

Lecture 14 | Example of a double point

group: $222^d = \{E, C_{2x}, C_{2y}, C_{2z}, \bar{E}, \bar{E}C_{2x}, \bar{E}C_{2y}, \bar{E}C_{2z}\}$

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

$$C_{2y}C_{2x} = C_{2z}^{-1} = \bar{E}C_{2z}$$

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

Conjugacy classes: {E} 2 5

$$\begin{aligned}
 & C_{zx} C_{zy} C_{zx}^{-1} \\
 &= C_{zy} C_{zx}^{-1} \\
 &= \bar{E} C_{zy}
 \end{aligned}
 \quad \left. \begin{array}{l}
 \{ \bar{E} \} \\
 \{ C_{zx}, \bar{E} C_{zx} \} \\
 \{ C_{zy}, \bar{E} C_{zy} \} \\
 \{ C_{zz}, \bar{E} C_{zz} \}
 \end{array} \right\} \text{Conjugacy classes}$$

	E	C_{zx}	C_{zy}	C_{zx}	\bar{E}
T_1	1	1	1	1	1
T_2	1	1	-1	-1	1
T_3	1	-1	-1	1	1
T_4	1	-1	1	-1	1

also linear reps
of the ordinary
 Pt group

bar denotes
that it's a
double-valued
rep

$\overrightarrow{\Gamma}_5 | 2 \ 0 \ 0 \ 0 -2$

our spin- $\frac{1}{2}$ irrep

$$\Gamma_5(C_{2x}) = -i\sigma_x$$

$$\bar{\Gamma}_5(C_{2y}) = -i\sigma_y$$

$$\tilde{\Gamma}_5(C_{2z}) = -i\sigma_z$$

One last thing we have ignored - time-reversal symmetry

\hat{T} - the operator that implements time-reversal
on Hilbert space

$$\hat{T} \xrightarrow{\text{---}} \hat{T}^{-1} = \xleftarrow{\text{---}}$$

$$\hat{T} \xrightarrow{\text{---}} \hat{T}^{-1} = -\xrightarrow{\text{---}}$$

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

$$\exists T [x_i, p_j] T^{-1} = T i\hbar T^{-1} \delta_{ij}$$

$$\left[\begin{smallmatrix} T x_i T^{-1}, T p_j T^{-1} \\ \end{smallmatrix} \right]$$

$$- \left[\begin{smallmatrix} x_i, p_j \\ \end{smallmatrix} \right]$$

$$-i\hbar s_{ij} = T(i\hbar\delta_{ij})T^{-1} \quad T(i\hbar\delta_{ij})T^{-1} = -i\hbar s_{ij}$$

impossible if T is unitary

$\rightarrow T$ is antunitary

What is an antiunitary operator

①

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

②

$$\langle Tr|Tw\rangle = \langle w|v\rangle = \langle v|w\rangle^*$$

(compare w/ unitary operators)

$$\begin{aligned} \rightarrow \langle Uv|Uw\rangle &= \langle v|w\rangle \\ \langle v|U^+Uw\rangle \end{aligned}$$

③ If T is an antiunitary operator, then
 $\overline{T^2}$ is unitary

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

for any $|v\rangle, |w\rangle \Rightarrow T^2$ is unitary

If we have a basis $\{|v_i\rangle\}$ for Hilbert Space, there is a useful representation of

T : for any $|v\rangle$ we have

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

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

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

We can define a unitary matrix

$$U_T^{j|i} = \langle v_i | T v_j \rangle$$

$$\sum_i a_i^* \langle v_j | T v_i \rangle = U_T^{j|i} a_i^*$$

$U_T K$

$$= \boxed{U_T^{j|i} K} a_i^*$$

"complex conjugation operation"

Lets specialize to T being time-reversal

$T \hat{x} T^{-1} = \overrightarrow{x}$ \Rightarrow we want TR to commute
with all spatial symmetries

$\rightarrow T^2$ commutes with all spatial symmetries

in any point or space group irrep ρ

$\rho(T^2)$ needs to commute w/ $\rho(g) \forall g \in G$

\rightarrow Schur's lemma: $\rho(T^2) = \lambda \text{Id}$

$$T^2 = U_T K U_T^* K = \boxed{U_T U_T^*}$$

w/ continuous rotational Symmetry for each irreducible block

$$U_T U_T^* = \lambda$$



$$U_T = \lambda U_T^T$$

$$U_T^{-1} = U_T^*$$

$$(U_T^*)^{-1} = U_T^T$$

$$U_T^T = \lambda U_T \Rightarrow U_T = \lambda^2 U_T^T$$

$$\Rightarrow \lambda = \pm 1$$

\rightarrow Spin-statistics theorem: $\lambda = +1$ for single-valued

irreps

$\lambda = -1$ for double-valued

irreps

$$(T^2 |\psi\rangle = (-1)^F |\psi\rangle)$$

So for systems w/ TR, we want to extend our notion of reps and irreps to

allow for a representation of TRS as
an antiunitary operator

↪ corepresentations

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

	E	\bar{E}	C_{2z}	\bar{C}_{2z}^{-1}
T_1	1	+1	1	1
T_2	1	+1	-1	-1
$\rightarrow \bar{T}_3$	1	-1	-i	+i ↗
\bar{T}_4	1	-1	+i	-i ↗

an up spin transforms
in this irrep

a down spin transforms
in this irrep

Let's consider \bar{F}_3 : $\nexists \bar{F}_3(T) = U_T K$

$$[\bar{F}_3(T), \bar{F}_3(C_{27})] = 0$$

$$(\bar{F}_3(T))^2 = -1$$

\rightarrow to form an irreducible corepresentation,
we need $\bar{F}_3 \oplus \bar{F}_4 \equiv \bar{F}_3 \bar{F}_4$

$$\bar{F}_3 \bar{F}_4 (G_{2z}) = \begin{pmatrix} \bar{F}_3(G_{2z}) & 0 \\ 0 & \bar{F}_4(G_{2z}) \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & e+i \end{pmatrix} = -i \sigma_z$$

$$\bar{F}_3 \bar{F}_4 (\tau) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} k = i \sigma_y k$$

we say $\bar{F}_3 \bar{F}_4$ is { an irreducible corepresentation
physically irreducible representation }

$$(\alpha_x K)^2 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} K \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} K$$

$$= \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(\alpha_y K)^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} K \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} K = - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We can figure out what irrep can be extended to coreps by noting the following:

Given an antisymmetry T , w/ $T^2 = \pm 1$
we can define a bilinear form

$$B(v, w) = \langle Tv | w \rangle$$

$$\begin{aligned} B(v, aw_1 + bw_2) &= \langle Tv | (aw_1 + bw_2) \rangle \\ &= B(v, w_1)a + B(v, w_2)b \end{aligned}$$

$$B(av_1 + bv_2, w) = aB(v_1, w) + bB(v_2, w)$$

$$\begin{aligned}
 B(w, v) &= \langle Tw | v \rangle \\
 &= \langle Tv | T^2 w \rangle \\
 &= \pm B(v, w)
 \end{aligned}$$

$$\begin{aligned}
 B(\rho(g)v, \rho(g)w) &= \langle T\rho(g)v | \rho(g)w \rangle \\
 &= \langle Tv | w \rangle = B(v, w)
 \end{aligned}$$

Since we want T to commute with $\rho(g)$

representation for matrices

This goes the other way too; given B we
can construct \overline{T}

$$\varphi_v(w) = B(v, w)$$

||

$$\varphi_r = \sum_i \varphi_v(v_i) \langle v_i | \equiv \langle Tr |$$

$$\textcircled{1} \quad B: V \times V \rightarrow \mathbb{C}$$

$v \triangleright w \mapsto B(v, w)$

$$\textcircled{2} \quad B: V \rightarrow \boxed{V^*}$$

$v \mapsto \varphi_v = B(v, \cdot)$

$$\rho(g) | v \mapsto \langle v | \rho^+(g)$$

Schur's lemma: β can only exist if
 ρ and ρ^+ are isomorphic as
representations \rightarrow all characters χ_ρ are

real
↑

See Fulton & Harris

"Representation Thy:
A first course")