligned}
\hat{b}_1 &= \frac{2\pi \hat{a}_2 \times \hat{a}_3}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)}, \\
&= \frac{2\pi a^2/4\left(\left(\hat{z} + \hat{x}\right) \times \left(\hat{x} + \hat{y}\right)\right)}{a^3/4}, \\
&= \frac{2\pi}{a}\left(\hat{y} + \hat{z} - \hat{x}\right).
\end{aligned} \tag{8}$$

Now the next one

$$\begin{aligned}\hat{b}_2 &= \frac{2\pi\hat{a}_3 \times \hat{a}_1}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)},\\ &= \frac{2\pi a^2/4\,((\hat{x}+\hat{y}) \times (\hat{y}+\hat{z}))}{a^3/4},\\ &= \boxed{\frac{2\pi}{a}\left(\hat{z}+\hat{x}-\hat{y}\right),}\end{aligned} \tag{9}$$

And the last one,

$$\begin{aligned}\hat{b}_3 &= \frac{2\pi\hat{a}_1 \times \hat{a}_2}{\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)},\\ &= \frac{2\pi a^2/4\,((\hat{y}+\hat{z}) \times (\hat{z}+\hat{x}))}{a^3/4},\\ &= \boxed{\frac{2\pi}{a}\left(\hat{x}+\hat{y}-\hat{z}\right).}\end{aligned} \tag{10}$$

And now we see, that the vectors defined in eqs. 8-10 are parallel to the primitive vectors of the BCC structure defined in eqs. 4-6. **Therefore, the reciprocal lattice of a FCC one is a BCC one.** ■

As we know, if we take now the $\hat{b}$ vectors of our resulting BCC structure and calculate the resulting reciprocal ones, we will go back to the original lattice, which was a FCC lattice (the reciprocal of the reciprocal lattice is the original). **Therefore, the reciprocal of a BCC lattice is an FCC one.** ■

b. Volumes

Solution: We now that the volume of the primitive cell is given by the box product. In eq. 7 we calculated the volume of the initial lattice. Let's now calculate the volume of the lattice formed by the $\hat{b}$ vectors.

$$\begin{aligned}\hat{b}_1 \cdot (\hat{b}_2 \times \hat{b}_3) &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left((\hat{z}+\hat{x}-\hat{y}) \times (\hat{x}+\hat{y}-\hat{z})\right),\\ &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left(\hat{y}-\hat{x}+\hat{z}+\hat{x}+\hat{y}+\hat{z}\right),\\ &= \frac{(2\pi)^2}{a^2}\hat{b}_1 \cdot \left(2\hat{y}+2\hat{z}\right),\\ &= \frac{(2\pi)^3}{a^3}2\left(\hat{y}+\hat{z}-\hat{x}\right) \cdot \left(\hat{y}+\hat{z}\right),\\ &= \frac{(2\pi)^3}{a^3}2\left(1+1\right),\\ &= \frac{(2\pi)^3}{a^3}4,\\ &= \frac{(2\pi)^3}{a^3/4}.\end{aligned} \tag{11}$$

If we remember, the volume of the direct lattice was $a^3/4$, hence, **the volume of the reciprocal cell is $v_{rec} = (2\pi)^3/v_{dir}$**. Where v_{rec} is the colume of the reciprocal cell, and v_{dir} the volume of the direct cell.

2 Exercise 2 - Reciprocal lattice 2

a. Reciprocal basis 2D

Solution: To tackle this problem it is useful to remember the following relation between the vectors of the direct and reciprocal basis

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}. \tag{12}$$

Now if we take vectors in two dimensions, this yields the following matrix equation

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} \begin{pmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{pmatrix} = 2\pi \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{13}$$

If we solve the equation for $\mathcal{B}$ then we have

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} = \frac{2\pi}{a_{1x}a_{2y} - a_{1y}a_{2x}} \begin{pmatrix} a_{2y} & -a_{2x} \\ -a_{1y} & a_{1x} \end{pmatrix}. \tag{14}$$

The vectors given in the assignment for the direct basis give us the matrix $\mathcal{A}$

$$\mathcal{A} = \begin{pmatrix} a & a/2 \\ 0 & a \end{pmatrix}, \tag{15}$$

therefore

$$\begin{pmatrix} b_{1x} & b_{1y} \\ b_{2x} & b_{2y} \end{pmatrix} = \frac{2\pi}{a^2} \begin{pmatrix} a & -a/2 \\ 0 & a \end{pmatrix} = \begin{pmatrix} 2\pi/a & -\pi/a \\ 0 & 2\pi/a \end{pmatrix}. \tag{16}$$

Hence, the primitive vectors of the reciprocal lattice are

$$\vec{b}_1 = \begin{pmatrix} 2\pi/a \\ -\pi/a \end{pmatrix}, \quad \vec{b}_2 = \begin{pmatrix} 0 \\ 2\pi/a \end{pmatrix}. \tag{17}$$

The respective drawings of the first and second Brillouin zones can be seen in fig. 1

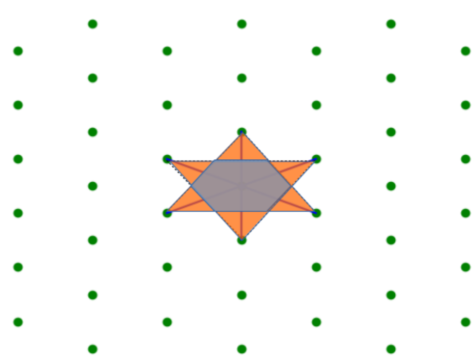

Figure 1: First (hexagon) and second (star) Brillouin zones.

b. Areas of the Brillouin zones

Solution: First we need to remember that all Brillouin zones have the same area. Then we only need to calculate the area of the first one. From fig. 1 we can see that the length apothem is half of the size of the vector $(0, 2\pi/a)$, that is $ap = \pi/a$. Now, by doing simple trigonometry and recalling that all the triangles inside the hexagon are equilateral, since it is a regular hexagon, we will have that the length of each side of the hexagon is equal to $b = 2ap/\sqrt{3}$. This result comes as a consequence of Pythagoras theorem. Finally, if we remember that the area of an hexagon is $6 * b * ap/2$ we find

$$A = \frac{6b(ap)}{2} = \frac{6(ap)^2}{\sqrt{3}} = \frac{2(\sqrt{3})^2\pi^2}{a^2\sqrt{3}} = \boxed{\frac{2\sqrt{3}\pi^2}{a^2}}. \tag{18}$$

3 Exercise 3 - Lattice planes

a. Reciprocal orthogonal vectors

Solution: A lattice is such that all points can be written as a linear combination of three primitive vectors

$$\vec{r} = n_1 a_1 + n_2 a_2 + n_3 a_3, \quad n_1, n_2, n_3 \in \mathbb{Z}. \tag{19}$$

We can do the same for the reciprocal lattice now

$$\vec{G} = hb_1 + kb_2 + lb_3, \quad h, k, l \in \mathbb{Z}. \tag{20}$$

We are going to prove now that the reciprocal lattice vector with components (h, k, l) lies perpendicular to the lattice plane with Miller indexes (hkl). To span the plane we can take the difference between the primitive vectors (naturally rescaling them with suitable coefficients), so a famili of lattice planes can be generated with linear combinations of the following vectors

$$\frac{\vec{a_1}}{h'} - \frac{\vec{a_2}}{k'}, \tag{21}$$

and

$$\frac{\vec{a_3}}{l'} - \frac{\vec{a_2}}{k'}. \tag{22}$$

Their vector product must be perpendicular to such plane, so let's see what it yields

$$\left(\frac{\vec{a_1}}{h'} - \frac{\vec{a_2}}{k'}\right) \times \left(\frac{\vec{a_3}}{l'} - \frac{\vec{a_2}}{k'}\right) = -\frac{1}{h'k'}(\vec{a_1} \times \vec{a_2}) - \frac{1}{k'l'}(\vec{a_2} \times \vec{a_3}) - \frac{1}{h'l'}(\vec{a_3} \times \vec{a_1}), \tag{23}$$

if we multiply this suspicious equation by $-2\pi h'k'l'/(\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3}))$ we get

$$2\pi \left(h' \left(\frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \right) + k' \left(\frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \right) + l' \left(\frac{\vec{a_3} \times \vec{a_1}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \right) \right), \tag{24}$$

this vector however is parallel to the vector shown in eq. 20, by definition, and therefore such vector is also perpendicular to the lattice plane. We can do the same process for all latice planes, and therefore we have proven that we can find this vectors perpendicular for all of them. Naturally if we take this arguments in reverse we will find that given this vectors, we can find lattice planes perpendicular to them. The question now is, where do we place them? That's why we need the second part of this exercise.

Now let's calculate the distance from the origin to the lattice plane (hkl), this distance is

$$\begin{aligned} d'_{hkl} &= \frac{a_1}{h'} \cos\angle(\vec{a_1}, \vec{G}_{hkl}), \\ &= \frac{a_1}{h'} \frac{\vec{a}_1 \cdot \vec{G}_{hkl}}{a_1 G_{hkl}}, \\ &= \frac{2\pi}{G_{hkl}} \frac{h}{h'}, \\ &= \frac{2\pi}{G_{hkl}} p. \end{aligned} \tag{25}$$

Therefore the shortest length of one of this vectors to a lattice plane is

$$\boxed{G_{hkl} = \frac{2\pi}{d_{hkl}}}. \tag{26}$$

Where $d_{hkl} = d'_{hkl}/p$. Once again we can take the arguments backwards and prove that given the lattice vectors $\vec{G}$ we will find a family of lattice planes perpendicular to them and separated by a distance d_{hkl}. ■

4 Exercise 4 - Periodic functions

a. Fourier expansion

Solution: First we know that the eigenfunctions of a Hermitian operator are orthogonal. Second, we know that $i\nabla$ is a hermitian operator (basically because the momentum is hermitian). And we now that the eigenfunctions of such an operator are plane waves

$$i\nabla e^{-iG_n \cdot r} = e^{-iG_n \cdot r}. \tag{27}$$

Therefore we know that

$$\langle e^{-iG_n \cdot r} | e^{-iG_m \cdot r} \rangle = V \delta_{nm}. \tag{28}$$

Where V is the volume over which we are integrating (since the plane waves are not normalized already). Hence, if we take this last equation with $m = 0$ we will find

$$\int_{\mathcal{V}} e^{-iG_n \cdot r} dr = V \delta_{n0}, \tag{29}$$

Solving the equation for delta will yield

$$\frac{1}{V} \int_{\mathcal{V}} e^{-iG_n \cdot r} dr = \delta_{n0}. ■ \tag{30}$$

Once we have this proving the fourier expansion is easy.

$$
\begin{aligned}
F(r) &= \sum_n F_n \exp{(iG_n \cdot r)}, \\
F(r)\exp{(-iG_m \cdot r)} &= \sum_n F_n \exp{(iG_n \cdot r)} \exp{(-iG_m \cdot r)}, \\
\int_{\mathcal{V}} F(r)\exp{(-iG_m \cdot r)} &= \int_{\mathcal{V}} \sum_n F_n \exp{(iG_n \cdot r)} \exp{(-iG_m \cdot r)}, \\
\int_{\mathcal{V}} F(r)\exp{(-iG_m \cdot r)} &= \sum_n F_n \int_{\mathcal{V}} \exp{(iG_n \cdot r)} \exp{(-iG_m \cdot r)}, \\
\int_{\mathcal{V}} F(r)\exp{(-iG_m \cdot r)} &= \sum_n F_n V \delta_{mn}, \\
\int_{\mathcal{V}} F(r)\exp{(-iG_m \cdot r)} &= F_m V. \qquad (31)
\end{aligned}
$$

Since m is a mute index we can actually name it however we want, in this case n. So from eq. 31 we conclude

$$
F_m = \frac{1}{V}\int_{\mathcal{V}} F(r)\exp{(-iG_m \cdot r)}.\blacksquare \qquad (32)
$$

b. Integral over Brillouin zone

Solution: Let's take different cases first when $n = -m$

$$
\frac{V}{(2\pi)^3}\int_{BZ} \cancelto{1}{\exp{[ik \cdot (R_{-m} + R_m)]}} dk = \frac{V}{(2\pi)^3}\int_{BZ} dk, \qquad (33)
$$

But we know that the volume of the Brillouin zone is $(2\pi)^3/V$, hence

$$
\frac{V}{(2\pi)^3}\int_{BZ} dk = 1. \qquad (34)
$$

If $n \neq -m$ we will have

$$
\frac{V}{(2\pi)^3}\int_{BZ} \exp{[ik \cdot (R_n + R_m)]} dk = \frac{V}{(2\pi)^3} \left. \frac{\exp{[ik \cdot (R_n + R_m)]}}{ik \cdot (R_n + R_m)} \right|_{\partial BZ}, \qquad (35)
$$

If we center the Brillouin zone in the origin, it can help us. Because the k vectors of the Brillouin zone are periodic in such zone. So they will have to have the same values the boundaries of the Brillouin zone ∂BZ but at opposite sides, so they will actually cancel each other (since we centered the Brillouin zone on the origin). Other way to see this is that we are integrating a function over its period, so the result will be zero. Therefore we conclude

$$
\frac{V}{(2\pi)^3}\int_{BZ} \exp{[ik \cdot (R_n + R_m)]} dk = 0. \qquad (36)
$$

And finally we have

$$
\frac{V}{(2\pi)^3}\int_{BZ} = \delta_{n,-m} \qquad (37)
$$

c. Deltas 1

Solution: For this I will show how it's done for 1D and the extension will be easy to do. First we need to consider the lattice function

$$f(x) = \sum_{n=-\infty}^{\infty} \delta(x - na). \tag{38}$$

This represents a function with period a, so we can also expand in fourier series the same function

$$f(x) = \sum_{h=-\infty}^{\infty} c_h \exp\left(i2\pi h \frac{x}{a}\right). \tag{39}$$

We are interested on the coefficients c_h, so lets do that

$$\begin{aligned} c_h &= \frac{1}{|a|} \int_{-a/2}^{a/2} f(x) \exp\left(i2\pi h \frac{x}{a}\right) dx, \\ &= \frac{1}{|a|} \int_{-a/2}^{a/2} \sum_{n=-\infty}^{\infty} \delta(x - na) \exp\left(i2\pi h \frac{x}{a}\right) dx, \\ &= \frac{1}{|a|} \int_{-a/2}^{a/2} \delta(x) \exp\left(i2\pi h \frac{x}{a}\right) dx, \\ \frac{1}{|a|}&. \end{aligned} \tag{40}$$

Therefore

$$\sum_{n=-\infty}^{\infty} \delta(x - na) = \frac{1}{|a|} \sum_{h=-\infty}^{\infty} \exp\left(i2\pi h \frac{x}{a}\right) = \frac{1}{|a|} \sum_{h=-\infty}^{\infty} \exp\left(ik_x x\right). \tag{41}$$

If we extend this procedure to 3D we will find

$$\sum_{n=-\infty}^{\infty} \delta(k - G_n) = \frac{V}{(2\pi)^3} \sum_{n=-\infty}^{\infty} \exp\left(ik \cdot r_n\right). \tag{42}$$

d. Last one

Solution: Now lets consider the following lattice function

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} \delta(r - R_n) = \\ &= FT^{-1}\left(\frac{1}{B^N} \frac{1}{V} \sum_{h=-\infty}^{\infty} \delta\left(r' - \frac{2\pi}{k}(h_1 b_1 + \cdots + h_N b_n)\right)\right), \\ &= \frac{1}{V} \int_{-\infty}^{\infty} \sum_{h=-\infty}^{\infty} \delta\left(r - \frac{2\pi}{k}(h_1 b_1 + \cdots + h_N b_n)\right) \exp(ikr' \cdot r) dr', \\ &= \frac{1}{V} \sum_{h=-\infty}^{\infty} \exp[i2\pi \left((h_1 b_1 + \cdots + h_N b_n) \cdot r\right], \end{aligned}$$

$$\boxed{= \frac{1}{V} \sum_{h=-\infty}^{\infty} \exp[iG_n \cdot r]. \blacksquare \qquad (43)}$$