# Symmetry operations

$$\{\vec{R}_n\} \xrightarrow{S} \{\vec{R}_n'\}$$

order $\{\vec{R}_n\}$ and $\{\vec{R}_n'\}$

if they are equal $\Rightarrow$ $S$ is a symmetry operation

$$\{\vec{R}_n\} \xrightarrow{S'} \{\vec{R}_n'\}$$

$$\{\vec{R}_n\} \xrightarrow{S''} \{\vec{R}_n''\}$$

if $\{\vec{R}_n'\} = \{\vec{R}_n''\}$ $\Rightarrow$ $S'$ is equiv. to $S''$

| | $E$ | $i$ | $C_2\vert x$ | |
|---|---|---|---|---|
| $E$ | $E$ | $i$ | $C_2/x$ | |
| $i$ | $i$ | $E$ | $C_2\vert x \otimes i$ | ... |
| $C_2\vert x$ | $C_2/x$ | $i \otimes C_2\vert x$ | $E$ | |
| ⋮ | | | | |

Crystal systems and lattice centering:

Primitive: lattice points only on the corners

Body centered: Primitive + a point at the center of the cell

face centered: Primitive + points at the center of all faces

base centered: Primitive + 2 lattice points in the middle of parallel faces

$(A, B, C)$

In principle, there are $7 \times 6 = 42$ Bravais lattices

After symmetry reduction $\Rightarrow$ 14 Bravais lattices in 3D.

## 4.2. Bloch theorem

$h$ and $T_{\vec{R}_n}$ commute

$$T_{\vec{R}_n} h \, \varphi_{0_i}(\vec{r}) = h \, T_{\vec{R}_n} \varphi_{0_i}(\vec{r})$$

$\Rightarrow$ $\varphi_{0_i}(\vec{r})$ and $T_{\vec{R}_n} \varphi_{0_i}(\vec{r})$ have are both eigenfunctions of $h$ and also have the same eigenvalue

Two cases:

1) $\varepsilon_{0_i}$ is non-degenerate

$\Rightarrow$ $\varphi_{0_i}(\vec{r})$ and $T_{\vec{R}_n} \varphi_{0_i}(\vec{r})$ are physically equivalent

$$T_{\vec{R}_n} \varphi_{0_i}(\vec{r}) = e^{i\alpha} \varphi_{0_i}(\vec{r}) \qquad \alpha(\vec{R}_n) \in \mathbb{R}$$

$$T_{\vec{R}_n} T_{\vec{R}_m} \varphi_{0_i}(\vec{r}) = e^{i\alpha(\vec{R}_n)} e^{i\alpha(\vec{R}_m)} \varphi_{0_i}(\vec{r})$$

$$T_{\vec{R}_n + \vec{R}_m} \varphi_{0_i}(\vec{r}) = e^{i\alpha(\vec{R}_n + \vec{R}_m)} \varphi_{0_i}(\vec{r})$$

$$\Rightarrow \quad \alpha(\vec{R}_n + \vec{R}_m) = \alpha(\vec{R}_n) + \alpha(\vec{R}_m)$$

$$\alpha(j \vec{R}_n) = j \, \alpha(\vec{R}_n) \qquad \underline{j \in \mathbb{Z}}$$

$\Rightarrow \quad \alpha(\vec{R}_n)$ is linear in $R_n$

$$\alpha(\vec{R}_n) = \vec{k}\,\vec{R}_n$$

Therefore,

$$T_{\vec{R}_n} f_{0_i}(\vec{r}) = f_{0_i}(\vec{r}+\vec{R}_n) = e^{i\vec{k}\vec{R}_n} f_0(\vec{r})$$

The vector $\vec{k}$ labels the eigenvalues of $T_{\vec{R}_n}$ and the eigenfunctions of $f_{0_i}(\vec{r})$

2) The eigenvalues are f-fold degenerate.

<u>Prove yourself</u>

Summary:

$T_{\vec{R}_n}$ and h have the same eigenvalues and eigenfunctions.

We can label them by $\vec{k}$

From this point, we will write $f_{\vec{k}}(\vec{r})$ and $\varepsilon_{\vec{k}}$.

The statement

$$T_{\vec{R}_n} f_{\vec{k}}(\vec{r}) = f_{\vec{k}}(\vec{r}+\vec{R}_n) = e^{i\vec{k}\vec{R}_n} f_{\vec{k}}(\vec{r})$$

is called <u>Bloch theorem</u>.

Ansatz:

$$f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{\vec{k}}(\vec{r})$$

$$T_{\vec{R}_n} f_{\vec{k}}(\vec{r}) = e^{i\vec{k}(\vec{r}+\vec{R}_n)} u_{\vec{k}}(\vec{r}+\vec{R}_n)$$

Because $f_{\vec{k}}(\vec{r})$ satisfies Bloch theorem

$$T_{\vec{R}_n} f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{R}_n} f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{R}_n} e^{i\vec{k}\vec{r}} u_{\vec{k}}(\vec{r})$$

$$\Longrightarrow \quad u_{\vec{k}}(\vec{r}+\vec{R}_n) = u_{\vec{k}}(\vec{r})$$

The function $u_{\vec{k}}(\vec{r})$ has the periodicity of the Bravais lattice

<u>Second formulation of Bloch theorem</u>

$$f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{\vec{k}}(\vec{r})$$

If $V^{eff} \equiv const$

$$f_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V_g}} e^{i\vec{k}\vec{r}}$$

## 4.3. Reciprocal lattice

$$e^{i\vec{k}'\vec{r}} \stackrel{?}{=} e^{i\vec{k}\vec{r}}$$

$$\vec{k}' = \vec{k} + \vec{G}_m$$

$$\vec{G}_m \vec{R}_m = 2\pi N \qquad N \in \mathbb{Z}$$

The set of points $\{\vec{G}_n\}$ is the reciprocal lattice of a Bravais lattice $\{\vec{R}_n\}$.

Second definition:

All vectors that satisfy

$$e^{i\vec{G}_n\vec{R}_n} = 1$$ form a reciprocal lattice $\forall\ \vec{R}_n$ in the Bravais lattice

What are the basis vectors of the reciprocal lattice:

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

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

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

$\Omega$ - the volume of the Wigner Seitz cell.

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

$$\Rightarrow \vec{G}_n = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3,\ m_i \in \mathbb{Z}$$

Proof that $\vec{G}_n$ is a reciprocal lattice:

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

$$\vec{G}_m \vec{R}_n = 2\pi(m_1 n_1 + m_2 n_2 + m_3 n_3)$$

$$\Rightarrow e^{i \vec{G}_m \vec{R}_n} = 1$$

What is the Wigner-Seitz cell of the reciprocal lattice? It is called

<u>1st Brillouin zone</u>.

The point at $\vec{k} = 0$ is called $\Gamma$.

Due to translational invariance of $v^{eff}$:

$$v^{eff}(\vec{r}) = \sum_{\ell} v^{eff}(\vec{G}_\ell) e^{i \vec{G}_\ell \vec{r}}$$

$$\vec{G}_\ell \cdot \vec{R}_n = 2\pi N$$

For $\psi_{\vec{k}}(\vec{r})$:

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} \sum_m C_{\vec{G}_m}(\vec{k}) e^{i\vec{G}_m \vec{r}}$$

The Kohn-Sham equations:

$$\sum_m \frac{\hbar^2}{2m}(\vec{k} + \vec{G}_m)^2 C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k} + \vec{G}_m)\vec{r}} +$$

$$\sum_\ell v^{eff}(\vec{G}_\ell) \sum_m C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k} + \vec{G}_m + \vec{G}_\ell)\vec{r}} =$$

$$= \varepsilon(\vec{k}) \sum_m C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k} + \vec{G}_m)\vec{r}}$$

Separate for $C_{\vec{G}_m}(\vec{k})$:

$$\frac{\hbar}{2m}(\vec{K}+\vec{G}_n)^2 C_{\vec{G}_n}(\vec{K}) +$$

$$\sum_m v^{eff}(\vec{G}_n - \vec{G}_e) C_{\vec{G}_m}(\vec{K}) =$$

$$= \mathcal{E}(\vec{K}) C_{\vec{G}_n}(\vec{K})$$

The only coefficients that are coupled by $v^{eff}(\vec{G}_n - \vec{G}_m)$, are those that differ by $\vec{K}$,

$\Rightarrow$ The plane-wave $e^{i\vec{K}\vec{r}}$ is coupled with other plane waves $e^{i(\vec{K}+\vec{G}_m)\vec{r}}$

$$\sum_m h_{n,m} C_{\vec{G}_m}(\vec{K}) = \mathcal{E}(\vec{K}) C_{\vec{G}_n}$$

$$h_{n,m} = \frac{\hbar^2}{2m}(\vec{K}+\vec{G}_n)^2 \delta_{n,m} + v^{eff}(\vec{G}_n - \vec{G}_m)$$

Label the eigenfunctions as

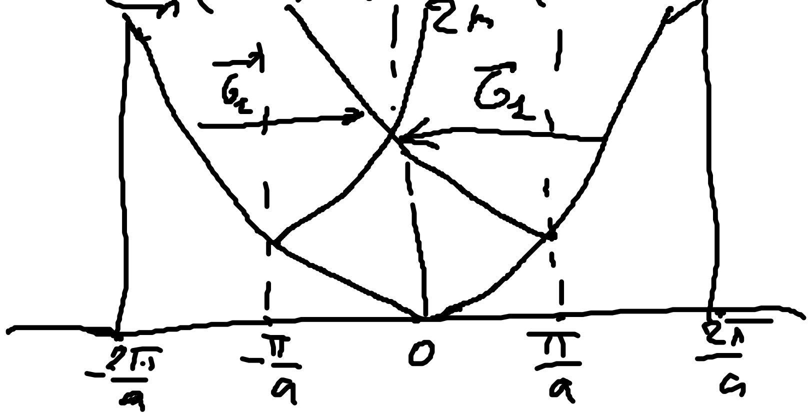
$$f_{n,\vec{K}}(\vec{r}), \quad \mathcal{E}_n(\vec{K})$$

K-point

band index

1D electron system in a weakly varying potential

$$\varepsilon_n(\vec{K}) \approx \frac{\hbar^2}{2m}\left(\vec{K}+\vec{G}_m\right)^2$$




1st BZ