Lecture 13

Lessons so far

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

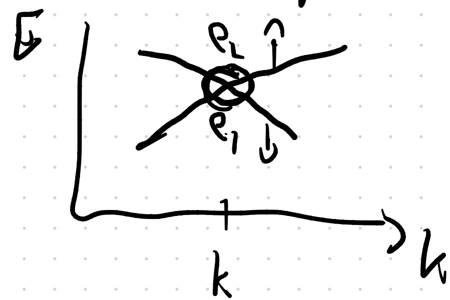
$$\rho_k : G_k \to U(N)$$

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

② Schur's lemma: all states transforming in the same irrep of G_k → these states must be degenerate

→ these degeneracies can't be split by any perturbation that respects the space group symmetries

(3) Schur's lemma: if bands cross, and if the bands carry different irreps of G_k → these



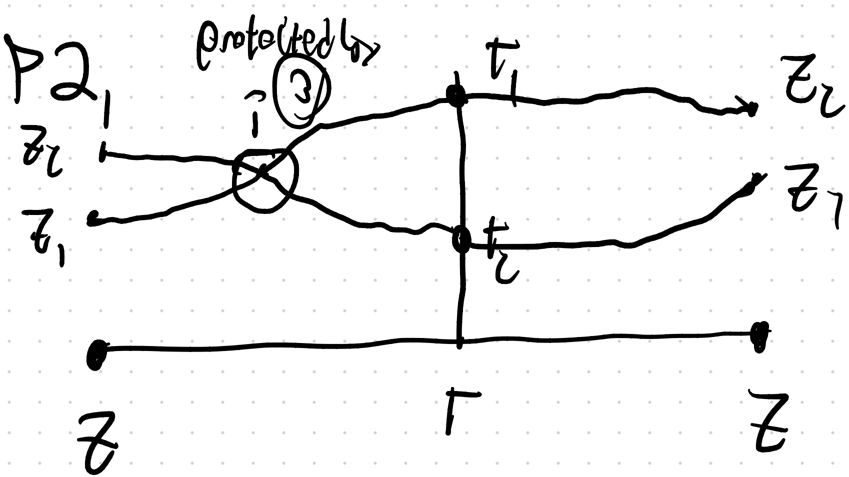
$\langle 1 | H | 2 \rangle = 0$

$$H = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix}$$

→ these crossings can be moved, but not removed

(4) Nonsymmorphic groups → compatibility relations force groups of bands to be connected

Ex $P2_1$



Two last ingredients:

1. spin orbit coupling and symmetry
2. time-reversal symmetry

So far: $G < \mathbb{R}^3 \rtimes O(3)$ space groups as a subgroup of the Euclidean group

2π rotation about $\hat{n}$ $\to$ identity E

This is a problem for spin-$\frac{1}{2}$ particles

This is OK as long as there's no SOC:

$$H_{electrons} = \underset{\substack{\uparrow \\ \text{independent} \\ \text{of spin}}}{H_0} \otimes \sigma_0 \leftarrow \text{2x2 identity matrix on spin-}\tfrac{1}{2}$$

for every space group symmetry $U_g = U_g^{coords} \otimes U_g^{spin}$

No SOC : $[H, U_g] = 0 \Rightarrow [H_0, U_g^{coord}] = 0$

enhanced symmetry $\to G \times SO(2)$ $[H, Id \otimes SU(2)] = 0$
$\downarrow soc$
G^d

If we have spin-orbit coupling (H depends on spin)

we have to use half-integer spin representations of $SU(2)$

Reminder: $(\hat{n}, \theta) = g \in SU(2)$ $\quad$ $\hat{n}$ a unit vector in 3d (on the sphere S^2)

$l = \frac{1}{2}$ representation of $SU(2)$ $\quad$ $\theta \in [-2\pi, 2\pi)$

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

$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ pauli matrices defining representation

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

$$= \cos\frac{\theta}{2}\sigma_0 - i\sin\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}$$

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

$$= -\sigma_0$$

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

$\bar{E}$ "a 2π rotation)

$\bar{E}^2 = E \in SU(2)$ the identity

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

$$\rho(\bar{E}) = \begin{cases} +Id & \text{for } l \in \mathbb{Z} \text{ (spinless electrons)} \\ -Id & \text{for } l \in \mathbb{Z}+\frac{1}{2} \text{ (s.o.c. Hamiltonians)} \end{cases}$$

For groups w/ only rotations: $SO(3) = SU(2)/\{E, \bar{E}\}$

G that only contains rotations

$$G < \mathbb{R}^3 \rtimes SO(3) = \mathbb{R}^3 \rtimes SU(2) / \{E, \bar{E}\}$$

we can' define $G^d < \mathbb{R}^3 \rtimes SU(2)$

$$G^d / \{E, \bar{E}\} = G \qquad G^d \text{ double (space) group}$$

Example of how this works $D_2 < SO(3) = \{E, C_{2x}, C_{2y}, C_{2z}\}$

in $SO(3) > D_2$: $C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = E \qquad C_{2x}C_{2y} = C_{2z} = C_{2y}C_{2x}$

constructing D_2^d: look @ $l = \frac{1}{2}$ representation of $SU(2)$

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

$$\rho_{\frac{1}{2}}(C_{2i}^2) = (-i\sigma_i)^2 = -\sigma_0 = \rho_{\frac{1}{2}}(\bar{E}) \checkmark$$

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

in the double group D_2^d

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

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

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

$$D_2 = D_2^d / \{E, \bar{E}\}$$

HW 1: $\varphi: Q \to D_2$

$$\ker \varphi = \{E, \bar{E}\}$$

$$D_2 = \frac{D_2^d < SU(2)}{\{E, \bar{E}\}}$$

$$\wedge$$

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

to construct double groups: take a point or space group G view it as a subgroup of $SU(2)$ add whatever factors of $\bar{E}$ are needed

$SU(2) = Spin(3)$ - transformation of spinors in 3D

If we also have reflections:

$\bar{G} < O(3)$

$$\frac{Spin(3)}{\{E, \bar{E}\}} \cong SO(3)$$

$$? \to \frac{Pin(3)}{\{E, \bar{E}\}} = O(3)$$

Two possibilities

Inversion $I: (x, y, z) \to (-x, -y, -z) \in O(3)$

$$\mathrm{Pin}(3) \ni I^2 = \begin{cases} E & \mathrm{Pin}_-(3) \\ \bar{E} & \mathrm{Pin}_+(3) \end{cases}$$

Physical intuition: spin-$\frac{1}{2}$ carries angular momentum and magnetic moment $\Rightarrow$ spin-$\frac{1}{2}$ transforms like $\vec{L} = \vec{r} \times \vec{p}$

$\Rightarrow$ $I^2 = E$ on spin-$\frac{1}{2}$ $\Rightarrow$ $\mathrm{Pin}_-(3)$ is the "physical" choice

$$\mathrm{Pin}_-(3) = SU(2) \times \{E, I\}$$

When we have SOC: H_{soc} is symmetric under

⊕ double space group

$$T < G^d < \mathbb{R}^3 \rtimes \mathrm{Pin}_3(3) \rightarrow$$ 220 double space groups

Hermann–Maugin notation for double groups

(ordinary point/space group symbol)^d

$D_2 = 222$

$Q = 222^d$

H_{soc} is symmetric under $G^d \rightarrow$ its eigenstates transform in irreps of G^d

$\eta : G^d \rightarrow U(V)$ a double group representation

$$\eta(\bar{E}) = \begin{cases} +\mathrm{Id} \to \text{ we get back ordinary reps of } G \text{ "single-valued representations"} \\ -\mathrm{Id} \to \text{ "double-valued representations"} \end{cases}$$

Example $Q = 222^d$ double group of D_2

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

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

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

→ 5 conjugacy classes (HW1)

$E = \{E\}$

$\bar{E} = \{\bar{E}\}$

$C_{2i} = \{C_{2i}, \bar{E}C_{2i}\}\ x3$

	E	C_{2x}	C_{2y}	C_{2z}	$\bar{E}$
A	+1	1	1	1	1
B_1	+1	-1	-1	1	1
B_2	+1	-1	1	-1	1
B_3	+1	-1	-1	1	1
$\bar{\Gamma}_5$	2	0	0	0	-2

$8 = 1 + 1 + 1 + 1 + x^2$
$\rightarrow 2$

$\rho_{\frac{1}{2}} \downarrow Q = \rho_{\bar{\Gamma}_5}$

SOC → states **must** transform in double valued representations

$\rho_{\bar{\Gamma}_5}(C_{2i}) = -i\sigma_i$

$\rho_{\bar{\Gamma}_5}(E) = \sigma_0 \quad \rho_{\bar{\Gamma}_5}(\bar{E}) = -\sigma_0$

H symmetric under $Q = \mathbb{Z}_2\mathbb{Z}_2\mathbb{Z}_2^d$

$\rightarrow$ all states $2\times$ degenerate and transforming in $\bar{F}_5$

Note: SOC example

(2) Next time