Symmetry operations

$$\{\vec{R_n}\} \xrightarrow{S} \{\vec{R_n'}\}$$

order $\{\vec{R_n}\}$ and $\{\vec{R_n'}\}$

if they are equal => S is a symmetry operation

$$\{\vec{R_n}\} \xrightarrow{S'} \{\vec{R_n'}\}$$

$$\{\vec{R_n}\} \xrightarrow{S''} \{\vec{R_n''}\}$$

if $\{\vec{R_n'}\} = \{\vec{R_n''}\}$ => 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

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

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

Two cases:

1) ε_{0i} is non-degenerate

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

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

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

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

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

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

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

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

Therefore,

$$T_{\vec{R}_n} \varphi_{0i}(\vec{r}) = \varphi_{0i}(\vec{r}+\vec{R}_n) = e^{i\vec{k}\vec{R}_n}\varphi_0(\vec{r})$$

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

e) The eigenvalues are f-fold degenerate.

Prove yourself

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 $\varphi_{\vec{k}}(\vec{r})$ and $\varepsilon_{\vec{k}}$.

The statement

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

is called Bloch theorem.

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

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

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

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 $v^{eff} \equiv \text{const}$

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

4.3. Reciprocal lattice

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

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

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

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:

$$\vec{b_1} = \frac{2\pi}{\Omega}(\vec{a_2} \times \vec{a_3})$$

$$\vec{b_2} = \frac{2\pi}{\Omega}(\vec{a_3} \times \vec{a_2})$$

$$\vec{b_3} = \frac{2\pi}{\Omega}(\vec{a_2} \times \vec{a_2})$$

Ω - the volume of the Wigner Seitz cell.

$$\Omega = \vec{a_1}(\vec{a_2} \times \vec{a_3})$$

$$\Rightarrow \vec{G_n} = m_1\vec{b_1} + m_2\vec{b_2} + m_3\vec{b_3}, \quad m_i \in \mathbb{Z}$$

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 Γ.

Due to translational invariance of v^{eff}:
$$v^{eff}(\vec{r}) = \sum_{l} v^{eff}(\vec{G}_l) e^{i\vec{G}_l \vec{r}}$$
$$\vec{G}_l \cdot \vec{R}_n = 2\pi N$$

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:
$$\sum_{m} \frac{\hbar^2}{2m}(\vec{k}+\vec{G}_m)^2 C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k}+\vec{G}_m)\vec{r}} +$$
$$\sum_{l} v^{eff}(\vec{G}_l) \sum_{m} C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k}+\vec{G}_m+\vec{G}_l)\vec{r}} =$$
$$= \varepsilon(\vec{k}) \sum_{m} C_{\vec{G}_m}(\vec{k}) e^{i(\vec{k}+\vec{G}_m)\vec{r}}$$

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

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

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

$$= \varepsilon(\vec{K})\, C_{\vec{G}_n}(\vec{K})$$

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 $e^{i(\vec{K}+\vec{G}_n)\vec{r}}$

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

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

Label the eigenfunctions as

$$f_{n,\vec{K}}(\vec{r}), \quad \varepsilon_n(\vec{K})$$

$\vec{K}$: K-point

n: band index

1D electron system in a weakly varying potential

$$\varepsilon_n(\vec{k}) \simeq \frac{\hbar^2}{2m}\left(\vec{k} + \vec{G}_n\right)^2$$