Lecture 13

Announcements: HW 2 is due Thursday 3/6 @ 11:59pm

Recall: electrons have spin $\frac{1}{2}$, under a 2π rotation, spinors get a -1

For rotations introduce double groups
- subgroups of $SU(2)$

$\bar{E} \in SU(2)$ represents a 2π rotation

$\eta(\bar{E}) = -Id$ for spin-$\frac{1}{2}$

- to construct double groups use

$$\begin{array}{ccc} SU(2)/\{E,\bar{E}\} & \cong & SO(3) \\ \vee & & \vee \\ \bar{G}^d/\{E,\bar{E}\} & \cong & \bar{G} \end{array}$$

Ex: D_2 whose double group $D_2^d = Q$ from HW1

$SU(2) \cong Spin(3)$ - transformations of spinors in 3D space

For rotations & reflections

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

$SO(3)$ - rotations

$O(3)$ - rotations & reflections

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

$$\mathrm{Pin}(3)/\{E,\bar{E}\} \cong O(3)$$ ← we need an extension of $O(3)$ satisfying this

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

physical spin-$\frac{1}{2}$ carries a magnetic moment, and so spin-$\frac{1}{2}$ should transform like magnetic moment under inversion symmetry

$I^2 = E$ on spins ← $\mathrm{Pin}_-(3)$ as the physical group

$$Pin_-(3) = SO(2) \times \{E, I\}$$

$$\mathcal{Z}(Pin_-(3)) = \{E, \bar{E}\} \times \{E, I\}$$
$$\mathbb{Z}_2 \times \mathbb{Z}_2$$

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

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

($Pin_+(3)$:
$I^2 = \bar{E}$
$I\bar{E} = \bar{E}I$)

$$\mathcal{Z}(Pin_+(3)) = \{E, \bar{E}, I, I\bar{E}\} = \mathbb{Z}_4$$

For any group G
define $Z < G$
Z center of G

$$Z = \{z \in G \mid zg = zg \ \forall g \in G\}$$

$$H_{no\text{-}soc} = \boxed{H_0} \otimes \boxed{\sigma_0}$$

identity on spins

$$U_g = \boxed{U_g^{coords}} \otimes \cancel{U_g^{spin}}$$

For spin-$\frac{1}{2}$ particles w/ SOC

H_{soc} is symmetric under double space groups

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

Ex: $D_2^d = Q \qquad (222^d)$

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

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

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

if η is an irrep of a double group G^d

Q has 5 conjugacy classes

$\{E\}$

$\{\bar{E}\}$

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

$\{C_{2y}, \bar{E}C_{2y}\}$ → 5 irreducible representations

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

$$\eta(\bar{E}) = \begin{cases} +\eta(E) & \eta \text{ has kernel} \supset \{E, \bar{E}\} \Rightarrow \eta \text{ is a rep of } G = G^d/\{E,\bar{E}\} \\ -\eta(E) & \text{– spin-}\tfrac{1}{2} \text{ or "double-valued" representations} \end{cases}$$

	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

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

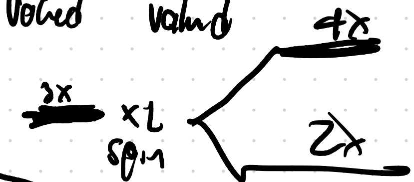
$\rho_{\bar{\Gamma}_5}(\bar{E}) = -\sigma_0$

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

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

In 432
T_2 : $l = 1$
$1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$

single-valued double valued



Notation: Hermann-Maugin symbol for double groups:

$(\text{ordinary symbol})^{d}$

$\bar{E} \leftarrow {}^{d}1$

② Time-reversal symmetry (TRS) T

on operators on Hilbert space

$T\vec{x}T^{-1} = \vec{x}$ → T cannot be unitary

$T\vec{p}T^{-1} = -\vec{p}$ if it preserves $[x_i, p_j] = i\hbar\delta_{ij}$

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

$$\| $$

$$T(i\hbar\delta_{ij})T^{-1} \not\longleftrightarrow = -i\hbar\delta_{ij}$$

Resolution: T has to be an antiunitary operator

antiunitary operators satisfy:

① $\langle Tv|Tw\rangle = (\langle v|w\rangle)^* = \langle w|v\rangle$

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

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

To see how antiunitary operators are represented let $\{|v_i\rangle\}$ be a basis

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

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

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

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

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

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

We can say T is represented by $B_{ij}(T)K$

complex conjugation on scalars

Note $B(T)$ is unitary

$$\left(B(T)^\dagger B(T)\right)_{ik} = \sum_j B^\dagger_{ij}(T)\, B_{jk}(T)$$

$$= \sum_j \langle Tv_i | v_j\rangle \langle v_j | T v_k\rangle$$

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

Ex: Isolated spin-$\frac{1}{2}$ particle $\{|\uparrow\rangle, |\downarrow\rangle\}$

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

on spin $\frac{1}{2}$ "T is represented by $i\sigma_y K$"

Let T be antiunitary $\rightarrow$ T^2 is a unitary operator

T^2 is unitary
$$T^2(\alpha|v\rangle + \beta|w\rangle) = \alpha T^2|v\rangle + \beta T^2|w\rangle$$
$$\langle T^2 v|T^2 w\rangle = \langle Tw|Tv\rangle = \langle v|w\rangle$$

$$B(T^2) = B(T)\mathcal{K}\underbrace{B(T)\mathcal{K}}$$ ← For TRS in particular

$$= B(T)B^*(T)$$

T^2 should commute with all spatial symmetries

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

$$\lambda\, Id = B(T)B^*(T) \Rightarrow \lambda B^T(T) = B(T)$$

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

$$\lambda = \pm 1$$

$\lambda = +1$ for integer spins (single-valued representations)

Spin-statistics theorem

$\lambda = -1$ for half-integer spins
(double valued representations

$$\Rightarrow \quad T^2 = \bar{E}$$

We want Ⓐ $Tg = gT$ for all $g \in G$ - TRS
commutes w/
spatial symmetries

let $\rho: G \to U(V)$ be an irrep of G
if T can be represented on the Hilbert space V

$$B(T)K\rho(g) = \rho(g)B(T)K$$

(A) $\rho^*(g) = B^{-1}(T)\, \rho(g)\, B(T)$

(B) $B(T) B^*(T) = \rho(\bar{E})$

Its <u>not</u> always possible to satisfy (A) and (B) on the Hilbert space V

Example: point group $2^d = \{E, C_{2z}, \bar{E}, C_{2z}\bar{E}\}$

	E	$\bar{E}$	C_{2z}	$C_{2z}\bar{E}$	
Γ_1	1	1	1	1	single valued
Γ_2	1	1	-1	-1	
$\bar{\Gamma}_3$	1	-1	$-i$	i	double valued

$\bar{\Gamma}_4 \,|\, 1 \quad -1 \quad i \quad -i$

on a spin-$\frac{1}{2}$ $\quad C_{2z} \quad e^{-i\frac{\pi}{2}\sigma_z} = \begin{array}{cc} & \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} & \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \end{array}$

$\bar{\Gamma}_3 - V_3 = \{|\uparrow\rangle\}$

$\bar{\Gamma}_4 - V_4 = \{|\downarrow\rangle\}$

$\bar{\Gamma}_3(C_{2z}) = -i \qquad \bar{\Gamma}_4(C_{2z}) = +i$

$+i \neq -i \rightarrow$ no way to represent TRS on V_3 or V_4 alone

To make a T-invariant representation

$$\bar{\Gamma}_3\bar{\Gamma}_4 = \bar{\Gamma}_3 \oplus \bar{\Gamma}_4$$

$$\bar{\Gamma}_3\bar{\Gamma}_4(C_{2z}) = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z$$

$$\bar{\Gamma}_3\bar{\Gamma}_4(T) = i\sigma_y \mathcal{K}$$

representations w/ both unitary & antiunitary elements

corepresentations

$\bar{\Gamma}_3\bar{\Gamma}_4$ is reducible as a representation of 2^d

but as a corepresentation it's irreducible

"physically irreducible"

Herman-Maugin symbol for TRS $1'$

$2^{\circ}\underline{1}'$ or $21'$