Lecture 12

Announcements: · HW1 solutions posted, grades returned
· HW2 is due 3/6

Recap: Representations of little groups:

$G > G_k$:

G_k is symmorphic. $\rho(\{\bar{g}|\vec{t}\}) = e^{-i\vec{k}\cdot\vec{t}}\,\eta(\bar{g})$ where η is a representation of $\overline{G}_k = G_k/T$ - "little cogroup"

G_k nonsymmorphic - representations ρ of G_k are from <u>projective representations</u> of $\overline{G}_k$

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

if $\{\bar{g}_1|\vec{d}_1\}, \{\bar{g}_2|\vec{d}_2\} \in \bar{G}_k$

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

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

cocycle

$$c(\bar{g}_1,\bar{g}_2) = -\vec{k}\cdot(\bar{g}_1\vec{d}_2+\vec{d}_1-\vec{d}_3) = -\vec{k}\cdot\vec{t}_{12}$$

Example $P2_1$

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

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

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

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

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

$$\vec{b}_1 = \frac{2\pi}{a_2 b_1 - a_1 b_2}\left(-b_2\hat{x} + a_2\hat{y}\right) \qquad \Gamma : (0,0,0)$$

$$\vec{b}_2 = \frac{2\pi}{a_1 b_2 - b_2 a_1}\left(-b_1\hat{x} + a_1\hat{y}\right) \qquad Z : (0,0,\tfrac{1}{2})$$

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

$\boxed{G_\Gamma = P2_1 = G_Z}$ the whole space group

Irreps of G_Γ : G_Γ is nonsymmorphic.

But $k_\Gamma = \vec{0}$

$$c(\bar{g}_1, \bar{g}_2) = \cdot \; k_T \cdot t_{12} = 0$$

So even for nonsymmorphic G_T, irreps of G_T are inherited from irreps of $\overline{G_T} = \bar{G}$

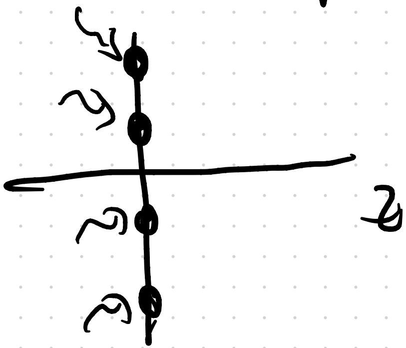
$$\rho_\Gamma(\{E|\vec{t}\}) = e^{-i0\cdot k} = \underline{1}$$

$$\rho_\Gamma(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\}) = \eta(C_{2z}) \quad \eta \text{ is a point group representation}$$

irreps of $\bar{G} = \langle \underline{E}, \underline{C_{2z}} \rangle$

$$C_{2z}^2 = E$$

two irreps



	E	2_1	t
Γ_1	1	1	1
Γ_2	1	-1	1

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

Next: G_Z

if ρ_Z is a irrep

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

$$\rho_Z(\{E|\vec{t}\}) = e^{-i(\frac{1}{2}\vec{b}_3)\cdot\vec{t}}$$

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

$$= e^{-i\pi t_3}$$

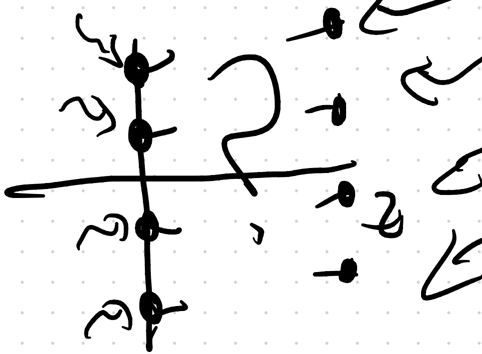
$$\rho_Z(\{C_{2t}|\tfrac{1}{2}\vec{e}_3\}) = \alpha$$

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

$$\alpha = \pm i$$

two irreps

	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; Γ; eigenstates $|\psi_{n\Gamma}\rangle$

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

Γ_1 Γ_2

and at Z, eigenstates $|\psi_{nZ}\rangle$

$U_{\{C_{2z}|\frac{1}{2}\vec{e}_3\}}|\psi_{nZ}\rangle = \pm i|\psi_{nZ}\rangle$

Z_1 Z_2

How do we connect little group reps at different points?

Let $\vec{k}$ be some special point w/

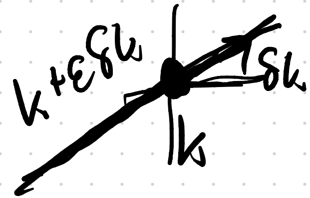
$$G_k > T$$

consider $\vec{k} + \varepsilon \vec{\delta k}$

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

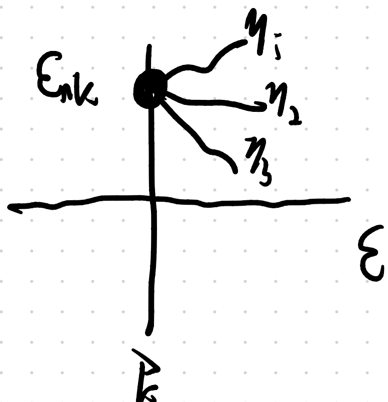
Little group of this line:

$$G_{k+\varepsilon\delta k} = \{ g \in G \mid g(k+\varepsilon\delta k) = k + \varepsilon \delta k \text{ for all } \varepsilon \}$$



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

so lets say we have $\{|\psi_{n\vec{k}}\rangle\}$ trasforming in an irrep ρ_k of G_k



then these states transform in a representation $\rho_k \downarrow G_{k+\epsilon\delta k}$

$$= \bigoplus \eta_i$$

η_i are irreps of $G_{k+\epsilon\delta k}$

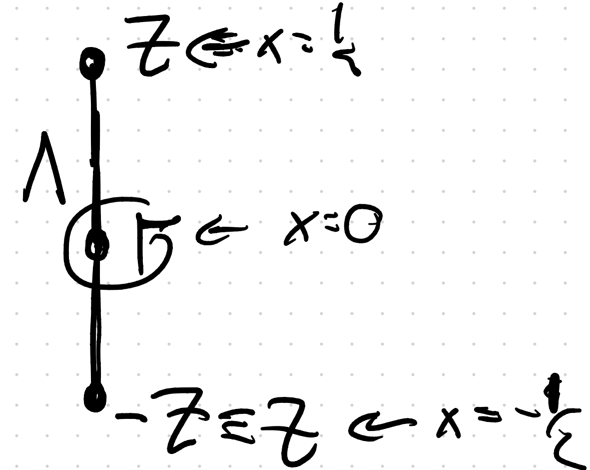
Compatibility relations tell us how irreps change as we change $\vec{k}$

Lets apply compatibility relations to $P2_1$

Γ: $(0,0,0)$

Z: $(0,0,\frac{1}{2})$

Λ: $(0,0,x)$ $\quad x \in (-\frac{1}{2}, \frac{1}{2})$



$G_\Lambda \neq G$ the full space group

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

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

	E	2_1	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

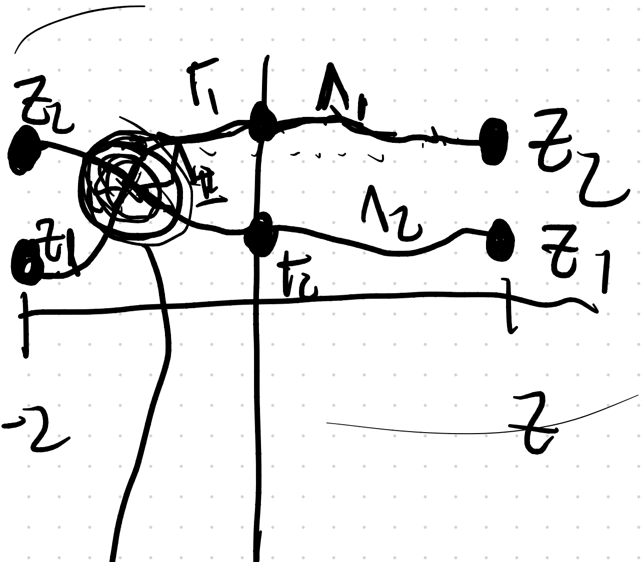
	E	2_1	$\vec{t}$
Z_1	1	$+i$	$e^{-i\pi t_3}$
Z_2	1	$-i$	$e^{-i\pi t_3}$

Compatibility relations

$\Gamma: x \to 0$

$\Lambda_1 \leftarrow \Gamma_1$

$\Lambda_2 \leftarrow \Gamma_2$



Schur's lemma

$\Lambda_1 \quad \Lambda_2$

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

$\Lambda_1 \leftarrow Z_2$

$\Lambda_2 \leftarrow Z_1$

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

$\Lambda_1 \leftarrow Z_1$

$\Lambda_2 \leftarrow Z_2$

$$H(x) \quad \begin{array}{cc} & \\ \left(\begin{matrix} \underline{\mathcal{E}_{11}(x)} & \boxed{0} \\ 0 & \underline{\mathcal{E}_{22}(x)} \end{matrix}\right) & \begin{matrix} \Lambda_1 \\ \Lambda_2 \end{matrix} \end{array}$$

Lesson: Compatibility relations for nonsymmorphic groups cause bands to be connected → Moveable but nonremovable band crossings

Bands in $P2_1$ come in connected groups of 2

Two last ingredients: (1) Spin

(2) Time-reversal symmetry

<u>Spin</u>: Electrons have spin-$\frac{1}{2}$

So for $G < \mathbb{R}^3 \rtimes O(3)$ in this group

a 2π rotation is the identity

This is OK if no spin orbit coupling

$$H_{electrons} = \underbrace{H_0}_{\text{spin-independent}} \otimes \sigma_0$$

σ_0: 2x2 identity matrix on spin-$\frac{1}{2}$

for every $g \in \mathbb{R}^3 \rtimes O(3)$

$$U_g = U_g^{coordinates} \otimes U_g^{spin}$$

$U_g^{coordinates}$: $e^{i(r \times p)}$

U_g^{spin}: spin rotation

$$0 = [H_{electron}, U_g]$$

No SOC : $[H_{electron}, U_g^{coordinates}]$

If we do have SOC, need to use representations of SU(2) to figure out U_g^{spin}

Reminder $(\hat{n}, \theta) = g \in SU(2)$

$\hat{n}$ a vector on S^2

$\theta \in [-2\pi, 2\pi)$

$l = \frac{1}{2}$ representation of SU(2)

$$\rho_{\frac{1}{2}}((\hat{n}, \theta)) = e^{-i \hat{n} \cdot \vec{\sigma}/2\, \theta}$$

$\vec{\sigma}$ a vector of 2x2 Pauli matrices

$$\rho_{\frac{1}{2}}(r(\hat{n}, 2\pi)) = \rho_{\frac{1}{2}}(r(\hat{n}, -2\pi)) = -\sigma_0$$

$$\rho_{\frac{1}{2}}(r(\hat{n}, 0)) = \sigma_0$$

$$(\hat{n}, \theta = \pm 2\pi) \equiv \bar{E} \in SU(2)$$

$$\bar{E}^2 = E$$

To encode this we will take $E(3)$ and extend it with $\bar{E}$

$$\rho(\bar{E}) = Id \quad \text{for } l \in \mathbb{Z} \text{ integer spin}$$

$$\rho(\bar{E}) = -\mathrm{Id} \quad \text{for } l \in \mathbb{Z} + \tfrac{1}{2}$$

in any representation ρ $\qquad SU(2)/\{E,\bar{E}\} = SO(3)$

For groups only containing rotations:

$$G < \mathbb{R}^3 \rtimes SO(3)$$
$$\downarrow$$
$$G^d < \mathbb{R}^3 \rtimes SU(2)$$

$$G^d/\{E,\bar{E}\} = G$$

Ex: Point group $D_2 < SO(3) = \{E, C_{2x}, C_{2y}, C_{2z}\}$

$$C_{2x}C_{2y} = C_{2y}C_{2x} = C_{2z}$$

$$C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = E$$

In $SU(2)$ we can look in the defing $l=\frac{1}{2}$ rep

$$\rho_{\frac{1}{2}}(C_{2i}) = e^{-i\pi\sigma_i/2} = \cancel{\cos\frac{\pi}{2}} - i\sin\frac{\pi}{2}\sigma_i = -i\sigma_i$$

$$\rho_{\frac{1}{2}}(C_{2x})\rho_{\frac{1}{2}}(C_{2y}) = (-i\sigma_x)(-i\sigma_y) = i\sigma_z = \rho_{\frac{1}{2}}(C_{2z})$$

$$= \rho_{\frac{1}{2}}(\bar{E})\rho_{\frac{1}{2}}(C_{2y})\rho_{\frac{1}{2}}(C_{2x})$$

so in $SU(2)$: $C_{2x}C_{2y} = \bar{E}C_{2y}C_{2x}$

$$C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = \bar{E}$$

Double group $D_2^d = \{E, C_{2x}, C_{2y}, C_{2z}, \bar{E}, \bar{E}C_{2x}, \bar{E}C_{2y}, \bar{E}C_{2z}\} = Q$

$$SU(2) \to Q/\{E, \bar{E}\} = D_2$$

$$\wedge$$

$$SU(2)/\{E, \bar{E}\} = SO(3)$$

For rotations: view double group as a subgroup of $SU(2)$