Lecture 14

Recap: e^-'s have spin-$\frac{1}{2}$

with spin-orbit coupling $\mathbb{E}(3)$ alone is not enough to understand rotations & reflections

$$\frac{\mathrm{Pin}_-(3)}{\{E,\bar{E}\}} \cong O(3) \qquad \frac{SU(2)}{\{E,\bar{E}\}} = SO(3)$$

$$\mathbb{E}(3) \cong \mathbb{R}^3 \rtimes \mathrm{Pin}_-(3)$$

"double" space groups are subgroups of this

multiplication table for G^d inherited from $SU(2)$

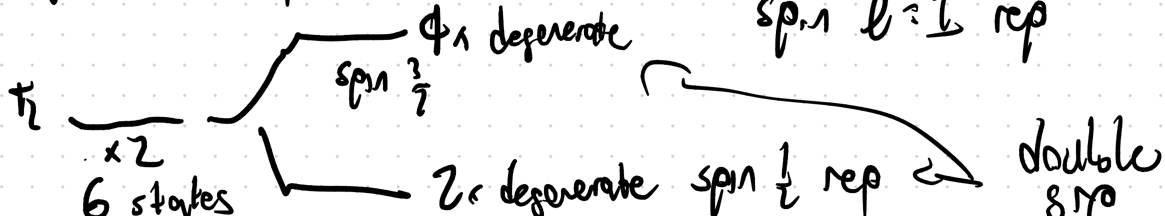
representations $\quad \eta(\bar{E}) = \begin{cases} +\mathrm{Id} \to \text{ordinary "single-valued" rep of } G \\ -\mathrm{Id} \to \text{"double-valued" rep} \end{cases}$

relevant for spin-$\frac{1}{2}$ electrons

No SOC $\quad H = H_0 \otimes \sigma_0$

Ex: point group 432 $\quad T_2$ irrep (3 dimensional)

spin $l = 1$ rep



megs

$$1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$$

Now: Time reversal symmetry $\quad T$

On operators on Hilbert space

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

$$T \vec{p} T^{-1} = -\vec{p} \qquad [T x_i T^{-1}, T p_j T]$$

$$= -i\hbar \delta_{ij}$$

$$\neq T [x_i, p_j] T^{-1}$$

$\Rightarrow$ T cant be a unitary operator

T has to be antiunitary (antilinear)

an operator T is antiunitary

1. $T|v\rangle = |Tv\rangle$
   $T|w\rangle = |Tw\rangle$

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

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

To see how we can represent an antiunitary operator, pick a basis $\{|v_i\rangle\}$ for our Hilbert space

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

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

$$T|v\rangle = T\left(\sum_i a_i |v_i\rangle\right)$$

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

insert Identity $\sum_j |v_j\rangle\langle v_j|$

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

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

We can say that T is represented by

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

unitary

complex conjugation of scalars

$$K|v_i\rangle = |v_i\rangle$$
$$K(a_i|v_i\rangle) = a_i^*|v_i\rangle$$

Note $B(T)$ is a unitary matrix

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

$$= \sum_j \langle Tv_i|v_j\rangle\langle v_j|Tv_k\rangle$$

$$= \langle Tv_i|Tv_k\rangle = \langle v_k|v_i\rangle = \delta_{ik}$$

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

$$T|\uparrow\rangle = -|\downarrow\rangle$$
$$T|\downarrow\rangle = +|\uparrow\rangle$$
$\leftarrow$ QFT lore

$$B_{\sigma\sigma'}(T) = \langle\sigma|T\sigma'\rangle = \begin{pmatrix} \langle\uparrow|T\uparrow\rangle & \langle\uparrow|T\downarrow\rangle \\ \langle\downarrow|T\uparrow\rangle & \langle\downarrow|T\downarrow\rangle \end{pmatrix}$$

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

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

$$T\left(\sum_{i=\uparrow\downarrow} \alpha_i |\sigma_i\rangle\right) = \sum_j |\sigma_j\rangle B_{\sigma_j\sigma_i}(T)\alpha_i^*$$

Let T is antiunitary, T^2 must be a unitary operator

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

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

$$= \langle Tw | Tv\rangle = \langle v | w\rangle$$

T^2 is unitary

$$B(T^2) = (B(T)K)(B(T)K) = B(T)B^*(T)$$

we expect T to commute w/ all spatial symmetries

$\to$ T^2 commutes w/ all spatial symmetries

Lets say we have an irrep B, of a symmetry group G

$$[B(T^2), B(g)] = 0 \text{ for all } g \in G$$

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

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

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

$$\lambda^2 = 1$$

$\lambda = \pm 1$

spin-statistics theorem : $\lambda = +1$ for integer spins (single-valued representations)

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

$T^2 = \underline{E} \in \underline{Pin_-(3)}$

Given a point or space group G (double group) and an irreducible representation $\rho : G \to U(V)$

we want to construct $\rho(T) = B(T)\mathcal{K}$

where :

① $[\rho(T), \rho(g)] = 0$

② $(\rho(T))^2 = B(T)B^*(T) = \rho(\bar{E})$

It is not always possible to satisfy these two properties on the Hilbert space V

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

	E	C_{2z}	$\bar{E}$	$\bar{E}C_{2z}$
Γ_1	1	1	1	1
Γ_2	1	-1	1	-1
$\bar{\Gamma}_3$	1	$-i$	-1	i
$\bar{\Gamma}_4$	1	i	-1	$-i$

Consider $\bar{\Gamma}_3$ irrep $\bar{\Gamma}_3 : G \to V_3$

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

$\Gamma_3(T) \stackrel{?}{=} \alpha K \qquad [\Gamma_3(T), \Gamma(C_{2z})] = 2i\alpha K \neq 0$

$\Rightarrow$ no way to represent T on V_3

same problem for V_4

On a single spin-$\frac{1}{2}$ $\quad \rho_{\frac{1}{2}}(C_{2z}) = e^{-i\frac{\pi}{2}\sigma_z} = \begin{array}{cc|c} |\uparrow\rangle & |\downarrow\rangle & \\ \end{array}$

$$\begin{array}{c|c} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

$V_3 = \{|\uparrow\rangle\}$

$V_4 = \{|\downarrow\rangle\}$

To make a time-reversal invariant representation

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

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

reducible when viewed as a rep. of 2d

but if we include TRS it is not reducible

"physically irreducible"

Hermann-Mauguin symbol for TRS $1'$

co-representation of a group w/ TRS

- a representation of the group
+
an antiunitary operator for TRS

$\bar{\Gamma}_3 \bar{\Gamma}_4$ is an irreducible corepresentation of $2^{d}1'$

How does Time-reversal symmetry (TRS) act on $\vec{k}$

start w/ $|\psi_{n\vec{k}}\rangle$ $\quad U_{\vec{t}}|\psi_{nk}\rangle = e^{-i\vec{k}\cdot\vec{t}}|\psi_{nk}\rangle$

consider $T|\psi_{n\vec{k}}\rangle$ - what crystal momentum does this have?

$$U_{\vec{t}} T |\psi_{nk}\rangle = T(U_{\vec{t}} |\psi_{nk}\rangle)$$
$$= T(e^{-i\vec{k}\cdot\vec{t}} |\psi_{nk}\rangle)$$
$$= e^{-i(-\vec{k})\cdot\vec{t}} (T|\psi_{nk}\rangle)$$

$\rightarrow$ $T|\psi_{nk}\rangle$ has crystal momentum $-\vec{k}$

If $-\vec{k} \equiv k$ mod a reciprocal lattice vector, TRSGG$_k$

$\uparrow$

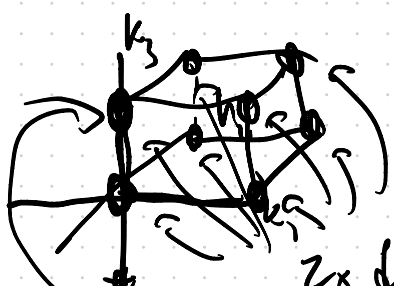
$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 \qquad k_j \in [-\tfrac{1}{2}, \tfrac{1}{2})$$
$$-\vec{k} = -k_1\vec{b}_1 - k_2\vec{b}_2 - k_3\vec{b}_3$$

equivalent when $2k_i = (0, 1)$

$k_i = (0, \frac{1}{2})$

8 $\underbrace{\text{time-reversal invariant momenta}}_{\text{(TRIM)}}$ in the Brillouin zone

$$\frac{n_1}{2}\vec{b}_1 + \frac{n_2}{2}\vec{b}_2 + \frac{n_3}{2}\vec{b}_3 \qquad n_i \in \{0, 1\}$$



2x degeneracies

$PZ^d 1'$

here

little cogroup $G_k/T < \overline{G}_k$

nothing to do w/ corepresentations