

Lecture 9

- HW 1 Due today on gradescope

Given $k \in$ 1st Brillouin Zone of a space grp G

$$G_k = \left\{ \{\bar{g}|\bar{j}\} \in G \text{ s.t. } \bar{g}k \equiv k \text{ modulo a recip. lattice vector} \right\}$$

$$\overline{G}_k = G_k / T \quad - \text{the point group of } G_k \text{ (little coset group)}$$

- G_k symmorphic \Rightarrow irreps of G_k determined from irreps of \overline{G}_k
- G_k nonsymmorphic \Rightarrow projective representations of \overline{G}_k

Alternative point of view on projective reps:

Projective rep: \bar{G}_k , cocycle $e^{iC(\bar{g}_1, \bar{g}_2)}$: $\bar{G}_k \times \bar{G}_k \rightarrow H$

This same set of data defines a central extension

consider $\{e^{-i\vec{k} \cdot \vec{t}} \mid \vec{t} \in T\} = H$

our cocycles $e^{iC(\bar{g}_1, \bar{g}_2)}: \bar{G}_k \times \bar{G}_k \rightarrow H$

ex: $k = \frac{1}{2}\vec{b}_1 + \frac{1}{2}\vec{b}_2 + \frac{1}{2}\vec{b}_3$

$$\vec{t} = \eta_1 \vec{e}_1 + \eta_2 \vec{e}_2 + \eta_3 \vec{e}_3 \quad \vec{k} \cdot \vec{t} = -i\pi(n_1 + n_2 + n_3) \quad e^{\vec{k} \cdot \vec{t}} = e^{-i\pi(n_1 + n_2 + n_3)} \rightarrow H = \{1, -1\}$$

using C , we can construct $\bar{G}_k \times_c H$ a central

extension of \widehat{G}_k by H

elements of $\widehat{G}_k \times_c H$ are (\bar{g}, h) $\bar{g} \in \widehat{G}_k$

$$(\bar{g}_1, h_1)(\bar{g}_2, h_2) = (\bar{g}_1 \bar{g}_2, h_1 h_2 e^{ic(\bar{g}_1, \bar{g}_2)})$$

Ordinary representations of $\widehat{G}_k \times_c H$ are projective

reps of \widehat{G}_k w/ cocycle $e^{ic(\bar{g}_1, \bar{g}_2)}$

$H \hookrightarrow \widehat{G}_k \times_c H$

$$h \mapsto (E, h)$$

$$(\bar{g}_1, h_1)(\bar{g}_2, h_2) = (\bar{g}_1 \bar{g}_2, h_1 h_2 e^{iC(\bar{g}_1, \bar{g}_2)})$$

$$= (E, h_1 h_2 e^{iC(\bar{g}_1, \bar{g}_2)}) (\bar{g}_1 \bar{g}_2, 1)$$

Consider a projective rep ρ_k of \widehat{G}_k w/ cocycle C

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

↓
an ordinary representation of $\widehat{G}_k \times_c H$

$$\rho_k((\bar{g}, h)) = h \rho_k(\bar{g})$$

$$\begin{aligned}
 \rho_k((\bar{g}, h)) \rho_k(g_1, \bar{h}_1) &= h_1 h_2 \rho_k(\bar{g}_1) \rho_k(\bar{g}_2) \\
 &\stackrel{\text{def}}{=} h_1 h_2 e^{iC(\bar{g}_1, \bar{g}_2)} \rho_k(\bar{g}_1, \bar{g}_2) \\
 &= \rho_k((\bar{g}_1, \bar{g}_2, h_1 h_2 e^{iC(\bar{g}_1, \bar{g}_2)}))
 \end{aligned}$$

From here on out, we will work w/ ordinary reps of central extensions

$$\begin{aligned}
 \rho_k(E) \rho_k(\bar{g}) &= e^{iC(E, \bar{g})} \rho_k(\bar{g}) \\
 &\uparrow \\
 I + \rho_k(E) &= \text{Identity Matrix}
 \end{aligned}$$

We can show

$$\bar{G}_k X_C H \quad \bar{G}_k X_{C'} H$$

then if

$$e^{ic(\bar{g}_1, \bar{g}_2)} = \frac{e^{ib(\bar{g}_1)} e^{ib(\bar{g}_2)}}{e^{ib(\bar{g}_1, \bar{g}_2)}} e^{ic'(\bar{g}_1, \bar{g}_2)}$$

then $\bar{G}_k X_C H \simeq \bar{G}_k X_{C'} H$

$$(\bar{g}, h) \rightarrow (\bar{g}, e^{ib(\bar{g})} h)$$

One useful fact:

The 1st BZ of every
Space Group contains
 $k_F = Q\bar{b}_1 + Q\bar{b}_2 + Q\bar{b}_3$

The center of a group G
is the set $Z(G) = \{g \in G \text{ s.t. } \forall g' \in G$
 $gg' = g'g\}$

$$=(0,0,0) \leftarrow \Gamma_{\text{point}}$$

1st: $G_\Gamma = G$

2nd: $e^{-ik_\Gamma \cdot \vec{r}} = e^{-i0} = 1$

\rightarrow even for nonsymmorphic grps, irreps of G_Γ are determined by irreps of the pt group \overline{G}

the center is on grp b/c

if $g_1, g_2 \in Z(G)$, $g_1 g_2 g_1^{-1} = g_2 g_1^{-1}$
 $\therefore g_1, g_2 \in Z(G)$

Ex: $P2_1 = G$ ① Nonsymmorphic

- ② Point group C_2
- ③ Primitive lattice

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

$$\{C_{2z} | \vec{e}_3/2\} \subset G$$

$$\langle \vec{e}_1, \vec{e}_2, \{C_{2z} | \vec{e}_3/2\} \rangle = G$$

$$\vec{b}_i \cdot \vec{e}_j = 2\pi \delta_{ij} \quad \vec{k} = (k_1, k_2, k_3) = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3$$

① Γ point $\vec{k} = (0, 0, 0)$ for any irrep ρ_Γ of G_Γ

$$\rho_\Gamma(\{C_{2z} | \vec{e}_3\})^2 = \rho_\Gamma(\{C_{2z} | e_3\})^2$$

$$\begin{aligned} &= \rho_\Gamma(\{\mathbb{E} | \vec{e}_3\}) = e^{-i0 \cdot \vec{e}_3} \xrightarrow{\text{Id}} \text{Id} \\ &= \text{Id} \end{aligned}$$

irreps of G_Γ
are labelled by
 T_i

$$\bar{G}_\Gamma = \langle E, C_{2z} \rangle$$

ρ_Γ	E	C_{2z}
Γ_1	1	1

ρ_{Γ_1} is the trivial rep.

$$F_2 \mid 1 -1$$

Let's look at $B = (\frac{1}{2}, 0, 0) \quad (\frac{1}{2}\vec{b}_1)$

$$\begin{aligned} C_{22}(\frac{1}{2}, 0, 0) \\ = (-\frac{1}{2}, 0, 0) \\ = k_B - \vec{b}_1 \end{aligned}$$

$$G_B = \langle \{E|\vec{t}\}, \{C_{22}|e_3/2\} \rangle$$

$$P_{B_i}(\{E|\vec{t}\}) = e^{-i\vec{k}_B \cdot \vec{t}} = e^{-i\frac{1}{2}(\vec{b}_1 \cdot \vec{t})}$$

$$= e^{-i\pi t_1}$$

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

$$P_{B_i}(\{C_{22}|e_3/2\}) = P_{B_i}(\{E|\vec{e}_3\}) = e^{-i\frac{1}{2}\vec{b}_1 \cdot \vec{e}_3} = 1$$

e	$\{E \vec{t}\}$	$\{C_{0z} e_3/z\}$
B_1	$e^{-i\pi t_1}$	I
B_2	$e^{-i\pi t_1}$	$-I$

Let's look at a point where we get something different

$$Z = (0, 0, \frac{1}{2}) \Rightarrow k_z = \frac{1}{2} \vec{b}_3$$

$$G_Z = \langle \{E|\vec{t}\}, \{C_{0z}|e_3/z\} \rangle$$

$$e_{Z_i}(\{E|\vec{t}\}) = e^{-i k_z \cdot \vec{t}} = e^{-i \pi t_3}$$

$$\rho_{Z_1}(\{C_{23} | e_3/z\})^2 = \rho_{Z_1}(\{E | \vec{e}_3\}) = e^{-i\pi} = -1$$

$$\begin{array}{c|cc} e & \{E | \vec{e}\} & \{C_{23} | e_3/z\} \\ \hline z_1 & e^{-i\pi t_3} & i \\ z_2 & e^{-i\pi t_3} & -i \end{array}$$

What does this tell us:

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

$$H \text{ has the symmetries of } G \Rightarrow U_g^\dagger H U_g = H$$

$$\rightarrow U_g |\Psi_{nk}\rangle = \sum_m |\Psi_{mgl}\rangle \beta_{mn}^k(g)$$

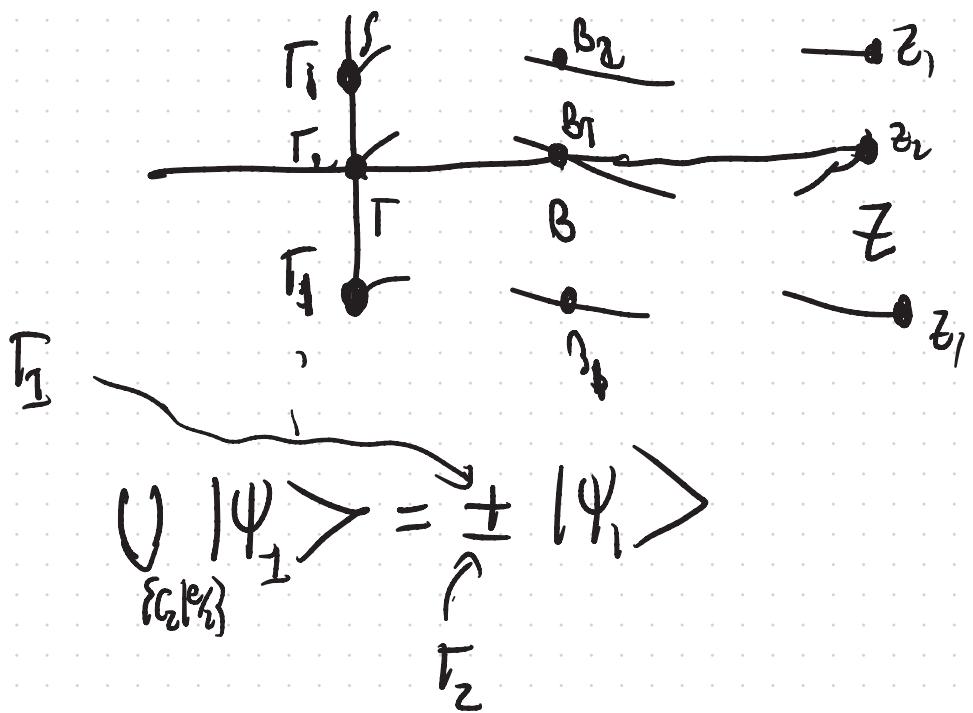
$$\text{and } H\left(\sum_n |\Psi_{n\bar{g}k}\rangle \langle B_{nn}^k(g)|\right) = E_{nk} \left(\sum_n |\Psi_{n\bar{g}k}\rangle \langle B_{nn}^k(g)|\right)$$

for $g \in G_k$ this says that

$\sum_n |\Psi_{nk}\rangle \langle B_{nn}^k(g)|$ is also an eigenstate w/ energy E_{nk} .

$\rightarrow \{|\Psi_{n_1 k}\rangle, |\Psi_{n_2 k}\rangle, |\Psi_{n_3 k}\rangle, \dots\}$ transform in a representation of G_k with $\rho_k(g) = [B_{nn}^k(g)]_{nn}$

$|\Psi_i\rangle$



What we've learned

- ① Bloch states w/ crystal momentum \vec{k} transform in reps of G_k

- ② All states that span a given map are degenerate, and the degeneracy cannot be lifted w/o breaking a symmetry (Schur's Lemma)

Notes:

- ① Bilbao Crystallographic Server (BCS) uses a passive convention for translations
- ② BCS defaults to "unique b-axis" description

$$\{C_{2,3,4,6} \mid \vec{d}\}$$

$$\{C_n | \vec{\theta}\}^\wedge = \{E | \vec{\theta}\}$$

the component of \vec{d} along the axis of rotation

$\propto \boxed{\frac{M}{n}} \times$ a lattice translation

2_1	6_1
3_1	6_2
3_2	6_3
4_1	6_4
4_2	6_5
t_3	