Lecture 10

Reminder: $\vec{k}_*$ be a vector in the BZ

space group G

little group $G_{\vec{k}_*} = \left\{ \{\bar{g}|\vec{d}\} \in G \mid \bar{g}\vec{k}_* = \vec{k}_* \bmod \check{T} \right\}$

$$G_{k_*} < G$$

if $g_{k_*} \in G_{k_*}$

$$U_{g_*}|\psi_{nk_*}\rangle = \sum_m |\psi_{m\bar{g}k_*}\rangle B^{k_*}_{mn}(g_{k_*})$$

$$= \sum_m |\psi_{mk_*}\rangle B^{k_*}_{mn}(g_{k_*})$$

$$B^{k_*}_{mn}(g_{k_*}) = \langle \psi_{mk_*} | U_{g_{k_*}} | \psi_{nk_*} \rangle$$

$\{ B^{k_*}_{mn}(g_*) \mid g_* \in G_{k_*} \}$ forms a represetentation of the little group

Schur's lemma: Eigenstates of H w/ crystal momentum k_* transform in irreps of G_{k_*} and states transforming in the same irrep are degenerate

Example: space group $G = \underset{\text{primitive centering}}{P}\underbrace{432}_{\text{octahedral point group}}$ Symmorphic space group

Primitive Bravais lattice vectors

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

$$G = \langle \vec{e}_1, \vec{e}_2, \vec{e}_3, C_{4z}, C_{3,111} \rangle$$

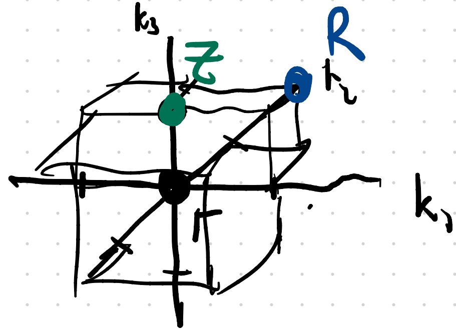
$\hookrightarrow$ primitive reciprocal lattice vectors

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$ $\quad$ $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

$\vec{b}_2 = \frac{2\pi}{a}\hat{y}$

Conventions

Γ is $\vec{k}=0$



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

$\Gamma: (k_1, k_2, k_3) = (0,0,0)$

$Z: (k_1, k_2, k_3) = (0, 0, \frac{1}{2})$

$R: (k_1, k_2, k_3) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

① Γ point $\vec{k}=0$

For any $\{\bar{g} | \vec{d}\} \in G$

$\bar{g}\vec{k} = 0$ if $\vec{k} = 0$

$G_\Gamma \cong G$ the entire space group

Translations are always in the little group of any $\vec{k}$

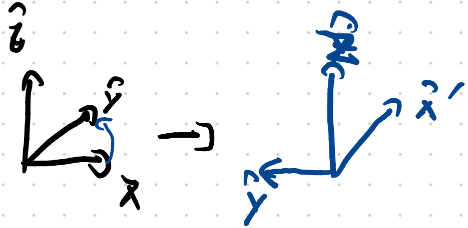
$\{E | \vec{t}\}$, $E\vec{k} = \vec{k}$

$\downarrow$

little groups are space groups

② R point $\vec{k}_R = \frac{1}{2}\vec{b}_1 + \frac{1}{2}\vec{b}_2 + \frac{1}{2}\vec{b}_3 = \frac{\pi}{a}(\hat{x}+\hat{y}+\hat{z})$

$T < G_R$

C_{4z}: 

$\hat{x} \to \hat{y}$

$\hat{y} \to -\hat{x}$

$\hat{z} \to \hat{z}$

$$C_{4z}\vec{k}_R = \frac{\pi}{a}(\hat{y} - \hat{x} + \hat{z})$$

$$\stackrel{?}{=} k_R + \vec{b}$$

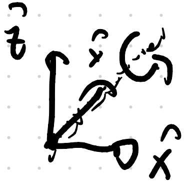
$$C_{4z}\vec{k}_R + \vec{b}_1 = \vec{k}_R$$

$$\to \quad C_{4z} \in G_R$$

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$ $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

$\vec{b}_2 = \frac{2\pi}{a}\hat{y}$

$C_{3,111}$



$C_{3,111}$: $\hat{x} \to \hat{y}$
$\hat{y} \to \hat{z}$
$\hat{z} \to \hat{x}$

$C_{3,111} k_R = k_R \qquad C_{3,111} \in G_R$

$G_R = G$ the entire space group $P432$

③ $Z \qquad k_Z = \frac{1}{2}\vec{b}_3 = \frac{\pi}{a}\hat{z}$

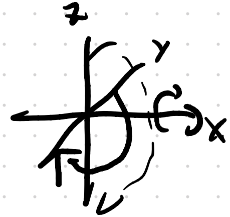
$\{E|\vec{t}\} \in G_Z$

$C_{4z} \in G_Z$

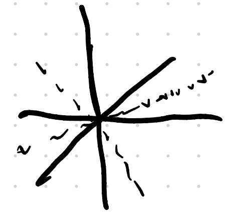
$C_{3,111} k_Z = \frac{\pi}{a}\hat{x}$

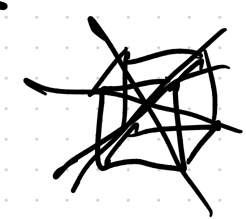
$C_{3,111} k_Z - k_Z = \frac{\pi}{a}(\hat{x} - \hat{z}) = \frac{1}{2}(\vec{b}_1 - \vec{b}_3)$

$\Rightarrow C_{3,111} \notin G_{k_z}$

C_{2x}: 

$\hat{x} \to \hat{x}$
$\hat{y} \to -\hat{y}$
$\hat{z} \to -\hat{z}$





$$C_{2x} k_z = -\frac{\pi}{a}\hat{z} = k_z - \vec{b}_3 \qquad C_{2x} \in G_{k_z}$$

$$G_z = \langle T, C_{4z}, C_{2x} \rangle = P422 < P432$$

To look these up: • Bradley & Cracknell
• cryst.ehu.es "Krec"

$$432 = 422 \cup (422)C_3 \cup (422)C_3^{-1}$$

Lessons: ① For any $\vec{k}$ $T < G_k$ $\Rightarrow$ G_k is a space group and a subgroup of G (space subgroup of G)

② For any space group $G_\Gamma = G$

③ If G is symmorphic then G_k is symmorphic for every k

(if G is nonsymmorphic, then some k have nonsymmorphic little groups)

$\Rightarrow$ G symmorphic $\quad G = \bigcup_{i=0}^{n-1} T\bar{g}_i \quad \{\bar{g}_i\} = \bar{G}$

$$G_k < G \quad \text{and} \quad T < G_k$$

$$G_k = \bigcup_{j=0}^{M-1} T\bar{g}_j = T\bar{G}_k$$

$\bar{G}_k = G_k/T$ point group of the little group

"little cogroup"

$$\bar{G}_k < \bar{G}$$

Representations of little groups G_k of k

- $T \triangleleft G_k$ since G_k is a space group
- in any representation ρ_k of G_k for Bloch states

$$\rho_k(\{E|\vec{t}\}) = e^{-i\vec{k}\cdot\vec{t}}\, \mathrm{Id}$$

$\leftarrow$ since states w/ crystal momentum $\vec{k}$ transform "small/allowed" representations of G_k

in irrep $\vec{k}$ of T

① Easy case G_k is a symmorphic space group

$$G_k = T\bar{G}_k = \{\{E|\vec{t}\}\{\bar{g}_k|\vec{0}\}\}$$

$$\bar{G}_k = G_k/T$$

if ρ_k is a representation of G_k

$$\rho_k(\{\bar{g}_k|\vec{t}\}) = \rho_k(\{E|\vec{t}\}\{\bar{g}_k|0\})$$
$$= \rho_k(\{E|\vec{t}\})\rho_k(\{\bar{g}_k|0\})$$
$$= e^{-ik\cdot\vec{t}}\rho_k(\{\bar{g}_k|0\})$$

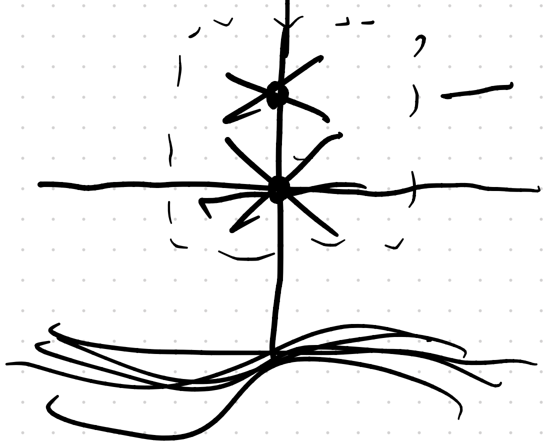
$\{\rho_k(\{\bar{g}_k|\vec{0}\}) \mid \bar{g}_k \in \bar{G}_k\}$ is a representation of $\bar{G}_k$

if η a representation of $\bar{G}_k$ then we can define $\rho_k(\{\bar{g}_k|\vec{t}\}) = e^{-ik\cdot t}\eta(\bar{g}_k)$

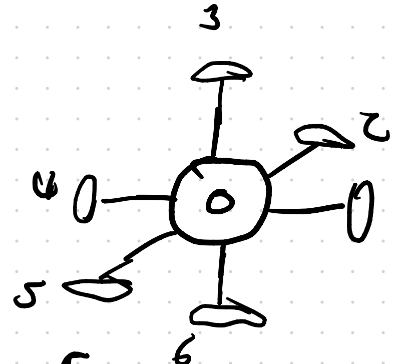
For symmorphic G_k irreps of G_k are determined by irreps of the point group $\bar{G}_k = G_k/T$

Ex: P432

Start at Γ $(k=\vec{0})$



$V = \{|\text{valence states}\rangle$



$$U(\vec{x}) = \sum_{\vec{t}} \sum_{i=0}^{6} V_i(\vec{x}-\vec{t})$$

is our periodic potential

Basis for valence states $\{$d orbitals on atom 0$\}$

$$V = \{|l=2, m\rangle, m=-2,-1,0,1,2\}$$

$G_\Gamma = G$ $\qquad \bar{G}_\Gamma = 432 = \langle C_{4z}, C_{3,111} \rangle$

$1 = \{E\}$

$4 = \{C_{4x}, C_{4y}, C_{4z}, \text{inverses}\}$

$2_{100} = \{C_{2x}, C_{2y}, C_{2z}\}$

$3 = \{C_{3\,111}, C_{3,1\bar{1}1}, \ldots\}$ 8

$2_{110} = \{C_{2x+y} \quad C_{2x-y} \quad C_{2x+z} \quad C_{2x-z} \quad C_{2y+z} \quad C_{2y-z}\}$

	1	4	2_1	3	2_{110}
A_1	1	1	1	1	1
A_2	1	-1	1	1	-1
E	2	0	2	-1	0
T_2	3	-1	-1	0	1
T_1	3	1	-1	0	-1

In the absence of $U(\vec{x})$ there 5 d orbitals are degenerate they transform in $l=2$ irrep $SO(3)$)

$$\rho_{\ell=2}(\hat{n},\theta) = e^{-\hat{n}\cdot\vec{J}\theta}$$

$$J_z = \begin{pmatrix} 2 & & & & \\ & 1 & & & \\ & & 0 & & \\ & & & -1 & \\ & & & & 2 \end{pmatrix} \qquad J_x = \frac{1}{2}\begin{pmatrix} 0 & 2 & & & \\ 2 & 0 & \sqrt{6} & & \\ & \sqrt{6} & 0 & \sqrt{6} & \\ & & \sqrt{6} & 0 & 2 \\ & & & 2 & 0 \end{pmatrix}$$

$$J_y = \frac{1}{2i}\begin{pmatrix} 0 & 2 & & & \\ -2 & 0 & \sqrt{6} & & \\ & -\sqrt{6} & 0 & \sqrt{6} & \\ & & -\sqrt{6} & 0 & 2 \\ & & & -2 & 0 \end{pmatrix}$$

Need to see how this 5-dimensional representation decomposes into irreps of G_T $\rightarrow$ tells us what

$h_{ab}(k=0) = \langle \varphi_{a\Gamma} | H | \varphi_{b\Gamma} \rangle$ can look like