Lecture 11

Recap: Little group G_k of a point $\vec{k}$ in the Brillouin zone (BZ)

$$G > G_k = \{ \{\bar{g}|\vec{d}\} \mid \bar{g}\vec{k} \equiv \vec{k} \mod \check{T} \}$$

"sewing matrix" for g_k

if $g_k \in G_k$ then $U_{g_k} |\psi_{nk}\rangle = \sum_m |\psi_{m\bar{g}k}\rangle B^k_{mn}(g_k)$

$g_k = \{\bar{g}|d\}$

$$= \sum_m |\psi_{mk}\rangle B^k_{mn}(g_k)$$

$\{ B^k_{mn}(g_k) \mid g_k \in G_k \}$ forms a representation of G_k under which $\{|\psi_{nk}\rangle\}$ transform

$$\boxed{B^k_{mn}(g) = \langle \psi_{m\bar{g}k} | U_g | \psi_{nk} \rangle}$$

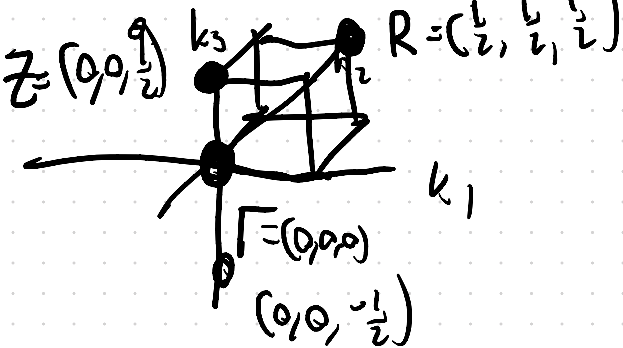
Example: Space group $P432$

P: primitive Bravais lattice

432: octahedral group

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

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



$$\left.\begin{aligned} \vec{b}_1 &= \frac{2\pi}{a}\hat{x} \\ b_2 &= \frac{2\pi}{a}\hat{y} \\ b_3 &= \frac{2\pi}{a}\hat{z} \end{aligned}\right\}$$ primitive reciprocal lattice vectors

① Γ point $\vec{k}=0$ $\quad \{\bar{g}|\vec{d}\} \in G \quad \bar{g}\vec{0} = \vec{0}$

$\Rightarrow G_\Gamma \cong G$ the little group of Γ is the whole space group

② R point $\vec{k} = \frac{1}{2}(\underbrace{\vec{b}_1 + \vec{b}_2 + \vec{b}_3})$

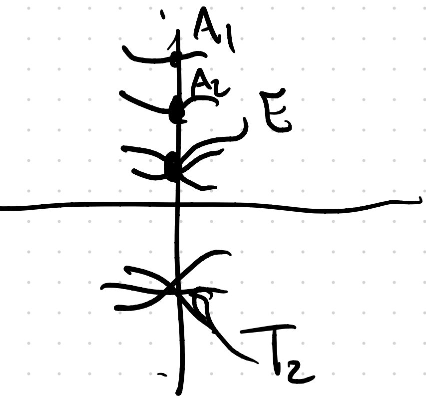
C_{4z}: $\hat{x} \to \hat{y}$
$\hat{y} \to -\hat{x}$
$\hat{z} \to \hat{z}$

$G_R = \langle T, C_{3,111}, C_{4z} \rangle$
$= G$

$C_{4z}R = \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
$= \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) - \vec{b}_1$

③ Z point $\vec{k} = \frac{1}{2}\vec{b}_2$

$G_Z = \langle T, C_{4z}, C_{2x} \rangle = P422$



kvec tool on cryst.ehu.es

"High symmetry" point $G_{\vec{k}+\delta\vec{k}} < G_k \quad \forall\ \delta k \neq 0$

Representations of Little Groups:

$T \triangleleft G_{\vec{k}}$ for every $\vec{k}$ → little groups are isomorphic to space groups

Two cases

1. G_k symmorphic
2. G_k is nonsymmorphic

↳ 1 easy G_k symmorphic $G \ni g_k = \{E|\vec{t}\}\{\bar{g}_k|0\}$

where $\bar{g}_k \in G_k/T = \bar{G}_k$ "little cogroup"

point group of the little group

if ρ_k is a representation of G_k

then $\rho_k(g_k) = \rho_k(\{E|\vec{t}\})\rho_k(\{\bar{g}_k|0\})$

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

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

given any rep η of $\bar{G}_k$

$\rightarrow$ $\rho_k(\{\bar{g}_k|\vec{t}\}) = e^{-i\vec{k}\cdot\vec{t}}\eta(\bar{g}_k)$ is a rep of $\bar{G}_k$

For symmorphic G_k, representations are determined from irreps of the point group $\bar{G}_k = G_k/T$ (little cogroup)

② G_k is nonsymmorphic is more interesting

$G_k = \bigcup_i T\{\bar{g}_i|\vec{d}_i\}$ at least one of the $\vec{d}_i$ is a fraction of a Bravais lattice translation

This means that there exist $\{\vec{g}_1|\vec{d}_1\}$, $\{\vec{g}_2|\vec{d}_2\}$

$$\{\bar{g}_1|\vec{d}_1\}\{\bar{g}_2|\vec{d}_2\} = \{\bar{g}_1\bar{g}_2|\underbrace{\vec{d}_1 + \bar{g}_1\vec{d}_2}_{=\vec{t}_{12}\neq 0}\} = \{E|\vec{t}_{12}\}\{\vec{g}_3|\vec{d}_3\}$$

Ex: twofold screw $\{C_{2z}|\tfrac{1}{2}\hat{z}\}$

$$\{C_{2z}|\tfrac{1}{2}\hat{z}\}\{C_{2z}|\tfrac{1}{2}\hat{z}\} = \{E|\vec{t}\}$$

this means in any representation

$$\rho_k(\{\bar{g}_1|d_1\})\rho_k(\bar{g}_2|d_2) = \rho_k(\{E|t_{12}\})\rho_k(\{\vec{g}_3|\vec{d}_3\})$$

$$= e^{-ik\cdot t_{12}}\, \rho_k(\{\bar{g}_3 | d_3\})$$

we can interpret this in two equivalent ways

but in representations of $\bar{G}_k$

$$\eta(\bar{g}_1)\,\eta(\bar{g}_2) = \eta(\bar{g}_3)$$

(A) Generalize our idea of representations

$$\rho_k(\bar{g}_1)\,\rho_k(\bar{g}_2) = e^{iC(\bar{g}_1,\bar{g}_2)}\,\rho_k(\bar{g}_1\bar{g}_2)$$

associative multiplication:

$$C(g_1, g_2) + C(g_1 g_2, g_3) = C(g_2, g_3) + C(g_1, g_2 g_3)$$

$$\rho_k(g_1)\big(\rho_k(g_2)\,\rho_k(g_3)\big)$$

$\rightarrow$ projective representation

representations of nonsymmorphic G_k are projective representations of $\bar{G}_k$ w/ c given by $e^{-ik\cdot t_n}$

Alternatively: $\bar{G}_k$ and extend it by $\{e^{-ik\cdot\vec{t}} \mid \vec{t}\in T\}$ and look for ordinary representations of this extension

Example: $P2_1$

$\vec{e}_1 = a_1\hat{x} + b_1\hat{y}$

$\vec{e}_2 = a_2\hat{x} + b_2\hat{y}$

$\vec{e}_3 = c\hat{z}$

$\{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\}$

$G = \langle T, \{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\}\rangle$

$\Gamma = (0,0,0)$ $\qquad Z = (0,0,\frac{1}{2})$

$G_\Gamma = G_Z = G$ the whole space group

Irreps of G_Γ: $\rho_\Gamma(\{E|\vec{t}\}) = e^{-i\vec{0}\cdot\vec{t}} = 1$

$$\rho_\Gamma(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\})^2 = \rho_\Gamma(\{E|\vec{e}_3\}) = 1$$

$\rightarrow$ Even when G_Γ is nonsymmorphic, its irreps are still determined from irreps of $\overline{G_\Gamma}$

	E	2_1	$\vec{t}$
Γ_1	1	1	1
Γ_2	1	-1	1

two irreps

at the Z point: $\vec{k} = \frac{1}{2}\vec{b}_3$ $\qquad \rho_Z(\{E|\vec{t}\}) = e^{-i\frac{1}{2}\vec{b}_3\cdot\vec{t}} = e^{-i\pi t_3}$

$\vec{t} = t_1\vec{e}_1 + t_2\vec{e}_2 + t_3\vec{e}_3$

$$\rho_Z(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\})^2 = \rho_Z(\{E|\vec{e}_3\}) = e^{-i\pi} = -1$$

$$\rho_Z(\{C_{2z}|\tfrac{1}{2}e_3\}) = \pm i$$

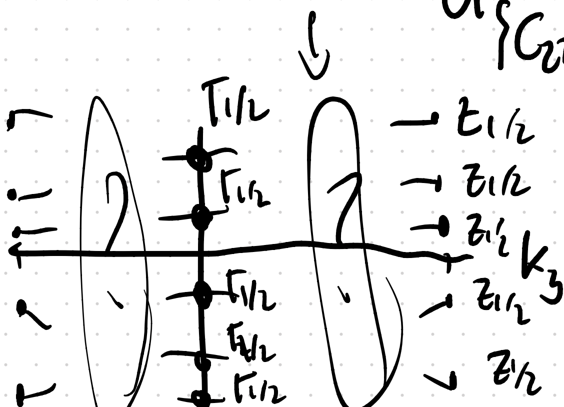
	E	2_1	$\vec{t}$
Z_1	1	$+i$	$e^{-i\pi t_3}$
Z_2	1	$-i$	$e^{-i\pi t_3}$

For electrons this means from Schur's lemma, all eigenstates $|\psi_{n\Gamma}\rangle$ transform as

$$U_{\{C_{2z}|\frac{1}{2}\vec{e}_3\}}|\psi_{n\Gamma}\rangle = \underset{\Gamma_2}{\overset{\Gamma_1}{\pm}}|\psi_{n\Gamma}\rangle$$

and all states $|\psi_{nZ}\rangle$ transform as

$$U_{\{C_{2z}|\frac{1}{2}e_3\}}|\psi_{nZ}\rangle = \underset{Z_2}{\overset{Z_1}{\pm}}\, i\,|\psi_{nZ}\rangle$$



$$\Lambda = (0,0,x) \qquad k_\Lambda = x\vec{b}_3$$

$x \to 0 \quad \Lambda \to \Gamma$

$x \to \frac{1}{2} \quad \Lambda \to Z$

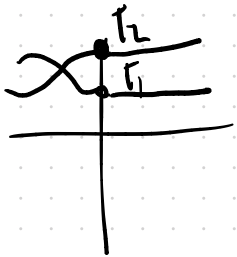
$x \to -\frac{1}{2} \quad \Lambda \to Z$

$G_\Lambda \cong G_\Gamma \cong G_Z \cong$ the full space group

$$\rho_\Lambda(\{E|\vec{t}\}) = e^{-2\pi i x t_3}$$

$$\rho_\Lambda(\{C_{2z}|\tfrac{1}{2}e_3\})^2 = \rho_\Lambda(\{E|\vec{e}_3\}) = e^{-2\pi i x}$$

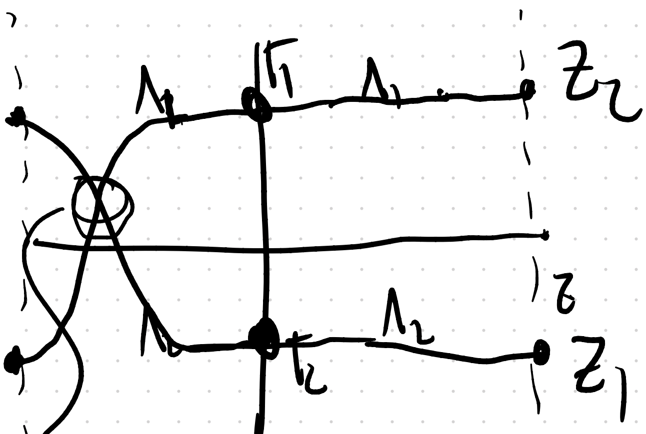
$$\rho_{\Lambda}(\{C_{2z}|\tfrac{1}{2}e_3\}) = \pm e^{-i\pi x}$$



	E	2_1	$\vec{t}$
Λ_1	1	$+e^{-i\pi x}$	$e^{-2\pi i x t_3}$
Λ_2	1	$-e^{-i\pi x}$	$e^{-2\pi i x t_3}$

	E	2_1	$\vec{t}$
Γ_1	1	1	1
Γ_2	1	-1	1

	E	2_1	$\vec{t}$
Z_1	1	$+i$	$e^{-i\pi t_3}$
Z_2	1	$-i$	$e^{-i\pi t_3}$



Schur's lemma

Compatibility relations:

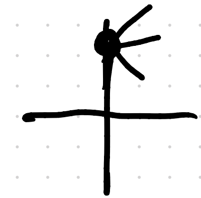
$$G_k \geq G_{k+\delta k}$$

then as $\delta k \to 0$

$H \cdot \begin{pmatrix} \varepsilon_{11} & 0 \\ 0 & \varepsilon_{22} \end{pmatrix}$

if I have states transforming in an irrep ρ_k of G_k then they better connect to states transforming

$$\rho_k \downarrow G_{k+\delta k \to 0} = \bigoplus_i \eta_i$$



as $x \to 0$ $\quad \Lambda_1 \to \Gamma_1$

$\qquad\qquad\;\; \Lambda_2 \to \Gamma_2$

$x \to \frac{1}{2}$ $\quad \Lambda_1 \to Z_2$

$\qquad\quad\;\; \Lambda_2 \to Z_1$

$x \to -\frac{1}{2}$ $\quad \Lambda_1 \to Z_1$

$\qquad\qquad\; \Lambda_2 \to Z_2$

$\to$ Bands in BZ, come in connected groups of two

→ Nonsymmorphic space groups have stable, unremovable band crossings