Lecture 11

Announcement - No office hours tomorrow
- Make up office hrs Mon 4pm

Recap: Little group G_k of a pt $\vec{k}$ in Brillouin Zone

$$G \supset G_k = \{\{R|\vec{d}\} \in G \mid R\vec{k} = \vec{k} \text{ modulo reciprocal lattice vectors}\}$$

$$R\vec{k} \equiv \vec{k}$$

equivalent modulo reciprocal lattice vectors

if $g_k \in G_k$ then $U_{g_k}|\psi_{nk}\rangle = \sum_m |\psi_{m\, g_k k}\rangle B^k_{mn}(g_k)$

$$= \sum_n |\psi_{nk}\rangle B^k_{nk}(g_k)$$

$\rightarrow$ $\boxed{\{B^k_k(g_k) \mid g_k \in G_k\} \text{ form a representation of the little group } G_k}$

Irreducible representations of G_k:

- G_k symmorphic - we can determine irreps from irreps of $\bar{G}_k = G_k/T$ (little cogroup)

- $G_{\Gamma=\vec{0}}$ irreps are also determined by irreps of $\overline{G}_{\Gamma=0} = \overline{G}$

- Nonsymmorphic $G_{\vec{k}}$ → we have to do more work

Example: $P2_1 = \langle T, \{C_{2z} | \tfrac{1}{2}\vec{e}_3 = \tfrac{1}{2}c\hat{z}\} \rangle$

$G_\Gamma \rightarrow$

	E	$\{C_2 \mid \tfrac{1}{2}\vec{e}_3\}$	$\{E \mid \vec{t}\}$
Γ_1	1	1	1
Γ_2	1	-1	1

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

$G_{Z=(\frac{1}{2}\vec{b}_3)} \rightarrow$

	E	$\{C_2 \mid \tfrac{1}{2}t_3\}$	$\{E \mid \vec{t}\}$
Z_1	1	$+i$	$e^{-i\pi t_3}$
Z_2	1	$-i$	$e^{-i\pi t_3}$

What does this tell us about electrons?

$$(*) \quad H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

$$U_{g_k}|\psi_{nk}\rangle = \sum_m |\psi_{mk}\rangle B^k_{mn}(g_k) \qquad g_k \in G_k$$

g_k is a symmetry of H =>

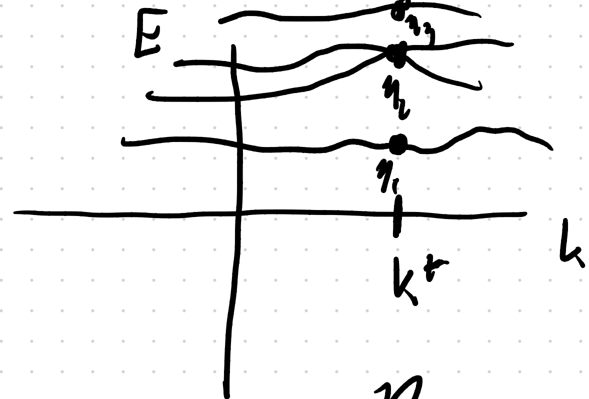
$$H U_{g_k} = U_{g_k} H$$

using this on *

$$H U_{g_k}|\psi_{nk}\rangle = U_{g_k} H|\psi_{nk}\rangle = E_{nk} U_{g_k}|\psi_{nk}\rangle$$

$U_{g_k} |\psi_{nk}\rangle$ is an eigenstate of H w/ eigenvalue E_{nk}. $\{|\psi_{nk}\rangle\}$ transforms in a reducible representation of G_k determined by $B^k_{nm}(g_k)$

Schur's lemma – this representation is reducible, and $B^k = \bigoplus_i \eta_i$, η_i irreducible, and states in the same representation are degenerate



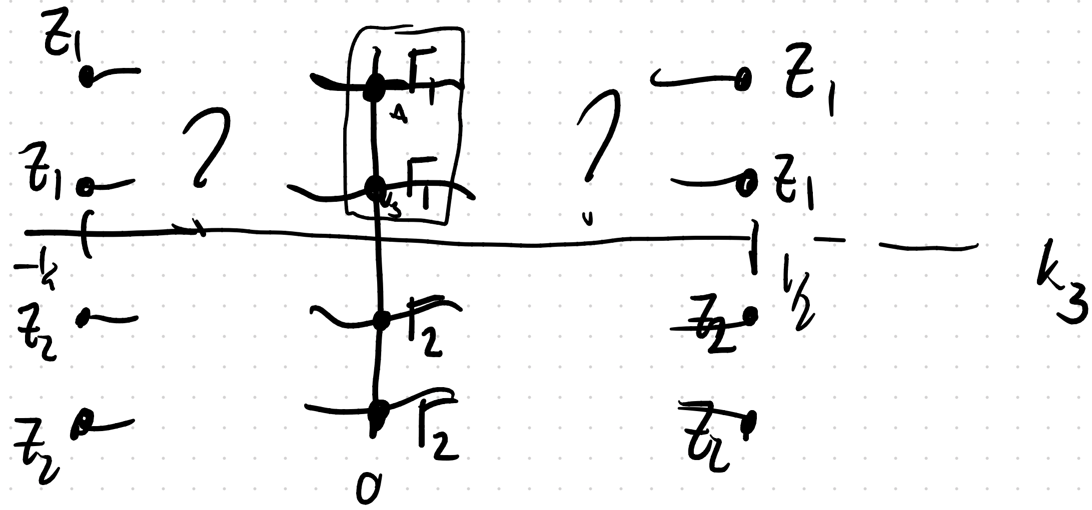
η_i irreps at G_{k^*}

In our PZ_1 example:

- all states at Γ can be labelled either Γ_1 or Γ_2
- all states at Z can be labelled either Z_1 or Z_2

$$H = \left(\begin{array}{c|c} H_{AA} & H_{AB} \\ \hline H_{BA} & H_{BB} \end{array}\right)$$

Ex



To connect these bands, we can look at <u>compatibility relations</u> for the space group

Idea: lets consider $\vec{k}$ and a nearby point

$\vec{k} + t\delta\vec{k}$ $\quad$ t real

$\delta\vec{k}$ is a fixed vector

$h \in G_{\vec{k}+t\delta\vec{k}}$ for all t then $h \in G_{\vec{k}+0\delta\vec{k}} = G_{\vec{k}}$

so the little group $\underbrace{G_{\vec{k}+t\delta\vec{k}}}_{\text{little group of the line } \{\vec{k}+t\delta\vec{k}\}} \subset G_k$

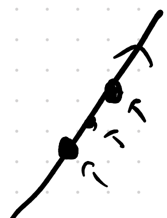
Given $\rho_k : G_k \to U(V)$ an irrep of G_k we can define $\rho_k \downarrow G_{\vec{k}+t\delta\vec{k}} = \eta$

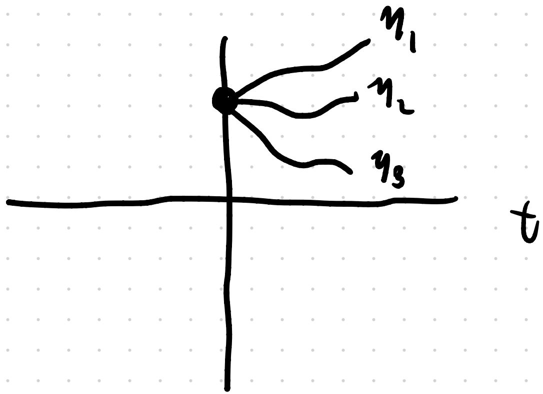
η is the restriction of ρ_k to $G_{\vec{k}+t\delta\vec{k}}$

$$\eta(h) = \rho_k(h) \quad \text{for } h \in G_{\vec{k}+t\delta\vec{k}}$$

$$\eta = \bigoplus_i \eta_i \quad \text{for } \eta_i \text{ irreps of } G_{\vec{k}+t\delta\vec{k}}$$

Ex





if $\rho_k \downarrow G_{\vec{k}+t\delta\vec{k}} = \eta_1 \oplus \eta_2 \oplus \eta_3$

$\rho_k \downarrow G_{\vec{k}+t\delta\vec{k}} = \bigoplus_i \eta_i$ are known as compatibility relations

Lets look at our $P2_1$ example

Γ $(0,0,0)$ Λ $(0,0,t)$ Z $(0,0,\frac{1}{2})$

$t \to 0 \quad \Lambda \to \Gamma$

$t \to \frac{1}{2} \quad \Lambda \to Z$

$$G_\Lambda = \langle T, \{C_{2z}|\tfrac{e_3}{2}\}\rangle \simeq G$$

Irreps of G_Λ

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

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

$$\downarrow$$

$$\rho_t(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\}) = \begin{cases} +e^{-i\pi t} \\ -e^{-i\pi t} \end{cases}$$

	E	$\{C_2\|\frac{1}{2}\vec{e}_3\}$	$\{E\|\vec{t}\}$
Γ_1	1	1	1
Γ_2	1	-1	1

	E	$\{C_{2z}\|\frac{1}{2}e_3\}$	$\{E\|\vec{t}\}$
Λ_1	1	$+e^{-i\pi t}$	$e^{-2\pi i t t_3}$
Λ_2	1	$-e^{-i\pi t}$	$e^{-2\pi i t t_3}$

$t \to \frac{1}{2}$ $\Lambda \to Z$

$\Lambda_1 \to Z_2$

$\Lambda_2 \to Z_1$

	E	$\{C_2\|\frac{1}{2}t_3\}$	$\{E\|\vec{t}\}$
Z_1	1	$+i$	$e^{-i\pi t_3}$
Z_2	1	$-i$	$e^{-i\pi t_3}$

$t \to -\frac{1}{2}$ $\Lambda \to Z$

$\Lambda_1 \to Z_1$

$\Lambda_2 \to Z_2$

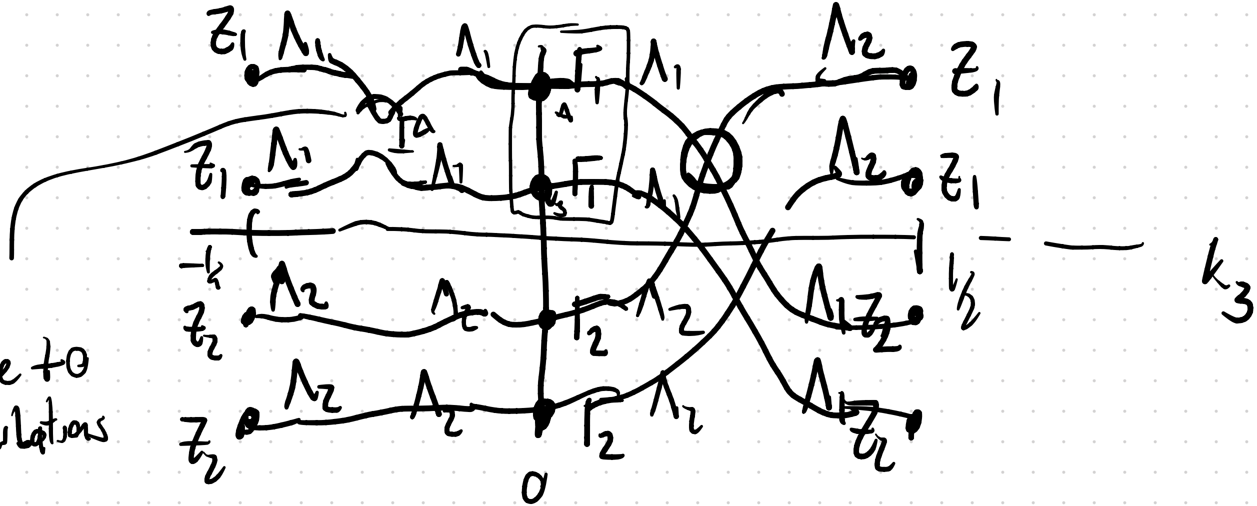
$t \to 0$; $\Lambda \to \Gamma$

$\Lambda_1 \to \Gamma_1$

$\Lambda_2 \to \Gamma_2$

$P2_1$

not stable to perturbations



$$H = \left(\begin{array}{c|c} \times & \Delta \\ \hline \Delta & \times \end{array}\right)$$

- Compatibility relations force bands to come in groups

the minimum number of isolated bands is 2 $\quad \Gamma_1 \to Z_1 \to \Gamma_2 \to Z_2$

- Nonsymmorphic space groups have stable, unremovable band crossings

Lessons so far

1. Bloch states w/ momentum $\vec{k}$ transform in representations of the little group G_k

2. All states that transform in the <u>same</u> irrep of G_k are degenerate, and this degeneracy can't be split w/o breaking a symmetry (Schur's Lemma)

(3) Schur's lemma – when bands cross, the crossing can't be gapped by small perturbations if the bands carry different irreps

(4) Screw (also glide) symmetries require nonremovable band crossings along high symmetry lines