4. Time reversal

As we will see Chern insulators, i.e. topological band-structures with non-vanishing Chern number are <u>not</u> invariant under time reversal. Since generalized symmetries play a key role in the classification of topological insulators we will now discuss them a bit more in detail

4.1. Wigner theorem and invariance transformations

a transformation $|\psi\rangle \longrightarrow G|\psi\rangle$ is called <u>invariance transformation</u> if $\forall \{|\psi\rangle, |\phi\rangle\} \in \mathcal{H}$ holds

(186) $$|\langle G\psi|G\phi\rangle| = |\langle\psi|\phi\rangle|$$

<u>Wigner (1931)</u>

invariance transformations are either

(187) <u>unitary</u> $$\langle G\psi|G\phi\rangle = \langle\psi|\phi\rangle$$

or

(188) <u>antiunitary</u> $$\langle G\psi|G\phi\rangle = \langle\psi|\phi\rangle^*$$

invariance transformations are called (generalized) <u>symmetry transformations</u> of a quantum system if and only if

(189) $$\boxed{GHG^{-1} = H} \quad \text{or} \quad \boxed{[H, G] = 0}$$

<u>properties of anti-unitary operators</u> (188)

- if G is anti-unitary $\Rightarrow$ G^2 is unitary

- every anti-unitary operator G can be written as product of a unitary operator U and the complex conjugation K

(190) $$\boxed{G = UK} \qquad U^+ = U^{-1}$$
$$Kf = f^*$$

or $G = K\tilde{U}$

- inverse

(191) $$G^{-1} = KU^+ \qquad (K^2 = 1)$$

- transformation of operators

$$A' = GAG^{-1} = UKAKU^+$$

since $KA = A^*K \Rightarrow$

(192) $$\boxed{A' = GAG' = UA^*U^+}$$

- transformation of matrix elements

$$A' = GAG^{-1} \quad \text{and} \quad |\psi'\rangle = G|\psi\rangle$$

$$\langle \psi' | A' | \phi' \rangle = \langle G\psi | G A G^{-1} | G\phi \rangle$$

$$= \langle G\psi | G A G^{-1} G \phi \rangle = \langle G\psi | G (A\phi) \rangle$$

(193)

$$= \langle \psi | A \phi \rangle^* = \langle \psi | A | \phi \rangle^*$$

4.2 time reversal of spinless particles

time reversal $T: \quad t \to -t$

(194) $$T \hat{x} T^{-1} \stackrel{!}{=} \hat{x} \qquad T \hat{p} T^{-1} = -\hat{p}$$

$$\Rightarrow T [\hat{x}, \hat{p}] T^{-1} = T i\hbar T^{-1} \stackrel{!}{=} -[\hat{x}, \hat{p}] = -i\hbar$$

thus T must be anti-unitary

(195) $$T = UK$$

it holds

(196) $$\boxed{T^2 = \pm 1}$$

proof: $T^2 = UKUK = UU^* K^2 = UU^*$
$= U (U^T)^{-1} \equiv A$

since $T^2 |\psi\rangle = e^{i\varphi} |\psi\rangle$

$\Rightarrow$ A is diagonal, i.e. $A = A^T$

$\Rightarrow$

$$U = A U^T \qquad U^T = U A^T = U A$$

thus $\quad U = AUA \qquad 1 = A^2 \qquad A = \pm 1 \;\square$

If

(197)
$$\boxed{T^2 = +1 \Rightarrow U = U^T} \quad \underline{\text{symmetric}}$$
$$\boxed{T^2 = -1 \Rightarrow U = -U^T} \quad \underline{\text{anti-symmetric}}$$

(A) action of T on spinless particles on a lattice

$$\hat{a}_e = \alpha \hat{x}_e + i\beta \hat{p}_e \qquad e \text{ position index}, \quad \alpha, \beta \in \mathbb{R}$$

(198)
$$\boxed{T \hat{a}_e T^{-1} = T(\alpha \hat{x}_e + i\beta \hat{p}_e) T^{-1} = \hat{a}_e}$$

time-reversal of real space operators

Thus we see that here

(199)
$$\boxed{U = \mathbb{1} \quad \text{i.e.} \quad T = K} \qquad \boxed{T^2 = +1}$$

Now lets construct time reversal for momentum-space operators

$$\hat{a}_e \stackrel{!}{=} T \hat{a}_e T^{-1} = T \frac{1}{\sqrt{L}} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_e} \tilde{a}_{\vec{k}} T^{-1}$$
$$= \frac{1}{\sqrt{L}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_e} T \tilde{a}_{\vec{k}} T^{-1} \stackrel{!}{=} \frac{1}{\sqrt{L}} \sum_{k} e^{i\vec{k}\vec{R}_e} \tilde{a}_{\vec{k}}$$

Thus

(200) $$\boxed{T\,\hat{a}_{\vec{k}}\,T^{-1} = \hat{a}_{-\vec{k}}}$$

Sanity check: $$\hat{p} = \sum_k \hbar\vec{k}\,\hat{a}^\dagger_k \hat{a}_k$$

$$T\hat{p}T^{-1} = \sum_k \hbar\vec{k}\,T\hat{a}^\dagger_k \hat{a}_k T^{-1}$$

$$= \sum_k \hbar\vec{k}\,\hat{a}^\dagger_{-k}\hat{a}_{-k} = -\sum_k \hbar\vec{k}\,\hat{a}^\dagger_k \hat{a}_k$$

$$= -\hat{p} \quad \checkmark$$

One recognizes that a single-particle hamiltonian

$$H = \sum_{\vec{k}} h(\vec{k})\,\tilde{c}^\dagger_{\vec{k}}\tilde{c}_{\vec{k}}$$

is time-reversal invariant (TR-invariant) if

$$THT^{-1} = \sum_{\vec{k}} T h(\vec{k}) T^{-1}\, T\tilde{c}^\dagger_{\vec{k}}\tilde{c}_{\vec{k}}T^{-1}$$

$$= \sum_k T h(\vec{k}) T^{-1}\,\tilde{c}^\dagger_{-\vec{k}}\tilde{c}_{-\vec{k}} \overset{!}{=} H$$

$\Rightarrow$

(201) $$\boxed{T h(\vec{k}) T^{-1} = h(-\vec{k})}$$ <u>TR invariant hamiltonian</u>

<u>Note:</u> $h(\vec{k})$ can still be a matrix if we have unit cells with more than one site;
since $T = K$ we have $h^*(\vec{k}) = h(-\vec{k})$

(B) Vanishing of Hall conductivity for TR invariant hamiltonians of spinless particles

TR invariance

$$h(\vec{k})|\psi(\vec{k})\rangle = T^{-1} h(-k) T |\psi(\vec{k})\rangle = \varepsilon_k |\psi(\vec{k})\rangle$$

i.e. if $|\psi(\vec{k})\rangle$ is eigenfunction of $h(\vec{k})$, then $T|\psi(\vec{k})\rangle$ is eigenfunction of $h(-\vec{k})$

Bloch functions $\quad u_{-\vec{k}} = T u_{\vec{k}} = u_{\vec{k}}^*$

$\Rightarrow$ Berry curvature

$$F_{\ell m}(\vec{k}) = -i\left(\langle \partial_\ell u_{\vec{k}} | \partial_m u_{\vec{k}}\rangle - \text{"}\ell \leftrightarrow m\text{"}\right)$$

$$= -i\left(\langle \partial_\ell u^*_{-\vec{k}} | \partial_m u^*_{-\vec{k}}\rangle - \text{"}\ell \leftrightarrow m\text{"}\right)$$

$$= -i\left(\langle \partial_m u_{-\vec{k}} | \partial_\ell u_{-\vec{k}}\rangle - \text{"}\ell \leftrightarrow m\text{"}\right)$$

$$= -F_{\ell m}(-\vec{k})$$

i.e integration over Brillouin zone $\int_{BZ} d\vec{k}\, F_{\ell m}(\vec{k}) = 0$

(202) $\quad \boxed{C = 0 \quad \text{i.e.} \quad \sigma_{xy} = 0}$

$\nexists$ QH-effect for spinless particles with TR symmetry

4.3 time reversal for particles with spin

In order to see how the spin transforms under time reversal, let us consider orbital angular momentum first

$$\vec{L} = \vec{r} \times \vec{p} \quad \Rightarrow \quad T\vec{L}T^{-1} = -\vec{L}$$

thus

(203) $$\boxed{T\hat{\vec{S}}T^{-1} = -\hat{\vec{S}}}$$

Can be achieved by rotation about arbitrary axis by π.
Convention : y-axis

(204) $$\boxed{T = e^{-i\pi\hat{S}_y}K}$$ i.e. $U = e^{-i\pi\hat{S}_y}$

$$T^2 = e^{-i\pi\hat{S}_y}Ke^{-i\pi\hat{S}_y}K = e^{-i\pi\hat{S}_y}e^{i\pi\hat{S}_y^*}$$

with $S_y^* = -S_y$ follows

(205) $$T^2 = e^{-2\pi i\hat{S}_y}$$

bosons / fermions

(206) $$\boxed{T^2 = 1} \qquad \boxed{T^2 = -1}$$

like pseudospin
or spinless particles

note: (206) holds for a single particle

Kramers theorem

> For a TR invariant fermionic Hamiltonian H every eigenstate is (at least) doubly degenerate

proof: $H|\psi\rangle = E|\psi\rangle$ and $[T, H] = 0$

$\Rightarrow$ also $T|\psi\rangle$ is eigenstate to energy E
but is this state orthogonal to $|\psi\rangle$?

$$\langle\psi|T\psi\rangle = \sum_{m,n} \psi_m^* U_{mn} K \psi_n$$

$$= \sum_{m,n} \psi_m^* U_{mn} \psi_n^* = \sum_{m,n} \psi_n^* (-U_{nm}) \psi_m^*$$

note $T^2 = -1 \Rightarrow U = -U^T$ see eq.(197)

$$= -\sum_{m,n} \psi_n^* U_{nm} K \psi_m = -\langle\psi|T\psi\rangle$$

$$\Rightarrow \quad \langle\psi|T\psi\rangle = 0 \qquad \square$$

time-reversal of lattice models of fermions (spin 1/2)

(207) $$H = \sum_{\vec{k}\sigma\sigma'} \hat{c}^{+}_{\vec{k}\sigma} h_{\sigma\sigma'}(\vec{k}) \hat{c}_{\vec{k}\sigma'}$$

how does T act on creation and annihilation operators of fermions? $\hat{c}^{+}_{\uparrow}$ creates a particle with spin up. $T\hat{c}^{+}_{\uparrow}T^{-1}$ should create a particle with reversed spin

$$\boxed{\begin{aligned} T\, c_{j\uparrow}\, T^{-1} &= c_{j\downarrow} \\ T\, c_{j\downarrow}\, T^{-1} &= -c_{j\uparrow} \end{aligned}} \tag{208}$$

Where we put a minus sign is a matter of convention but there has to be one in one of the two equations. On first glance this sounds odd since from (208) follows

$$T^2 \hat{c}_{j\uparrow} T^{-2} = -\hat{c}_{j\uparrow}$$

but $T^2 = T^{-2} = -1$. However $\hat{c}_{j\uparrow}$ reduces the number of particles by one!

$|\psi\rangle$ state with odd number of fermions (e.g. 1)

$$T^2 \hat{c}_{j\downarrow} \underbrace{T^{-2} |\psi\rangle}_{\text{single (odd number) particle}} = T^2 \hat{c}_{j\downarrow} (-|\psi\rangle)$$

$$= -T^2 |\tilde{\psi}\rangle$$

$|\tilde{\psi}\rangle = \hat{c}_{j\downarrow} |\psi\rangle$ has <u>even</u> number of particles i.e. $T^2 |\tilde{\psi}\rangle = +|\tilde{\psi}\rangle$

$$= -|\tilde{\psi}\rangle$$

$$= -\hat{c}_{j\downarrow} |\psi\rangle \quad \square$$

compact form $\qquad i\sigma^y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$$(209) \quad \boxed{\begin{aligned} T\, \hat{C}_{j\lambda}\, T^{-1} &= i\sigma^y_{\lambda\lambda'}\, \hat{C}_{j\lambda'} \\ T\, \underline{\hat{C}_j}\, T^{-1} &= i\underline{\underline{\sigma}}^y\, \underline{\hat{C}_j} \end{aligned}}$$

in real space

transformation to <u>Fourier space</u>

$$(210) \quad \boxed{T\, \underline{\tilde{C}}(k)\, T^{-1} = i\underline{\underline{\sigma}}^y\, \underline{\tilde{C}}(-k)}$$

Thus a single particle hamiltonian for spin 1/2 particles (here unit cell of 1)

$$(211) \qquad H = \sum_{\bar{k}\lambda\lambda'} h^{\lambda\lambda'}(\bar{k})\, \tilde{C}^+_{\lambda}(\bar{k})\, \tilde{C}_{\lambda'}(\bar{k})$$

is TR invariant, i.e. $[T, H] = 0$ or $THT^{-1} = H$

if

$$THT^{-1} = \sum_{k\lambda\lambda''} T h^{\lambda\lambda''}(\bar{k}) T^{-1}\, T \tilde{C}^+_{\lambda}(\bar{k})\, \tilde{C}_{\lambda''}(\bar{k}) T^{-1}$$

$$= \sum_{\substack{k\lambda\lambda'' \\ \lambda'\lambda'''}} h^{\lambda\lambda''}(\bar{k})^*\; i\sigma^y_{\lambda\lambda'}\, \tilde{C}^+_{\lambda'}(-\bar{k})\; i\sigma^y_{\lambda''\lambda'''}\, \tilde{C}_{\lambda'''}(-\vec{k})$$

$$= \sum_{\substack{k\lambda\lambda'' \\ \lambda'\lambda'''}} i(\sigma^{yT})_{\lambda'\lambda}\, h^{\lambda\lambda''}(-\vec{k})^*\; i\sigma^y_{\lambda''\lambda'''}\, \tilde{C}^+_{\lambda'}(\bar{k})\, \tilde{C}_{\lambda'''}(\bar{k})$$

thus for $THT^{-1} = H \Rightarrow$

(212) $$\boxed{h^{\lambda'\lambda'''}(\vec{k}) = i(\sigma^{yT})_{\lambda'\lambda}\, h^{\lambda\lambda''}(-\vec{k})^{*}\, i\sigma^{y}_{\lambda''\lambda'''}}$$

$$\underline{\underline{h}}(\vec{k}) = i\underline{\underline{\sigma}}^{yT}\,\underline{\underline{h}}(-\vec{k})^{*}\, i\underline{\underline{\sigma}}^{y}$$

(213) $$\boxed{\underline{\underline{h}}(\vec{k}) = \underline{\underline{\sigma}}^{y}\,\underline{\underline{h}}(-\vec{k})^{*}\,\underline{\underline{\sigma}}^{y}}$$

$\underline{h}$ 2×2 matrix for spin comp.

TR invariant spin 1/2 hamiltonians

- for general spin 1/2 hamiltonians (213) holds only for specific values of $\vec{k} = \vec{k}_0$

<u>$\vec{k}_0$: TR invariant points of $\underline{h}(\vec{k})$</u>