Lecture 11

- There was an error w/ Lecture 9 recording

Recap: let $\vec{k}_*$ in the Brillouin zone (BZ)

space group G

$$G > G_{k_*} = \{ \{\bar{g}|\vec{d}\} \in G \mid \bar{g}k_* \equiv k_* \bmod \check{T} \}$$

if $g_{k_*} \in G_{k_*}$ then $u_{g_{k_*}} |\psi_{nk_*}\rangle = \sum_m |\psi_{m\bar{g}k_*}\rangle B^{k_*}_{mn}(g_{k_*})$

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

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

$\{ B^{k_t}_{mn}(g_t) \mid g_{k_t} \in G_{k_t} \}$ form a representation of the little group

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

Example: Space group $\underbrace{P}_{\text{primitive Bravais lattice}}\underbrace{432}_{\text{octahedral point group}} \equiv G$

symmorphic

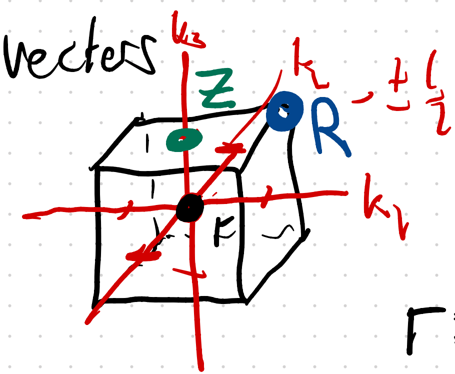
Primitive Bravais lattice vectors

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

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

Primitive reciprocal lattice vectors

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$
$\vec{b}_2 = \frac{2\pi}{a}\hat{y}$
$\vec{b}_3 = \frac{2\pi}{a}\hat{z}$



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

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

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

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

① Γ point $\vec{k}=0$

in <u>any</u> space group

$$\{g|\vec{d}\}\vec{0} = g\vec{0} = \vec{0}$$

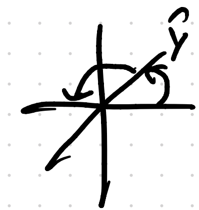
$G_\Gamma \cong G$ <u>always</u>

$\Rightarrow$ Γ point in any space group is invariant under the whole space group

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

$$= \frac{\pi}{a}(\hat{x}+\hat{y}+\hat{z})$$

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



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

$$C_{4z}k_R = \frac{\pi}{a}(\hat{y}-\hat{x}+\hat{z}) \stackrel{?}{=} k_R \mod \vec{t}$$

↓

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

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

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

$= \frac{\pi}{a}(\hat{x}+\hat{y}+\hat{z}) - \frac{2\pi}{a}\hat{x}$

$C_{4z} k_R = k_R - \vec{b}_1$

$\Rightarrow C_{4z} \in G_R$

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

$C_{3,111} k_R = k_R$

$\Rightarrow C_{3,111} \in G_R$

$\Rightarrow G_R \cong G$ the entire space group P432

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

$\{E|\hat{E}\} \in G_Z$ $\qquad\qquad C_{3,111} k_Z = \frac{\pi}{a}\hat{x} \neq k_Z \bmod \Upsilon$

$C_{4z} \in G_Z$

But: $C_{2x} k_Z = -\frac{\pi}{a}\hat{z} = k_Z - \frac{2\pi}{a}\hat{z} = k_Z - \vec{b}_3$

$\Rightarrow C_{2x} \in G_Z$

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

Lessons: 1. for any k, $T < G_k$ - G_k is a space group, and a subgroup of G (space subgroup of G)

2. for any space group G, $G_\Gamma = G$

3. if G is symmorphic, then G_k is symmorphic for all k

(if G is nonsymmorphic, some G_k are symmorphic and some G_k are nonsymmorphic)

To look up k-vectors & little groups:

- Bradley & Cracknell
- cryst.ehu.es "Kvec" tool

↳ G symmorphic ⇒

$$G = T\bar{G} = \bigcup_{i=0}^{n-1} T\bar{g}_0 \qquad \{\bar{g}_i\} = \bar{G}$$

if $G_k < G$ and $T < G_k$

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

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

Two cases: ① G_k is symmorphic

② G_k is nonsymmorphic

① Easy: G_k symmorphic $G_k = T\bar{G}_k = \{\{E|\vec{t}\}\{g_k|0\}\}$

$\bar{G}_k < \bar{G}$ and is a point group

$\bar{G}_k = G_k / T$ - "little cogroup"

point group of the little group

if ρ_k is a representation of G_k

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

$$= e^{-ik\cdot t}\,\underbrace{\rho_k(\{\bar{g}_k|0\})}_{\text{point group representation matrix for } \bar{G}_k}$$

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

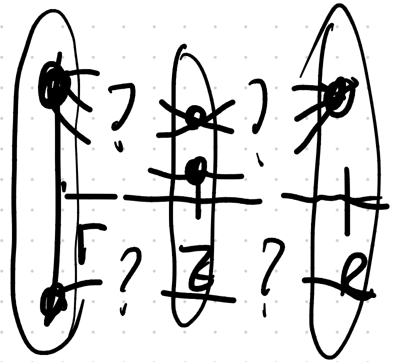
$\Rightarrow$ given any representation η of $\bar{G}_k$

we can contruct a representation

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

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

Ex: P432



can label states by irreps of G_k

$G_\Gamma = G_R = P432$

$\updownarrow$

irreps of 432

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

can have 1, 2, or 3 fold degenerate states at Γ and R

$G_Z = P422$

$\updownarrow$

irreps of 422

	dim
A_1	1
A_2	1

can have 1 or 2 fold degenerate states @ Z

B_1	1
B_2	1
E	2

(2) G_k nonsymmorphic - more interesting

$$G_k = \bigcup_{i=0}^{n-1} T\{\bar{g}_i | \vec{d}_i\} \qquad \{\bar{g}_i \mid i=0,\dots n\} = \overline{G_k}$$

but at least one $\vec{d}_i$ is a fraction of a Bravais lattice translation

$\Rightarrow$ there exists some $\{\bar{g}_1 | \vec{d}_1\}$, $\{\bar{g}_2 | \vec{d}_2\}$

s. t. $\qquad g_1'' \qquad g_2''$

$$g_1 g_2 = \{\bar{g}_1 | \vec{d}_1\}\{\bar{g}_2 | \vec{d}_2\} = \{\bar{g}_1\bar{g}_2 | \bar{g}_1\vec{d}_2 + \vec{d}_1\}$$

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

$$T \ni \vec{t}_{12} = \bar{g}_1\vec{d}_2 + \vec{d}_1 - \vec{d}_3$$

$$\left(\begin{array}{l} \text{Ex} \quad \{C_{2z} | \tfrac{1}{2}\hat{z}\} = g_1 = g_2 \\ \{C_{2z} | \tfrac{1}{2}\hat{z}\}\{C_{2z} | \tfrac{1}{2}\hat{z}\} = \{E | \hat{z}\}\{E | 0\} \end{array} \right)$$

this means that for any representation ρ_u

$$\underbrace{\rho_k(\{\bar{g}_1|\vec{d}_1\})}_{\bar{g}}\rho_k(\{\bar{g}_2|\vec{d}_2\}) = \rho_k(\{E|t_{12}\})\rho_k(\{g_1g_2|\vec{d}_3\})$$

$$\rho_k(\{E|t_{12}\}) = e^{-ik\cdot\vec{t}_{12}} \quad \text{twist}$$

but in $\bar{G}_k$,

$$\eta(\bar{g}_1)\eta(\bar{g}_2) = \eta(g_1g_2)$$

To accomodate this → generalize our idea of representatives

instead of representations η of $\bar{G}_k$, consider

$$\rho_k : \bar{G}_k \to U(V)$$

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

associativity:

$$\left(\rho_k(\bar g_1)\rho_k(\bar g_2)\right)\rho_k(\bar g_3) = e^{ic(\bar g_2,\bar g_3)}\rho_k(\bar g_1)\rho_k(\bar g_2\bar g_3)$$

$$= e^{ic(\bar g_2,\bar g_3)} e^{ic(\bar g_1,\bar g_2\bar g_3)} \rho_k(\bar g_1\bar g_2\bar g_3)$$

$$e^{ic(\bar g_1,\bar g_2)}\rho_k(\bar g_1\bar g_2)\rho_k(\bar g_3)$$

$$\shortparallel$$

$$e^{ic(\bar g_1,\bar g_2)} e^{ic(\bar g_1\bar g_2,\bar g_3)} \rho_k(\bar g_1\bar g_2\bar g_3)$$

$$c(\bar g_1,\bar g_2)+c(\bar g_1\bar g_2,\bar g_3)-c(\bar g_2,\bar g_3)-c(\bar g_1,\bar g_2\bar g_3)=0$$

"cocycle condition"

a map $\rho_k : \bar G_k \to GL(V)$ s.t.

$$\rho_k(\bar{g}_1)\rho_k(\bar{g}_2) = e^{ic(\bar{g}_1,\bar{g}_2)}\rho(g_1 g_2)$$

with c satisfying the cocycle condition

is a ~~projective representation~~

For nonsymmorphic G_k this is what we have

where $\bar{g}_1, \bar{g}_2 \in \overline{G_k}$

$$c(\bar{g}_1,\bar{g}_2) = -k \cdot t_{12} \quad \text{where } t_{12} = \bar{g}_1\vec{d}_2 + \vec{d}_1 - \vec{d}_{12}$$