

Lecture 8

We introduced the little groups

$$G_{\vec{k}} = \left\{ \{\vec{g} | \vec{t}\} \in G \mid \vec{g}\vec{k} \equiv \vec{k} \pmod{\vec{b}} \right\}$$

↓
 equivalent
 up to a
 reciprocal lattice
 vector

reciprocal
 lattice
 vector

$$g \in G_k \rightarrow \langle \psi_g | \Psi_{n\vec{k}} \rangle = \sum_m |\Psi_{m\vec{k}} \rangle B_{mn}(g)$$

$G_{\vec{k}}$ is isomorphic to a space group

$$\{\vec{E} | \vec{t}\} \vec{k} \equiv \vec{k}$$

↗
 $\overline{T} \subset G_k$
 bravais lattice

$T \subset G_k \subset G$

Example: P432

pt group 432

symmorphic
cubic

primitive cubic

$$\vec{t}_1 = a\hat{x}$$

$$\vec{t}_2 = a\hat{y}$$

$$\vec{t}_3 = a\hat{z}$$



$$\left\{ \begin{array}{l} T \subset G \quad T \subset \bar{G} \\ G = T \times \bar{G} \quad \bar{G}_k \ni \{C_{2z}|00\frac{1}{2}\} \\ \bar{G}/T = \bar{G} \quad G_k \ni \{C_{2z}|00e\} \\ \{C_{2z}|00\frac{1}{2}\}^2 = \{E|00\bar{1}\} \end{array} \right.$$

reciprocal lattice

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

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

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

$$432 = \langle C_{4z}, C_{3,111} \rangle$$

$$\textcircled{1} \quad \vec{k} = O\vec{b}_1 + O\vec{b}_2 + O\vec{b}_3 = (0, 0, 0) = \Gamma_{\text{part}}$$

$$G_\Gamma = \left\{ T, C_{43}, C_{3,111} \right\} \rightarrow G_\Gamma = G$$

For any space group G , $G_T = G$

$$\textcircled{2} \quad \vec{k} \text{ some generic randomly chosen pt } (k_1, k_2, k_3)$$

$$G_k = \{ T \} \quad \xrightarrow{\text{General position}} \quad \text{GP}$$

For any space group, the little grp $G_{sp} = T$

$$\textcircled{3} \quad \vec{k} = \frac{1}{2}\vec{b}_1 + \frac{1}{2}\vec{b}_2 + \frac{1}{2}\vec{b}_3 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \equiv R$$

$$G_R = \langle T, C_{43}, C_{3,111} \rangle \cong G = P432$$

$$C_{43}: \begin{array}{l} x \rightarrow -y \\ y \rightarrow x \\ z \rightarrow z \end{array} \quad \frac{1}{2}\hat{x} + \frac{1}{2}\hat{y} + \frac{1}{2}\hat{z} \rightarrow \frac{1}{2}\hat{x} - \frac{1}{2}\hat{y} + \frac{1}{2}\hat{z} \\ = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) - (0, 1, 0) \\ = R - \vec{b}_2$$

$$C_{3,111}: \begin{array}{l} x \rightarrow y \\ y \rightarrow z \\ z \rightarrow x \end{array}$$

$$\textcircled{4} \quad X_1 = \left(\frac{1}{2}, 0, 0\right)$$

$$G_{X_1} = \langle T, C_{2z}, C_{4x} \rangle \cong P422$$

$$C_{4x}\left(\frac{1}{2}, 0, 0\right) = \left(\frac{1}{2}, 0, 0\right)$$

$$C_{2z}\left(\frac{1}{2}, 0, 0\right) = \left(-\frac{1}{2}, 0, 0\right) = X_1 - \vec{b}_1$$

Now we want to construct irreps of the little
grps G_k of G

① G_k isomorphic to a symmorphic S.G.

② G_k isomorphic to a nonsymmorphic S.G.

If G is symmorphic, all G_k are symmorphic \leftarrow

If G is nonsymmorphic, at least some G_k are nonsymmorphic

G_k is symmorphic if $g_k \in G_k \Rightarrow g_k = \{E | \vec{t}\} \{ \bar{g}_k | \vec{0} \}$
for \bar{g}_k in \overline{G}

$G_{\vec{k}}$ is the little grp of \vec{t}

$$\{\bar{g} | \vec{0}\} \notin G_{\vec{k}} \quad k' = \{\bar{g} | \vec{d}\} \vec{k} = \bar{g} \vec{k}$$

$$G_{\bar{g}k} = \{\bar{g} | \vec{d}\} G_k \{ \bar{g} | \vec{0} \}^{-1}$$

① G_k is a symmorphic space group

$$\forall g_k \in G_k \quad g_k = \{E | \vec{t}\} \{ \bar{g} | 0 \} \text{ for } \bar{g} \in \overline{G_k} \subset \overline{G}$$

Say we have a rep. ρ of G_k

$$\rho(g_k) = \rho(\{E | \vec{t}\} \{ \bar{g} | 0 \})$$

$$= \rho(\{E | \vec{t}\}) \rho(\{ \bar{g} | 0 \})$$

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

↑
point group
of the little group
"little cagroup"

we are focusing on reps
on block wavefn's

$$\rho(E | \vec{t}) = e^{-i\vec{k} \cdot \vec{t}}$$

"Small representations"
"allowed reps"

So all we need to construct irreps of Symmorphic G_k is to construct irreps of $\overline{G}_k \leftarrow$ this is a point group!

The more complicated case: G_k nonsymmorphic

$$\{\bar{g}, | \vec{d}_1 \rangle\}, \{\bar{g}_2 | \vec{d}_2 \rangle\} \in G_k$$

$$\{\bar{g}, | \vec{d}_1 \rangle\} \{\bar{g}_2 | \vec{d}_2 \rangle\} = \{E | \vec{t}\} \{\bar{g}_1 \bar{g}_2 | \vec{d}_3 \rangle\}$$

$$\text{Ex: } \{\bar{g}, | \vec{d}_1 \rangle\} = \{C_{2z} | 00\frac{1}{2}\} = \{\bar{g}_2 | \vec{d}_2 \rangle\}$$

$$\{\bar{g}, | \vec{d}_1 \rangle\}^2 = \{E | 001\} \{E | \vec{Q}\}$$

U_g is a unitary (differential) operator

$B(g)$ is a very large (reducible) representation

\oplus a much smaller irrep

$$B(g) = \bigoplus_i P_i(g)$$

$$\text{f I picked } \rho(\{\bar{g}|\vec{d}\}) = \eta(\bar{g}) \quad \eta \text{ is a pt grp rep.}$$

$$\rho(\{\bar{g}, |\vec{d}_1\})\rho(\{g_1, |\vec{d}_1\}) = \eta(c_{zz})\eta(c_{zz}) = \eta(E) e^{-ik_0(001)}$$

There are two ways to resolve this:

① Lets stick to reps of the point grp \overline{G}_k , but:

$$\eta(\bar{g}_1)\eta(\bar{g}_2) = \eta(\bar{g}_1\bar{g}_2)e^{iC(\bar{g}_1, \bar{g}_2)} \leftarrow \begin{matrix} \text{projective} \\ \text{representations} \end{matrix}$$

$C(\bar{g}_1, \bar{g}_2)$ - 2-cocycle

f I have 3 pt group elements $\bar{s}_1, \bar{s}_2, \bar{s}_3$

$$\begin{aligned}
 (\eta(\bar{g}_1)\eta(\bar{g}_2))\eta(\bar{g}_3) &= \eta(\bar{g}_1\bar{g}_2)e^{iC(\bar{g}_1, \bar{g}_2)}\eta(\bar{g}_3) \\
 &= e^{iC(\bar{g}_1, \bar{g}_2)}\eta(\bar{g}_1\bar{g}_2\bar{g}_3)e^{iC(\bar{g}_1\bar{g}_2, \bar{g}_3)}
 \end{aligned}$$

$$\begin{aligned}
 \eta(\bar{g}_1)(\eta(\bar{g}_2)\eta(\bar{g}_3)) &= \eta(\bar{g}_1)\eta(\bar{g}_2\bar{g}_3)e^{iC(\bar{g}_2, \bar{g}_3)} \\
 &= \eta(\bar{g}_1\bar{g}_2\bar{g}_3)e^{iC(\bar{g}_1, \bar{g}_2\bar{g}_3)}e^{iC(\bar{g}_2, \bar{g}_3)}
 \end{aligned}$$

$$e^{i(C(\bar{g}_1, \bar{g}_2) + C(\bar{g}_1\bar{g}_2, \bar{g}_3) - C(\bar{g}_1, \bar{g}_2\bar{g}_3) - C(\bar{g}_2, \bar{g}_3))} = 1$$

"cocycle condition"

Given any f_n $b: \overline{G}_k \rightarrow \mathbb{R}$ we can define
a new projective representation

$$\gamma'(g) = e^{ib(\bar{g})} \gamma(\bar{g})$$

$$\gamma'(\bar{g}_1) \gamma'(\bar{g}_2) = e^{i(b(\bar{g}_1) + b(\bar{g}_2))} \gamma(\bar{g}_1) \gamma(\bar{g}_2)$$

$$= e^{i(b(\bar{g}_1) + b(\bar{g}_2))} e^{ic(\bar{g}_1, \bar{g}_2)} \gamma(\bar{g}_1, \bar{g}_2)$$

$$= e^{i(b(\bar{g}_1) + b(\bar{g}_2) - b(\bar{g}_1 \bar{g}_2))} e^{i c(\bar{g}_1 \bar{g}_2)} \eta(\bar{g}_1 \bar{g}_2)$$

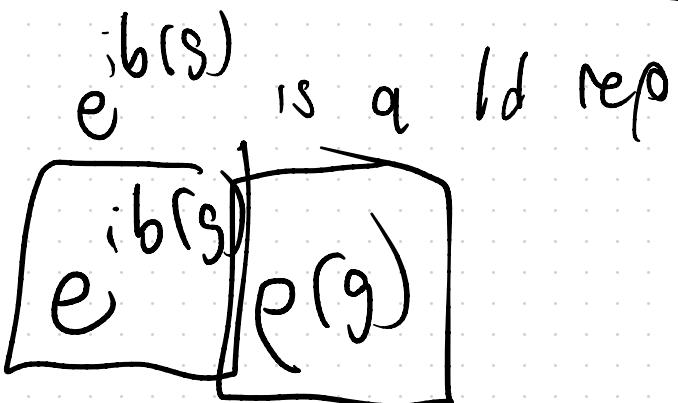
η' is also a projective rep w/ cocycle

$$c'(\bar{g}_1 \bar{g}_2) = c(\bar{g}_1 \bar{g}_2) + b(\bar{g}_1) + b(\bar{g}_2) - b(\bar{g}_1 \bar{g}_2)$$

$\tilde{c}(\bar{g}_1 \bar{g}_2) = b(\bar{g}_1) + b(\bar{g}_2) - b(\bar{g}_1 \bar{g}_2)$ is called a coboundary

$$\underbrace{e^{ib(g_1)} e^{ib(g_2)} e^{-ib(g_1 g_2)}}$$

$$\text{if } \underline{b(g_1 g_2)} = b(g_1) + b(g_2)$$



$$\rightarrow \underbrace{e^{ib(g_1)} e^{ib(g_2)}}_{= e^{ib(g_1 + g_2)}} = e^{ib(g_1 + g_2)}$$

$p_b: g \rightarrow e^{ib(g) \in U(1)}$ is a 1d rep

lets say, have a different rep ρ_2

$$\rho_2: g \rightarrow U(n)$$

$$\rho_2(g) = \begin{pmatrix} & \\ & \\ & \end{pmatrix}_{n \times n}$$

I can construct the tensor product rep

$$\rho_b \otimes \rho_2: g \rightarrow U(1) \otimes \underbrace{U(n)}$$

$$\rho_b \otimes \rho_2(g) = e^{ib(g)} \rho_2(g)$$

$$[\rho_b \otimes \rho_2](g_1) [\rho_b \otimes \rho_2](g_2) = e^{ib(g_1)} \rho_2(g_1) e^{ib(g_2)} \rho_2(g_2)$$

$$= e^{ib(s_1 s_2)} \rho_2(s_1 s_2) = [\rho_b \otimes \rho_2](s_1 s_2)$$

is a linear representation

The systematic study of cocycles & coboundaries
is called group cohomology

$$H^2(G, U(1)) = \frac{\{ \text{cocycles} \}}{\{ \text{coboundaries} \}}$$

our cocycles are $e^{ic(s_1, s_2)}$

$$\therefore c(c_{zz}, c_{zz}) = -1$$