Lecture 12

Lessons so far:

1. Bloch states $\{|\psi_{nk}\rangle\}_{n=1}^{N}$ w/ momentum $\vec{k}$ transform in representations of G_k

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

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

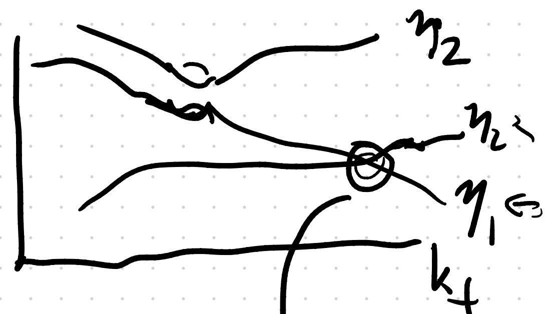
2. Schur's lemma: All states that transform in a given irrep of G_k are degenerate

3. Schur's lemma: When bands cross along lines, the crossing can't be gapped by small perturbations if the bands transform

in different irreps of the little group

$$k_t = t\hat{k} \quad t \in [0,1]$$

G_{k_t} - set of spacegroup elements that leave every point on the line invariant



η_i - irreps of G_{k_t}

$$H = \begin{pmatrix} H_{\eta_1\eta_1} & H_{\eta_1\eta_2} \\ H_{\eta_2\eta_1} & H_{\eta_2\eta_2} \end{pmatrix} = 0 \text{ if } \eta_1 \neq \eta_2$$

4. Screw (and glide) symmetries <u>require</u> nonremovable band crossings

Two last ingredients: 1. Spin
2. Time-reversal symmetry

$\boxed{\text{Conway et al, math/9911185}}$

Spin: electrons have spin $\frac{1}{2}$

so far $G < \mathbb{R}^3 \rtimes O(3)$

But for spin $\frac{1}{2}$ particles 2π rotation is not E

If we don't have spin-orbit coupling (SOC)

$$H_{electrons} = \underset{\substack{\uparrow \\ \text{spin-independent}}}{H_0} \otimes \sigma_0$$

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

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

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

U_g^{spin}: spin rotation

generated by $\vec{p}$ & $L = r \times p$

$$[H_{electron}, U_g] = 0 \Rightarrow [H_{elecron}, U_g^{coord}]$$

If we have SOC, we need to use reps of SU(2) to describe spin rotations

$(\hat{n}, \theta) = g \in SU(2)$ $\quad$ $\hat{n}$ - a vector on the sphere S^2

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

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

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

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

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

We can encode this in our study of space groups by extending $\mathbb{E}(3)$ by $\bar{E}$ s.t.

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

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

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

Ex: point group $D_2 < SO(3) = \{E, C_{2x}, C_{2y}, C_{2z}\} = 222$

$$C_{2i}^2 = E, \quad C_{2i} C_{2j} = C_{2j} C_{2i} \quad \forall i, j$$

In $SU(2)$ in the defining representation

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

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

$$\rho_{\frac{1}{2}}(C_{2i})\rho_{\frac{1}{2}}(C_{2j}) = \rho_{\frac{1}{2}}(\bar{E})\rho_{\frac{1}{2}}(C_{2j})\rho_{\frac{1}{2}}(C_{2i})$$

double group 222^d

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

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

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

$$D_2 \cong Q/\{E, \bar{E}\} \qquad SO(3) \cong SU(2)/\{E, \bar{E}\}$$

$$\begin{array}{ccc} D_2 & \cong & Q/\{E,\bar{E}\} \\ \wedge & & \wedge \\ SO(3) & \cong & SU(2)/\{E,\bar{E}\} \end{array}$$

For rotations: double point groups are subgroups of

$$SU(2) \cong Spin(3)$$

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

For reflections we need an extension of $O(3)$

$$Pin(3)/\{E,\bar{E}\} \overset{?}{\cong} O(3)$$

Two possibilities: $Pin(3) \ni I^2 = \begin{cases} E & Pin_-(3) \\ \bar{E} & Pin_+(3) \end{cases}$

physical spin-$\frac{1}{2}$ is like a magnetic moment $\to$ should transform like a magnetic moment under I

$$\Rightarrow \quad I^2 = E \text{ on spins} \quad \to \quad Pin_-(3)$$

$$Pin_-(3) = SU(2) \times \{E, I\} = \{g, gI \mid g \in SU(2), \; I_g = gI\}$$

For spin $\frac{1}{2}$ particles, w/ SOC, Hamiltonians are symmetric under (double) space groups

$$T < G < \underline{\mathbb{R}^3 \rtimes Pin_-(3)}$$

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

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

$$C_{2i}C_{2j} = \bar{E}C_{2j}C_{2i}$$

corresponds to ordinary pt group reps

If η is an irrep of a double group $\eta(\bar{E}) = \pm\eta(E)$

Correspond to spin-$\frac{1}{2}$ "double" representations

5 conjugacy classes:

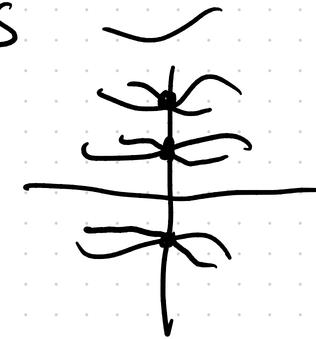
$\{E\}$

$\{\bar{E}\}$

$\{C_{2x}, \bar{E}C_{2x}\}$

$\{C_{2y}, \bar{E}C_{2y}\}$

$\{C_{2z}, \bar{E}C_{2z}\}$ $\rightarrow$ 5 irreps



	E	$\bar{E}$	C_{2x}	C_{2y}	C_{2z}
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	-2	0	0	0

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

$$\rho_{\Gamma_5}(C_{2i}) = -i\sigma_i$$

2d irrep inherited from SU(2))

$\boxed{\text{Electrons w/ SOC can } \underline{\text{only}} \text{ transform in irreps where } \rho(\bar{E}) = -\rho(E)}$

② Time-reversal symmetry (TRS)

on Hilbert space TRS T

$$T \vec{x} T^{-1} = \vec{x}$$

$$T \vec{p} T^{-1} = -\vec{p}$$

This means T cannot be unitary

$$[x_i, p_j] = i\hbar\,\delta_{ij} \qquad \text{but}$$

$$\underline{T[x_i, p_j]T^{-1}} = [Tx_iT^{-1}, Tp_jT^{-1}] = -[x_i, p_j]$$

$$= \underline{-i\hbar\,\delta_{ij}} = T(i\hbar\,\delta_{ij})T^{-1}$$

Resolution: T must be <u>antiunitary</u>:

① $T(\boxed{\alpha}|v\rangle + \beta|w\rangle) = \alpha^{*}T|v\rangle + \beta^{*}|w\rangle$

② $\langle Tv|Tw\rangle = \langle w|v\rangle = (\langle v|w\rangle)^{*}$

$(\langle Tv| = (T|v\rangle)^{\dagger} = |Tv\rangle^{\dagger}$

To see how antiunitaries are represented, introduce a basis $\{|v_i\rangle\}$

$$B_{ij}(T) = \langle v_i | T v_j \rangle$$

For any state $|v\rangle = \sum_i a_i |v_i\rangle$

$$T|v\rangle = \sum_i T a_i |v_i\rangle$$

$$= \sum_i a_i^* |T v_i\rangle$$

$$= \sum_{ij} a_i^* |v_j\rangle\langle v_j | T v_i\rangle$$

$$= \sum_{ij} |v_j\rangle B_{ji}(T) \overline{a_i^*}$$

We can say that T is represented by

$B_{ij}(T) \mathcal{K}$

complex conjugation on scalars

Note $B(T)$ is a unitary matrix

$$\left(B^\dagger(T) B(T)\right)_{ik} = \sum_j \langle T v_i | v_j\rangle\langle v_j | T v_k\rangle$$

$$= \langle T v_i | T v_j \rangle$$
$$= \langle v_j | v_i \rangle = \delta_{ij}$$

Ex: Spin-$\frac{1}{2}$ particles

$$T|\uparrow\rangle = -|\downarrow\rangle$$
$$T|\downarrow\rangle = |\uparrow\rangle$$

$$B_{\sigma\sigma'}(T) = \langle \sigma | T \sigma' \rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y$$

"T is represented by $i\sigma_y \mathcal{K}$"

Let T be antiunitary then T^2 is a unitary operator

$$T^2\big(\alpha|v\rangle + \beta|w\rangle\big) = \alpha T^2|v\rangle + \beta T^2|w\rangle$$

$$\langle T^2 v | T^2 w\rangle = \langle Tw|Tv\rangle = \langle v|w\rangle$$

$$B(T^2) = B(T)\mathcal{K}B(T)\mathcal{K} = B(T)\overset{*}{B}(T)$$

physically, we want $B(T^2) = \lambda\, \mathrm{Id}$

$$B(T)B^*(T) = \lambda \, \mathrm{Id}$$

$$B(T) = \lambda B^T(T)$$

$$= \lambda (B(T))^T = \lambda^2 (B^T(T))^T = \lambda^2 B(T)$$

$$\lambda^2 = 1$$

$$B(T^2) = \pm \mathrm{Id}$$

spin-statistics theorem: $\lambda = +1$ for integer spins

(single-valued reps)

$\lambda = -1$ for half integer spins

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

$$\langle v \mid Tw \rangle \stackrel{?}{=} \langle T^\dagger v \mid w \rangle$$

$$= \underline{\langle T^\dagger w \mid (T^\dagger)^2 v \rangle}$$

$$\langle v \mid T \mid w \rangle \qquad = \pm \langle T^\dagger w \mid v \rangle$$

$$= \pm \langle w \mid Tv \rangle$$

$$\langle T^\dagger v \mid w \rangle = \pm \langle w \mid Tv \rangle$$

$T \to T^\dagger$ has a complex conjugation <u>somewhere</u>

$$|\psi_{n\,k+\delta k}\rangle = \sum_n a_n(\delta k)\,\boxed{|\psi_{nk}\rangle}$$

$$\beta(v, w) = \langle Tv \mid w\rangle$$