# Lecture 12

Announcements: HW1 Solutions posted

Grades will be posted today

HW2 Due tonight

HW3 posted by end of day

due 10/16

Recap: Representations of little groups

$G_k < G$

$G_k$ symmorphic: $\rho(\{\bar{g}|\vec{t}\}) = e^{-ik\cdot\vec{t}}\eta(\bar{g})$

where $\eta$ is a representation of the little cogroup $\overline{G_k} = G_k/T$

$G_k$ nonsymmorphic: representations $\rho$ of $G_k$ are given by

## projective representations of $\bar{G}_k$

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

for coset representatives $\{\bar{g}_i | \vec{d}_i\}$ $\{\bar{g}_j | \vec{d}_j\} \in \bar{G}_k$

$$\{\bar{g}_i | \vec{d}_i\}\{\bar{g}_j | \vec{d}_j\} = \{E | \vec{t}_{ij}\}\{\bar{g}_{ij} | \vec{d}_{ij}\}$$

$$\boxed{\vec{t}_{ij} = \bar{g}_i \vec{d}_j + \vec{d}_i - \vec{d}_{ij}}$$

$\eta : \bar{G}_k \to U(V)$ $\qquad \eta(\bar{g}_i)\eta(\bar{g}_j) = e^{ic(\bar{g}_i, \bar{g}_j)}\eta(\bar{g}_{ij})$

cocycle $\quad c(\bar{g}_i, \bar{g}_j) = -\vec{k} \cdot \vec{t}_{ij}$

In practice: $H = \{ e^{-i\vec{k}\cdot\vec{t}} \mid t \in T \} < U(1)$

$e^{ic} \in H \quad \forall\, \bar{g}_i, \bar{g}_j$

can consider a larger group $\bar{G}_k \times_c H \ni (\bar{g}_i, h)$

$(\bar{g}_i, h_i)(\bar{g}_j, h_j) = (\bar{g}_i \bar{g}_j,\ h_i h_j e^{ic(\bar{g}_i, \bar{g}_j)})$

"central extension"

irreps of $\bar{G}_k \times_c H \iff$ projective reps of $\bar{G}_k$

$\rightarrow$ All tabulated in — Bradley & Cracknell Ch 5

- cryst. ehu. es

Example: $P2_1$ nonsymmorphic $2_1$ screw rotation

primitive Bravais lattice

$$\vec{e}_3 = c\hat{z}$$
$$\vec{e}_1 = a_1\hat{x} + b_1\hat{y}$$
$$\vec{e}_2 = a_2\hat{x} + b_2\hat{y}$$

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

$$P2_1 = \langle \vec{e}_1, \vec{e}_2, \vec{e}_3, \{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\} \rangle$$
$$= T\{E|\vec{0}\} \cup T\{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\}$$

$$\{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\}^2 = \{E|\vec{e}_3\}$$
$$= \{E|\vec{e}_3\}\{E|0\}$$

$$c(C_{2z}, C_{2z}) = -k \cdot \vec{e}_3$$

Brillouin zone: $\vec{b}_3 = \frac{2\pi}{c}\hat{z}$

$\vec{b}_1 = \frac{2\pi}{a_2 b_1 - a_1 b_2}(-b_2\hat{x} + a_2\hat{y})$

$\vec{b}_2 = \frac{2\pi}{a_1 b_2 - b_1 a_2}(-b_1\hat{x} + a_1\hat{y})$

$\Gamma$: $k = \vec{0}$

$Z$: $k = \frac{1}{2}\vec{b}_3$

$\Gamma$ point: $G_\Gamma = P2_1$ the entire space group

But note: for nonsymmorphic groups

$$C_k(\bar{g}_i, g_j) = -k \cdot t_{ij} \Rightarrow C_\Gamma(\bar{g}_i, \bar{g}_j) = 0$$

→ [even for nonsymmorphic groups, irreps of $G_\Gamma$

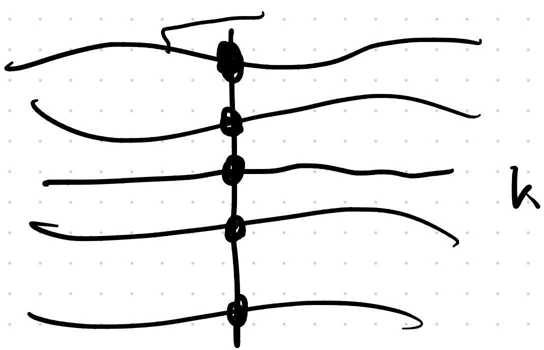
Coincide w/ irreps of $\bar{G}_\Gamma = \bar{G}$

In our case $\bar{G} = \{E, C_{2z}\}$

$C_{2z}^2 = E$

$\eta(C_{2z})^2 = \eta(E) = 1$

| | $E$ | $C_{2z}$ | $\vec{t}$ |
|---|---|---|---|
| $\Gamma_1 = A$ | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | -1 | 1 |



Next: $Z$ point $\vec{k} = \frac{1}{2}\vec{b}_3$ $\vec{t} = n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3$

$$G_Z = G = \left\langle T, \{C_{2z} | \tfrac{1}{2}\vec{e}_z\} \right\rangle$$

in any representation of $G_Z$, $\rho_Z(\{E|\vec{t}\}) = e^{-i\frac{1}{2}\vec{b}_3 \cdot \vec{t}}$

$= e^{-i\pi n_3}$

Abelian - irreps are 1d

$$\rho_Z(\{C_{2z} | \tfrac{1}{2}\vec{e}_z\}) = \alpha$$

$$\alpha^2 = \rho_Z(\{C_{2z} | \tfrac{1}{2} e_z\})^2 = \rho_Z(\{C_{2z} | \tfrac{1}{2} e_z\}^2) = \rho_Z(\{E | \vec{e}_z\})$$

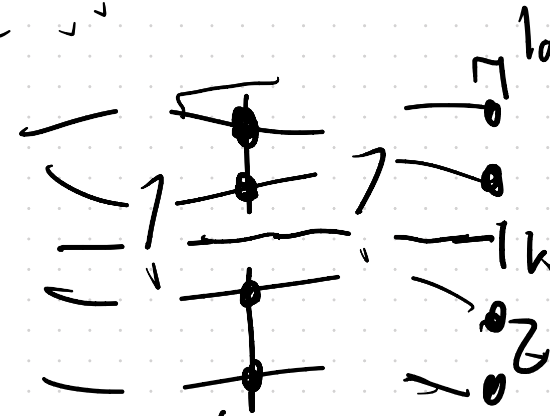
$= -1$

$\alpha = \pm i$

| | $E$ | $2_1$ | $\vec{t}$ |
|---|---|---|---|
| $Z_1$ | 1 | $+i$ | $e^{-i\pi n_3}$ |
| $Z_2$ | 1 | $-i$ | $e^{-i\pi n_3}$ |

projective rep of $\bar{G}_z$

labeled by $\tau_1$ or $\tau_2$



labeled by $t_1$ or $t_2$

Schurs lemma:

$\Gamma$ : $|\psi_{n\Gamma}\rangle$ eigenstates

$$U_{\{C_{2z}|\frac{1}{2}\vec{e}_3\}}|\psi_{n\Gamma}\rangle = \underset{t_1 \; t_2}{\pm} |\psi_{n\Gamma}\rangle$$

$Z$: eigenstates $|\psi_{nZ}\rangle$

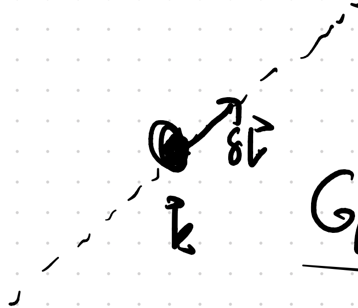
$$U_{\{C_{2z}|\frac{1}{2}e_3\}}|\psi_{nZ}\rangle = \overset{Z_1}{\underset{Z_2}{\pm}} i\,|\psi_{nZ}\rangle$$

How do we connect little group irreps at different k points?

Let k be some point in the BZ

w/ $G_k$ thats not trivial

consider $\vec{k} + \varepsilon\,\delta\vec{k} \rightarrow \varepsilon \in [0,1)$ this defines a line in the BZ




Little group for this line

$$G_{k+\epsilon\delta k} \doteq \{ g \in G \mid g(k+\epsilon\delta k) \equiv k+\epsilon\delta k \mod \vec{T} \text{ for all } \epsilon \}$$

intersection of little groups for all points on the line

$$G_{k+\epsilon\delta k} < G_k$$

so lets say we know at $\vec{k}$ we have $\{|\psi_{nk}\rangle\}$

transforming in an irrep $\rho_k$ of $G_k$


then $\{|\psi_{nk}\rangle\}$ transform in a representation

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

$\rho_k \downarrow G_{k+\epsilon\delta k}$ of $G_{k+\epsilon\delta k}$ as $\epsilon \to 0$

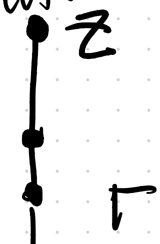
$\eta_i$ irreps $G_{k+\epsilon\delta k}$

compatibility relations. Tell us how irreps change as we vary $\vec{k}$

Lets apply compatibility relations to $P2_1$

$\Gamma: \vec{0} = \vec{k}$

$Z: \vec{k} = \frac{1}{2}\vec{b}_3$




$G = \langle e_1, e_2, e_3, \{C_{2z} | \frac{1}{2}\vec{e}_3\} \rangle$

$\Lambda \; * \quad \vec{k} = x\vec{b}_3 = x\frac{2\pi}{c}\hat{z}$

$(x \in [-\frac{1}{2}, \frac{1}{2}])$


$-z \equiv z$


$\hat{z}$

$G_\Lambda = G$ the full space group

$\rho_\Lambda(\{E|\vec{t}\}) = e^{-2\pi i x n_3}$

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

$= e^{-2\pi i x}$

| | $E$ | $2_1$ | $\vec{t}$ |
|---|---|---|---|
| $\Lambda_1$ | $1$ | $+e^{-i\pi x}$ | $e^{-2\pi i x t_3}$ |
| $\Lambda_2$ | $1$ | $-e^{-i\pi x}$ | $e^{-2\pi i x t_3}$ |

| | $E$ | $C_{2z}$ | $\vec{t}$ |
|---|---|---|---|
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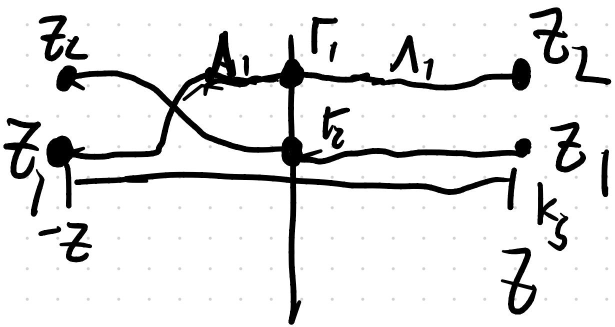
$\Gamma: \ x \to 0$

$\Gamma_1 \leftarrow \Lambda_1$

$\Gamma_2 \leftarrow \Lambda_2$




$Z: \ x \to \frac{1}{2}$

$\Lambda_1 \to Z_2$

$\Lambda_2 \to Z_1$

Nonsymmorphic groups

$\to$ compatibility relations force irreps to appear in groups

$Z: \ x \to -\frac{1}{2}$

$\Lambda_1 \to Z_1$

$\Lambda_2 \to Z_2$

in this case bands come in groups of 2