Lecture 9

Recap: 230 Space groups in 3D

- $T \triangleleft G$ - every space group has a Bravais lattice

73 symmorphic $G = T \rtimes \bar{G}$ ← point group

- $\bar{G} < G$ $\quad G = \bigcup_{i=0}^{n-1} T\{R_i|\vec{0}\}$ $\quad R_i \in \bar{G}$
- $g \in G \Rightarrow \{R|\vec{t}\}$ $\quad R \in \bar{G}, \vec{t} \in T$
- Hermann-Maugin notation [letter][pt group symbol]

157: Nonsymmorphic $\bar{G} \not< G$

$G = \bigcup_{i=0}^{n-1} T\{R_i|\vec{d}_i\}$ $\quad R_i \in \bar{G}$

at least one $\vec{d}_i$ must be

a fraction of a Bravais lattice translation

- Typically contain screw rotations or glide reflections
- Hermann-Mauguin symbol:
  - subscripts to indicate screws
  - letters for glide reflections

Space group symmetries and Band structure

Noninteracting Hamiltonian H invariant under space group G

Bravais lattice $T \triangleleft G$

point group $\bar{G}$

Translation symmetry $\rightarrow$ Bloch's theorem

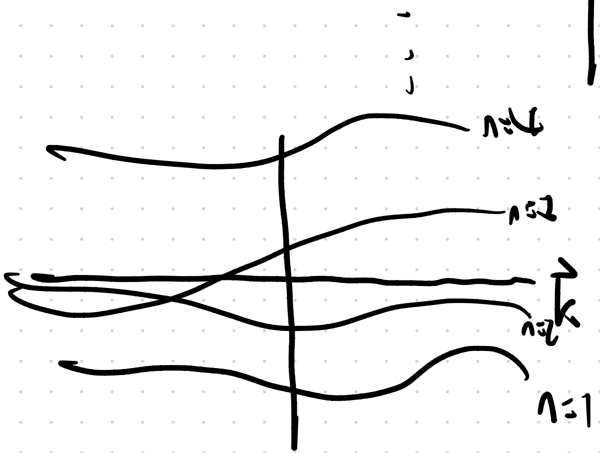
$$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

$$U_{\vec{t}}|\psi_{nk}\rangle = e^{-ik\cdot t}|\psi_{nk}\rangle$$

Hilbert space $\mathcal{H} = \bigcup_{\vec{k}\in BZ} \{|\varphi_{ak}\rangle\}$

$$U_t|\varphi_{ak}\rangle = e^{-ik\cdot\vec{t}}|\varphi_{a\vec{k}}\rangle$$

Schur's lemma $\langle\varphi_{a\vec{k}}|H|\varphi_{bk'}\rangle = h_{ab}(k)\delta_{kk'}$



E_{nk} are eigenvalues of $h_{ab}(k)$

$\boxed{\begin{array}{l} n, m \text{ - label energy eigenstates} \\ a, b, c, \text{ label general basis states in Hilbert space} \end{array}}$

What do symmetries like $\{g|\vec{d}\} \in G$ do to Bloch states?

$\bar{g} \in \bar{G}$

Unitary operator $U_{\{\bar{g}|\vec{d}\}}$ implements this transformation on Hilbert space of wavefunctions

$$\mathcal{U}_{\{\bar{g}|\vec{d}\}} \hat{X} \, \mathcal{U}^{-1}_{\{\bar{g}|\vec{d}\}} = \bar{g}\hat{X} + \vec{d}$$ on position operator

$$[H, \mathcal{U}_{\{\bar{g}|\vec{d}\}}] = 0$$ since G is the group of symmetries of H

$\mathcal{U}_{\{\bar{g}|\vec{d}\}} |\varphi_{a\vec{k}}\rangle \leftarrow$ What state is this

in particular How does it transform under our Bravais lattice.

- Same?
- ~~$\bar{g}k$~~

$$\mathcal{U}_{\{E|\vec{t}\}}\left(\mathcal{U}_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle\right) = \left(\mathcal{U}_{\{E|\vec{t}\}} \mathcal{U}_{\{\bar{g}|\vec{d}\}}\right) |\varphi_{ak}\rangle$$

$$\{\bar{g}|\vec{d}+\vec{t}\} = \{\bar{g}|\vec{d}\}\{E|\bar{g}^{-1}\vec{t}\}$$

$$= U_{\{E|\vec{t}\}\{\bar{g}|\vec{d}\}} |\psi_{ak}\rangle$$

$$= U_{\{\bar{g}|\vec{d}+\vec{t}\}} |\psi_{ak}\rangle$$

$$= U_{\{\bar{g}|\vec{d}\}} U_{\{E|\bar{g}^{-1}\vec{t}\}} |\psi_{ak}\rangle$$

$$= e^{-i\vec{k}\cdot(\bar{g}^{-1}\vec{t})} \left(U_{\{\bar{g}|\vec{d}\}} |\psi_{ak}\rangle\right)$$

is a translation by Bravais lattice vector $\bar{g}^{-1}\vec{t}$

But $\cdot$ is invariant under any rotation or reflection

$$\vec{k}\cdot(\bar{g}^{-1}\vec{t}) = (\bar{g}\vec{k})\cdot(\bar{g}\bar{g}^{-1}t) = \bar{g}k\cdot\vec{t}$$

$$u_{\{E|\vec{t}\}}\left(u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle\right) = e^{-i\,\bar{g}k\cdot\vec{t}}\left(u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle\right)$$

$u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle$ transforms in the irrep of T labelled by $\bar{g}k$ (has crystal momentum $\bar{g}k$)

↳ (if $\bar{g}\vec{k}$ is outside BZ we add $\vec{b}\in T$ to it)

Completeness:

$$u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle = \sum_{\substack{b \\ k'\in BZ}} \underbrace{|\varphi_{bk'}\rangle\boxed{\langle\varphi_{bk'}|}\, u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle}\ \ k'=\bar{g}k$$

$$= \sum_{b} |\varphi_{b\,\bar{g}k}\rangle \underbrace{\left(\langle\varphi_{b\,\bar{g}k}|u_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle\right)}_{=B^{\vec{k}}_{ba}(\{\bar{g}|\vec{d}\})}$$

$$\boxed{\langle \varphi_{bk'} | U_{\{E|\vec{t}\}} U_{\{\bar{g}|\vec{d}\}} | \varphi_{ak} \rangle}$$

$$= e^{-ik'\cdot t} \langle \varphi_{bk'} | U_{\{\bar{g}|\vec{d}\}} | \varphi_{a\vec{k}} \rangle$$

$$= \underline{e^{-i\bar{g}k\cdot\vec{t}}} \langle \varphi_{bk'} | U_{\{\bar{g}|\vec{d}\}} | \varphi_{a\vec{k}} \rangle$$

So $k' = \bar{g}k$ or $\langle \varphi_{bk'} | U_{\{\bar{g}|\vec{d}\}} | \varphi_{ak} \rangle = 0$

Sewing matrix for $\{\bar{g}|\vec{d}\}$

We can do the same thing in the basis $|\psi_{nk}\rangle$ of eigenstates of H

$$U_{\{\bar{g}|\vec{d}\}} |\psi_{nk}\rangle = \sum_m |\psi_{m\bar{g}k}\rangle \underbrace{\langle \psi_{m\bar{g}k} | U_{\{\bar{g}|\vec{d}\}} | \psi_{nk} \rangle}_{= B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\})}$$

Sewing matrix in Basis of Hamiltonian eigenstates

Because $[H, U_{\{\bar{g}|\vec{d}\}}] = 0$ we get two constraints:

$$[H, u_{\{\bar{g}|\vec{d}\}}]|\psi_{nk}\rangle = 0 = H\left(u_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle\right) - u_{\{\bar{g}|\vec{d}\}}\left(H|\psi_{nk}\rangle\right)$$

$$\boxed{H\left(u_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle\right) = E_{nk}\left(u_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle\right)}$$

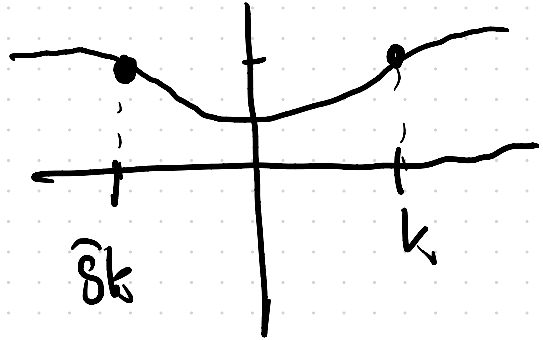
$$\| \qquad\qquad\qquad\qquad \|$$

$$\sum_m H|\psi_{m\bar{g}k}\rangle B^k_{mn}(\{\bar{g}|\vec{d}\})$$

$$\|$$

$$\sum_m E_{m\bar{g}k}|\psi_{m\bar{g}k}\rangle B^k_{mn}\{\bar{g}|\vec{d}\}$$

- $B^k_{mn}(\{\bar{g}|\vec{d}\}) = 0$ whenever $E_{nk} \neq E_{m\bar{g}k}$
- if there is a state $|\psi_{nk}\rangle$ w/ energy E_{nk}, then there is a state $u_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle$ w/ energy $E_{n\bar{g}k} = E_{nk}$



Something special happens when $\bar{g}k = k + \vec{b}$ for $\vec{b}$ of a reciprocal lattice vector

$$e^{-i\bar{g}k\cdot\vec{t}} = e^{-i(\vec{k}+\vec{b})\cdot\vec{t}} = e^{-ik\cdot\vec{t}}$$

$\Rightarrow \{|\varphi_{a\bar{g}k}\rangle\}$ and $\{|\varphi_{ak}\rangle\}$ actually span the same Hilbert space

$B^{k}_{ab}(\{\bar{g}|\vec{d}\}) = \langle \varphi_{a\bar{g}k} | U_{\{\bar{g}|\vec{d}\}} | \varphi_{bk} \rangle$ is a maps

the vector space $\{|\varphi_{ak}\rangle\}$ to itself

Given $\vec{k}_*$ in the Brillouin zone (BZ)

$$G_{k_*} = \{ \{\bar{g}|\vec{d}\} \in G \mid \bar{g}k_* = k_* \text{ modulo } \check{T} \}$$

$G_{k_*} < G$ is a subgroup of the space group

$\boxed{\text{The little group of } k_*}$

$\{ B^{k_*}_{ab}(g_*) \mid g_* \in G_{k_*} \}$ ← form a representation of

$$G_{k_*}$$

$$B^{k_*}_{ab}(g_*) = \langle \varphi_{a\bar{g}k_*} | U_{g_*} | \varphi_{bk_*} \rangle$$
$$= \langle \varphi_{ak_*} | U_{g_*} | \varphi_{bk_*} \rangle$$

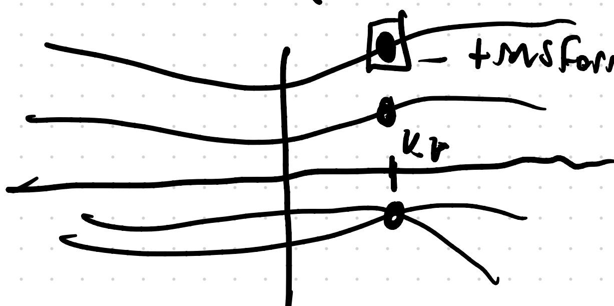
$$\boxed{h(\bar{g}k) B^k = B^k h(k)}$$

$$0 = \langle \varphi_{ak_*} | [H, U_{g_*}] | \varphi_{bk_*} \rangle$$
$$= \sum_c \langle \varphi_{ak_*} | H | \varphi_{ck_*} \rangle B^{k_*}_{cb}(g_*)$$
$$- \sum_c B^{k_*}_{ac}(g_*) \langle \varphi_{ck_*} | H | \varphi_{bk_*} \rangle$$

$$\Rightarrow \quad [B^{k_*}(g_*), h(k_*)] = 0$$

Schur's lemma: Eigenstates of H w/ crystal momentum k_* can be labelled by irreps of G_{k_*}

$$B^{k_*}(g_*) \cong \bigoplus_i \eta_i^{k_*} \qquad \text{irreps of } G_{k_*}$$



– transform in irreps of G_{k_*}

If $\eta_i^{k_*}$ has dimension >1

Schur's lemma $\Rightarrow$ these states are degenerate

Next time: Example of finding little groups