Lecture 9

The key feature of a crystal structure is it's periodicity. While describing the underlying physics, this periodic nature often comes into place. Another thing that is periodic in nature is wave. While describing the diffraction of electromagnetic wave by a periodic crystal structure, one introduces a a periodic crystal structure, one introduces a very important concept, namely the reciprocal lattice. There are many places in solid state physics where the reciprocal lattice is essential. We will discuss about the reciprocal lattice from few elementary features of the reciprocal lattice from a general point of view, without concentrating on the applications for now.

Definition of a reciprocal lattice

Consider a discrete set of ~~discrete~~ vectors $\vec{R}$ that constitutes a Bravais lattice, and a plane wave of the form,

$$\Psi_k(\vec{r}) = \Psi_0 \, e^{i\vec{k}\cdot\vec{r}} \qquad |\vec{k}| = \frac{2\pi}{\lambda}$$

where $\vec{k}$ is any arbitrary wave vector, and $\vec{R}$ is given by,

$$\vec{R} = n_1 \vec{a_1} + n_2 \vec{a_2} + n_3 \vec{a_3}$$

where $\vec{a_i}$'s are primitive translation vectors and $n_i \in \mathbb{Z}$.

For arbitrary $\vec{k}$, such a plane wave will not, of course have the periodicity (spatial) of the Bravais lattice, but for certain choices of $\vec{k}$ it will. "The set of all wave vectors $\vec{K}$ that yield plane waves with the periodicity of a given ~~Bravais~~ Bravais lattice is known as the reciprocal lattice".

It means, we are looking for all waves $\Psi_k(\vec{r})$ that remain unchanged when being shifted by any Bravais lattice vector $\vec{R}$. Formally,

$$\Psi_k(\vec{r}) = \Psi_k(\vec{r}+\vec{R})$$

$$\Rightarrow \Psi_0 e^{i\vec{k}\cdot\vec{r}} = \Psi_0 e^{i\vec{k}\cdot(\vec{r}+\vec{R})}$$

$$\Rightarrow e^{i\vec{k}\cdot\vec{r}} \times e^{i\vec{k}\cdot\vec{R}} = e^{i\vec{k}\cdot\vec{r}}$$

$$\boxed{\therefore e^{i\vec{k}\cdot\vec{R}} = 1} \quad \text{—— (1)}$$

for all $\vec{R}$ in the Bravais lattice.

Note that, the reciprocal lattice is defined with reference to a particular Bravais lattice. The Bravais lattice that determines a given reciprocal lattice is often referred to as the direct lattice.

Reciprocal lattice as a Bravais lattice

Since $\vec{R}$ is a discrete set of vectors, there must be some restrictions to the possible vectors $\vec{K}$ as well. The fact that the reciprocal lattice is itself a Bravais lattice follows from the definition of Bravais lattice (A Bravais lattice is a discrete set of vectors not all in one plane, closed under addition and subtraction), along withe the fact that, if $\vec{K_1}$ and $\vec{K_2}$ satisfies equation (1), so will their sum and differences.

Let's represent $\vec{K}$ with respect to some basis $\vec{b}_i$, given by,

$$\vec{K} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3$$

where $\vec{b}_i$'s are not further specified.

Since we are free to choose any basis $\{\vec{b}_i\}$ in order to represent the vectors $\vec{K}$, we choose the simplest one, that the basis $\{\vec{b}_i\}$ is orthogonal to the primitive translation vectors $\{\vec{a}_i\}$

$$\therefore \quad \vec{b}_i \cdot \vec{a}_j = 2\pi\, \delta_{ij}$$

where we have introduced a factor of 2π. δ_{ij} is the Kronecker delta, with, $\delta_{ij} = \begin{cases} 0 ; & i \neq j \\ 1 ; & i = j \end{cases}$

So, $\vec{b}_1 \cdot \vec{a}_1 = 1$, $\vec{b}_1 \cdot \vec{a}_2 = 0$, $\vec{b}_1 \cdot \vec{a}_3 = 0$ and so on so forth.

In this choice,

$$\vec{b}_1 \cdot \vec{a}_2 = 0 \qquad \text{and so} \quad \vec{b}_1 \perp \vec{a}_2 \text{ and } \vec{b}_1 \perp \vec{a}_3.$$
$$\vec{b}_1 \cdot \vec{a}_3 = 0$$

which means $\vec{b}_1 \parallel (\vec{a}_2 \times \vec{a}_3)$.

$$\therefore \quad \vec{b}_1 = c\, (\vec{a}_2 \times \vec{a}_3)$$

Again, $\vec{b}_1 \cdot \vec{a}_1 = 2\pi$

$$\Rightarrow c\, \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 2\pi$$

$$\therefore \quad c = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\therefore \quad \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Similarly,

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$
$$= \vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)$$
$$= \vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)$$

Now,

$$\vec{K} = K_1\vec{b_1} + K_2\vec{b_2} + K_3\vec{b_3} \quad \text{and} \quad \vec{R} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3}$$

$$\therefore \vec{K}.\vec{R} = (n_1K_1 + n_2K_2 + n_3K_3)\,2\pi$$

But, the condition for the reciprocal lattice was,

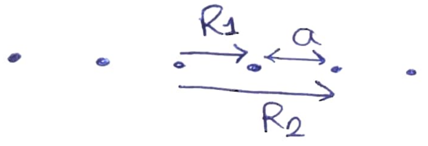
$$e^{i\vec{K}.\vec{R}} = 1, \quad \text{meaning} \quad \vec{K}.\vec{R} = 2\pi l \text{ with } l \in \mathbb{Z}$$

$$\boxed{\therefore \; n_1K_1 + n_2K_2 + n_3K_3 = l}$$

Since, n_1, n_2, n_3 are already integers, So, for the r.h.s. to be an integer for any choices of n_i's, K_i's must be integers as well.

Thus, the condition ① that $\vec{K}$ be a reciprocal lattice vector is satisfied by just those vectors that are linear combinations of the b_i's with integer coefficients K_i's. Thus, the reciprocal lattice is a Bravais lattice with $\vec{b_i}$'s being the primitive vectors.

What we have done here strictly applies to 3D Bravais lattice and it's reciprocal counterpart. Say, we want to see how the 1D Bravais lattice and it's reciprocal lattice would look like.



Consider the 1D Bravais lattice, with lattice constant a. Here, the position vector of any point is given by,

$$\vec{R} = n\vec{a}\,, \quad \text{where } \vec{a} = a\hat{i} \text{ is the basis vector}$$

We look for the $\vec{K}$ vectors for which,

$$\vec{K}\cdot\vec{R} = 2\pi l \quad \text{——— (11)}$$

Since its 1D, the basis vector in ~~reciproc~~ reciprocal lattice will be parallel to $\vec{a}$ (since if it is perpendicular, the equation (11) is only satisfied for $l=0$).

$$\therefore \vec{K} = K\vec{b} \quad \text{with} \quad \vec{b} = b\hat{a}$$

$$\therefore (11) \Rightarrow \quad Kb\hat{a}\cdot na\hat{a} = 2\pi l$$

$$\therefore \; k_n = \frac{2\pi}{ba} l$$

For $k_n = l$ (like in 3D), $b = \frac{2\pi}{a}$.

$$\boxed{\therefore \; \vec{K} = k \frac{2\pi}{a} \hat{a}}$$

where $k \in \mathbb{Z}$. This set of $\vec{K}$ vectors will constitute the reciprocal lattice. The unit is obviously $\left(\frac{1}{\text{length}}\right)$. One can confirm that indeed, for this set of vectors $\vec{K}$ the wave is periodic for any value of $\vec{R} = n\vec{a}$.

The reciprocal of the reciprocal lattice

Since the reciprocal lattice itself is a Bravais lattice, one can construct the reciprocal of the, 2nd reciprocal lattice, which turns out to be the direct lattice. The reciprocal lattice of the reciprocal lattice should satisfy the condition–

$$e^{i\vec{G}\cdot\vec{K}} = 1 \qquad \text{(III)}$$

for all $\vec{K}$ in the reciprocal lattice.

Since any direct lattice vector $\vec{R}$ has the same property, $(e^{i\vec{R}.\vec{K}} = 1)$, the set of vectors $\vec{G}$ are basically the set of vectors $\vec{R}$. Hence, all direct lattice vectors are in the reciprocal of reciprocal lattice. Furthermore, no other vectors can be, which is not in the direct lattice having the form $\vec{r} = x_1\vec{a_1} + x_2\vec{a_2} + x_3\vec{a_3}$ with at least one non-integar x_i. This is because, for the reciprocal lattice vector $\vec{K} = \Sigma K_i \vec{b_i}$, $e^{i\vec{K}.\vec{r}}$ will not be equal to 1, and the condition (iii) is violated. So, reciprocal of a reciprocal lattice is the direct lattice.

Reciprocal lattice in two dimension

For an infinite 2D Bravais lattice, defined by it's primitive vectors $\vec{a_1}$ and $\vec{a_2}$, it's reciprocal lattice can be determined by generating two reciprocal primitive vectors, such that,

$$\vec{K} = K_1\vec{b_1} + K_2\vec{b_2}$$

where $\vec{b_1}$ and $\vec{b_2}$ are ~~re~~ reciprocal primitive vectors and K_1, K_2 are integers as required by

$$\boxed{K_1 n_1 + K_2 n_2 = l}$$ for 2D.

How do we form the primitive vectors $\vec{b}_1$ and $\vec{b}_2$?

Again, we start with the requirement,

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

In matrix notation, we can write this as–

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

Multiplying with the inverse matrix on the right we get,

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

Transposing this so that we can read off the matrix column-by-column to get the b_is.

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

$$\therefore \begin{pmatrix} b_{1x} \\ b_{1y} \end{pmatrix} = \frac{2\pi}{a_{1x} a_{2y} - a_{1y} a_{2x}} \begin{pmatrix} a_{2y} \\ -a_{2x} \end{pmatrix}$$

and $\begin{pmatrix} b_{2x} \\ b_{2y} \end{pmatrix} = \frac{2\pi}{a_{1x}a_{2y} - a_{1y}a_{2x}} \begin{pmatrix} -a_{1y} \\ a_{1x} \end{pmatrix}$

One can explicitely write the primitive vectors as,

$$\vec{b}_1 = 2\pi \frac{Q\vec{a}_2}{\vec{a}_1 \cdot Q\vec{a}_2} \quad \text{and} \quad \vec{b}_2 = 2\pi \frac{Q(-\vec{a}_1)}{\vec{a}_2 \cdot Q(-\vec{a}_1)}$$

$$\therefore \vec{b}_2 = 2\pi \frac{Q\vec{a}_1}{\vec{a}_2 \cdot Q\vec{a}_1}$$

where Q is a $90°$ rotation matrix given by $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. You can easily check that $\vec{b}_1 \cdot \vec{a}_1 = 2\pi$, $\vec{b}_1 \cdot \vec{a}_2 = 0$ for the given b_i's, and so on so forth.

Important examples

(i) For a simple cubic Bravais lattice with the primitive cell with side length a, the primitive vectors of the direct lattice is,

$$\vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y}, \quad \vec{a}_3 = a\hat{z}$$

Now, $$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a^3} \times a^2 \hat{x}$$

$$\therefore \vec{b}_1 = \frac{2\pi}{a} \hat{x}$$

Similarly, $\vec{b}_2 = \frac{2\pi}{a} \hat{y}$ and $\vec{b}_3 = \frac{2\pi}{a} \hat{z}$.

So, the reciprocal of a simple cubic lattice is again a simple cubic lattice with cubic primitive cell of side $\frac{2\pi}{a}$.

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