8. \( \mathbb{Z}_2 \) topological invariant

For the minimal version of the Kane-Mele model with \( \lambda_x = \lambda_y = 0 \) we found that the total Chern number per band vanishes \( \text{Ch} = \text{Ch}_r + \text{Ch}_l = 0 \) but the difference could take two values \( |\text{Ch}_r - \text{Ch}_l| \in \{0, 2\} \). For \( \lambda_x, \lambda_y \neq 0 \) the latter is no longer quantized and we need to find a general \( \mathbb{Z}_2 \) topological invariant.

8.1 Kramers doublet of edge modes

A defining property of topological insulator was the existence of edge modes which are protected, i.e. do not allow for backscattering. Let's see how this looks like in the case of TR invariant systems.

Let \( \psi(x, k_y) \) be 1-particle edge mode (function of \( k_y \)) with energy \( E_0(k_y) \) in band gap.

Kramers theorem (p. 8) + TR invariance

\[ \begin{align*}
\Psi_2(x, k_y) & \text{ with } \Psi_2(x, -k_y) = -\Psi_1(x, k_y) \\
\text{with energy } E_0(k_y)
\end{align*} \]

Kramers doublet of edge modes
What happens at degeneracy points $k_y = 0, \pm \pi$?
Can $\psi_1$ scatter into $\psi_2$? i.e. is there any avoided crossing in the presence of a perturbation?

**No!**  
**Coupling is forbidden as long as there is TR invariance, i.e. as long as $H_{\text{pert}}$ is TR invariant**

**Proof:** perturbation $H_{\text{pert}}$, $T = \text{UK}$, $T^2 = -1$ (fermions)  
$\Rightarrow U^T = -U$

$$\langle T\phi | T\psi \rangle = \sum_{mpr} (U_{mp} \phi_p)^* U_{mr} \phi_r = \sum_{mpr} U_{mp} \phi_p U_{mr} \phi_r^*$$

$$= \sum_{mpr} U_{pm} U_{mr} \psi^*_p \phi_r = \langle \psi_1 \phi \rangle$$

choose $|T\psi\rangle = H_{\text{pert}}|\phi\rangle$  
$(|T\psi\rangle$ and $|\phi\rangle$ have same unperturbed energies)

$$T^2 |\psi\rangle = -|\psi\rangle = TT_{\text{pert}} |\phi\rangle = \frac{TT_{\text{pert}}}{\text{det}} |\phi\rangle = H_{\text{pert}} T |\phi\rangle$$

$\Leftrightarrow H_{\text{pert}}$ is TR invariant

$$\langle \psi_1 \phi | - \langle T\phi | H_{\text{pert}} | \phi \rangle = -\langle T\phi | H_{\text{pert}} | \phi \rangle$$

$$= -\langle T\phi | H_{\text{pert}} | \phi \rangle$$

(2.76)  
$$\langle T\phi | H_{\text{pert}} | \phi \rangle = 0 \quad \forall H_{\text{pert}} \text{ with } TH_{\text{pert}} T^{-1} = H_{\text{pert}}$$

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This can be generalized to multiple Kramers doublets if the number of doublets is odd. If the number of doublets is even, a coupling can exist (no proof here).

\[
\# \text{Kramers doublets} \quad \begin{cases} \text{even} & \quad \text{no protected edge modes} \\ \text{odd} & \quad \text{edge modes by \( TP \) symmetry protected} \end{cases}
\]

\[
\text{simple insulator} \quad \text{Z}_2 \text{ topological insulator}
\]

\section{8.2 \( \mathbb{Z}_2 \) invariant: zeroth of the Pfaffian \( \ast \)}

\textbf{(A) Pfaffian of an anti-symmetric matrix}

Let \( M_{jk} = - M_{kj} \) be a \( n \times n \) matrix.

\[
\begin{align*}
\text{If } n & = 2m+1, & \text{Pf}(M) & = 0 \\
\text{If } n & = 2m, & \text{Pf} & \text{ is a number}
\end{align*}
\]

\begin{equation}
(277)
\end{equation}

\textbf{Def:} \( TL \) set of all partitions of \( (1,2,3,\ldots,2m) \) into pairs (e.g., \((1,2);(3,4);\ldots\)). The total number of these partitions is \((2m-1)!!\).
Let $\alpha \in \pi : \{ (i_1, k_1), (i_2, k_2), \ldots, (i_m, k_m) \}$

where $i_1 < k_1$ and $i_1 < i_2 < i_3 < \ldots$

(2.38) Def: $M_{\alpha} = \text{sgn}(\alpha) M_{i_1 k_1} M_{i_2 k_2} \cdots M_{i_m k_m}$

where $\text{sgn}(\alpha)$ is $(-1)^p$ and $p$ is # of permutation needed

\[
\begin{array}{cccccc}
1 & 2 & 3 & 4 & \cdots & 2m \\
\downarrow & & & & & \\
\tilde{i}_1 & \tilde{k}_1 & \tilde{i}_2 & \tilde{k}_2 & \cdots & \tilde{k}_m
\end{array}
\]

(2.73)

\[\text{Pf} \left( \frac{M}{=} \right) = \sum_{\alpha \in \pi} M_{\alpha}\]

Proposition:

(2.80) \[\left( \frac{\text{Pf} (M)}{=} \right)^2 = \text{Det} (M)\]

(2.81) \[\text{Pf} \left( \frac{BM}{=} \right) = \text{Det} (B) \cdot \text{Pf} (M)\]

(2.82) \[\text{Pf} \left( \frac{L^T M}{=} \right) = \lambda^m \text{Pf} (M)\]

(2.83) \[\text{Pf} \left( \frac{M^T}{=} \right) = (-1)^m \text{Pf} (M)\]

Example: \[M = \begin{pmatrix} a & b \\
-b & a \end{pmatrix}\]

\[\text{Pf} (M) = a\]

\[H = \begin{pmatrix}
\lambda_1 & 0 & \cdots & 0 \\
0 & \lambda_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \lambda_m
\end{pmatrix}\]

\[\Rightarrow \text{Pf} (H) = \lambda_1 \lambda_2 \cdots \lambda_m\]
Let \( \{ | u_i(\vec{e}) \rangle \} \) be a Bloch eigenbasis of a TR invariant Hamiltonian. To characterize the effect of time reversal on these states consider the matrix

\[
H_{ij}(\vec{e}) = \langle u_i(\vec{e}) | T | u_j(\vec{e}) \rangle
\]

- \( H_{ij}(\vec{e}) \) is anti-symmetric

\[
H_{ij}(\vec{e}) = - H_{ji}(\vec{e})
\]

**Proof:**

\[
H_{ij}(\vec{e}) = \langle u_i | T | u_j \rangle = \langle u_i | U K | u_j \rangle
\]

since \( T = U K \) where \( T^2 = -1 \) \( \Rightarrow \) \( U^T = -U \) \( (U^+ = U^{-1}) \)

\[
\Rightarrow H_{ij} = (u_i(\vec{e})^*)_m \ U_{mn} \ (u_j(\vec{e})^*)_n
\]

\[
= - (u_j(\vec{e})^*)_n \ U_{mn} \ (u_i(\vec{e})^*)_m
\]

\[
= - \langle u_j(\vec{e}) | T | u_i(\vec{e}) \rangle = - H_{ji}(\vec{e}) \quad \square
\]

**Def:** \( \{ | u_i(\vec{e}) \rangle \}_o \) set of all eigenstates of \( H \) which are odd under TR

\( \{ | u_i(\vec{e}) \rangle \}_e \) set of all eigenstates of \( H \) which are even under TR

\[
T | u_i(\vec{e}) \rangle_o \perp \{ | u_i(\vec{e}) \rangle \}_o \quad T | u_i(\vec{e}) \rangle_e \in \{ | u_i(\vec{e}) \rangle \}_e
\]
Pfaffian of time reversal matrix

\[
\text{(287) \hspace{1cm}} \quad P(e) \equiv \text{Pf} \left[ \mathcal{M} (e) \right]
\]

- \( P(e) \) is not gauge invariant as
- \( |u_j(e)\rangle \rightarrow |u'_j(e)\rangle = R_{j,e} |u_j(e)\rangle \)

\[
\text{(x) \hspace{1cm}} \quad P(e) \rightarrow P'(e) = \text{Pf} \left[ R^* \mathcal{M} R'^* \right] = \det (R) P(e)
\]

but \( |P(e)| \) is gauge invariant

- Consider two bands i.e. \( (i,j) \in \{1,2\} \)

\[
\text{(288) \hspace{1cm}} \quad |P(e)| = 0 \quad \text{for all} \quad |u_{12}(e)\rangle \in \mathcal{J}_e
\]


\[
\text{(289) \hspace{1cm}} \quad |P(e)| = 1 \quad \text{for all} \quad |u_{i}(e)\rangle \in \mathcal{J}_e
\]

\[
\text{Thus \quad since} \quad \mathcal{N} = 0
\]

\[
\text{He} \quad \text{only} \quad M_{12} \neq 0 \quad \mathcal{M}_{12} = \langle u_{1}(e) | T | u_{2}(e) \rangle
\]

\[
\text{Since} \quad \langle u_{2}(e) | T | u_{2}(e) \rangle = 0 \quad \Rightarrow \quad |M_{12}| = 1
\]

We now argue that it is sufficient to look at
the Pfaffian only in half of the BZ.
Due to TR invariance we have

\[(290) \quad |u_j(-\bar{b})\rangle = B_{ji}(\bar{b}) \Gamma |u_i(\bar{b})\rangle\]

where $B_{ji}(\bar{b})$ is a unitary matrix, the sewing matrix.

![Diagram of U2, T, U1, k axis with labels -\pi, 0, \pi]

Thus

\[
P(-\bar{b}) = Pf[\langle u_i(-\bar{b}) | \Gamma | u_j(-\bar{b}) \rangle]\]

\[= \text{Det} [B^*] Pf[\langle u_m(\bar{b}) | \Gamma | u_n(\bar{b}) \rangle]^*\]

\[(291) \quad P(-\bar{b}) = \text{Det} [B^*] P(\bar{b})^*\]

i.e. if $P(\bar{b}) = 0 \Rightarrow P(-\bar{b}) = 0$ but phases of $P$ close to the degeneracy point have opposite chirality.

\[(292) \quad \nu = \frac{1}{2\pi i} \int_{C} d\bar{b} \bar{b} \log (P(\bar{b}))\]

- It is sufficient to consider only $B\bar{b}$

- An even number of vortices in half the BZ can be removed without closing of a band gap.
$Z_2$ topological invariant \textit{(without further proof)}

$I = \# \text{ of zeros of } P(\xi) \text{ in the half Brillouin zone} \pmod{2}$

\begin{equation}
I = \frac{i}{2\pi i} \oint_{C} \bar{\nu} \ln (P(\xi)) \mod 2
\end{equation}

Problem: This has no intuitive interpretation. How to measure $I$?

8.3 TR polarization

For the trivial QSH E we have seen that $Ch_1 - Ch_3$ is a topological invariant. $Ch_1$ characterizes the winding of $P_1$ in a closed parameter loop. We now want to generalize this to coupled spins

(A) 1D lattice with TR invariance

- Spinless particles $T = K$
- 1 band
\[ THT^{-1} = H \quad \Rightarrow \quad T\lambda(b)T^{-1} = \lambda(-b) \]

\[ T\lambda(b)T^{-1} = \lambda^*(b) = \lambda(-b) = \lambda(-\bar{\epsilon}) \]

\( T = -iS_yK \)

\[ \lambda(b) = \begin{pmatrix} iS_y \end{pmatrix} \lambda(-b)^* \begin{pmatrix} iS_y \end{pmatrix} \]

\[ \lambda(b) = \begin{bmatrix} h_{11}(b) & h_{12}(b) \\ h_{21}(b) & h_{22}(b) \end{bmatrix} = \begin{bmatrix} h_{22}^*(-b) - h_{21}^*(-b) \\ -h_{12}^*(-b) & h_{11}^*(-b) \end{bmatrix} \]

\[ \lambda(-b) = \begin{bmatrix} h_{22}(-b) - h_{12}(-b) \\ -h_{21}(-b) & h_{11}(-b) \end{bmatrix} \]

\[ \Sigma^\pm(b) = \frac{1}{2} \left( \lambda_{11} + h_{22} \pm \sqrt{\lambda_{11}^2 + 41h_{12}^2 - 2h_{11}h_{22} + h_{22}^2} \right)_b \]

\[ \Sigma^\pm(-b) = \frac{1}{2} \left( h_{22} + h_{11} \pm \sqrt{h_{22}^2 + 41h_{12}^2 - 2h_{11}h_{22} + h_{22}^2} \right)_b \]

\[ = \Sigma^\pm(b) \]
Kramers pairs

\[ \psi^I(-k) = e^{i \epsilon_k T} \psi^II(k) \]

Use Kramers pairs instead of \( \psi^I \) and \( \psi^II \) as \( \psi_c \) in the trivial case.

\[ \rightarrow \text{polarization of one of the two solutions in } \psi \text{ \ within BZ} \]

\[ \rightarrow \text{better: consider both solution but only in half BZ} \]

Polarization ( Zak phase) of one of the Kramers pairs

\[ P^s = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \sum_a \left< \psi^s_a(k) \right| \frac{\partial}{\partial k} \left| \psi^s_a(k) \right> \quad s=I,II \]

Sum over occupied bands \( a \)
Borey connection of Kramers pair

\[ A^s(k) = i \sum_a \langle u_a^s(k) | \partial_k | u_a^s(k) \rangle \quad s = I, \Pi \]

we can write (s = I)

\[ P^I = \frac{1}{2\pi} \int_0^\pi \text{d}k \left( A^I(k) + A^I(-k) \right) \]

relation between \( A^I(-k) \) and \( A^\Pi(k) \)

\[ A^I(-k) = -i \sum_a \langle u_a^I(-k) | \partial_k | u_a^I(-k) \rangle \quad \partial_{-k} = -\partial_k \]

\[ = -i \sum_a \langle Tu_a^\Pi(h) | \partial_k | Tu_a^\Pi(h) \rangle \]

\[ = -i \sum_a i \partial_k \chi_a \langle Tu_a^\Pi(h) | Tu_a^\Pi(h) \rangle \]

now \( T = U_k \quad U^* = (U^+)^T \) (drop band index \( a \))

\[ \langle Tu_a^\Pi(h) | \partial_k | Tu_a^\Pi(h) \rangle = (U^\Pi U^\Pi(h)^*)^* \partial_k U^\Pi U^\Pi(h)^* \]

\[ = U^\Pi U^\Pi(h) \partial_k U^\Pi(h)^* \]

\[ = \delta_{\Pi} \partial_k \chi U^\Pi(h) \]

\[ \text{part. integration} \quad \text{(sum convention!)} \]

\[ \Rightarrow \]

\[ A^I(-k) = A^\Pi(h) + \sum_a \partial_k \chi_a \]

\[ \text{(301)} \]

\[ \text{-125-} \]
\[ \rho^I = \frac{1}{2\pi} \int_{0}^{\pi} dk \left( A^I(k) + A^F(k) \right) + \frac{1}{2\pi} \int_{0}^{\pi} \sum_{\alpha} \partial_k \mathcal{Z}_{k\alpha} \]

(302) \[ \rho^I = \frac{1}{2\pi} \int_{0}^{\pi} dk \left( A^I(k) + A^F(k) \right) + \sum_{\alpha} (\mathcal{Z}_{k\alpha} - \mathcal{Z}_{k\alpha}) \]

We now want to express the last term \( \rho^I \) in terms of the saving matrix \((280)\)

\[ B_{ji}(\mathbf{b}) = \langle \mathbf{u}_j(-\mathbf{b}) | T | \mathbf{u}_i(\mathbf{b}) \rangle \]

Due to TR invariance:

(i) \[ U^I_{a}(-k) = e^{i\mathcal{Z}_{k\alpha}} U^I_{a}(k) \]

\[ T \left( U^I_{a}(-k) \right) = T e^{i\mathcal{Z}_{k\alpha}} T^{-1} T^{2} \left( U^I_{a}(k) \right) \]

\[ = -e^{-i\mathcal{Z}_{k\alpha}} U^I_{a}(k) \]

(ii) \[ U^F_{a}(-k) = -e^{i\mathcal{Z}_{-k\alpha}} U^F_{a}(k) \]

\[ \Rightarrow \]

\[ B^I_{mn}(k) = \langle U^I_{m}(-k) | T | U^I_{n}(k) \rangle = -\delta_{mn} e^{-i\mathcal{Z}_{-k\alpha}} \]

\[ B^F_{mn}(k) = -B^I_{mn}(-k) \]

\[ \Rightarrow \] B is block diagonal
(30.4) \[ B_{m,n}(k) = \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix} \begin{bmatrix} 0 & e^{i \pi n} \\ -e^{-i \pi n} & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ \vdots \end{bmatrix} \]

Thus, \[ \text{Pf}[B(k)] = \prod_{n \in \mathbb{N}} e^{i \pi n} \]

(30.5) \[ \sum_{\alpha} \left[ x_{\pi \alpha} - x_{0\alpha} \right] = i \ln \frac{\text{Pf}(B(\pi))}{\text{Pf}(B(0))} \]

This yields eventually

(30.6) \[ P^I = \frac{1}{2\pi} \int_{0}^{\pi} \left[ A^I(k) + A^{II}(k) \right] + i \ln \frac{\text{Pf}(B(\pi))}{\text{Pf}(B(0))} \]

= \text{A}(k) \text{ total Berry connection} 

An alternative expression which is simpler, but requires that one is able to identify ("follow" in any experimental implementation) one of the Kramer pairs

(30.7) \[ P^I = \frac{1}{2\pi} \int_{0}^{\pi} A^I(k) \]

Analogously, one finds

(30.8) \[ P^{II} = \frac{1}{2\pi} \int_{-\pi}^{0} \left( A^I(k) + A^{II}(k) \right) - i \ln \frac{\text{Pf}(B(\pi))}{\text{Pf}(B(0))} \]
the total polarization \( P = P^I + P^II \) reads

\[
P = \frac{1}{2\pi} \int_{-\pi}^{\pi} \, \text{d} n \left( A^I + A^II \right)
\]

We know however already that the total polarization is useless in a TR invariant system since its winding vanishes (\( \neq \) Chern number due to TR symmetry).

However: the difference, called TR-polarization

\[
P_I = P^I - P^II
\]

\[
(303) \quad \frac{1}{2\pi} \left\{ \int_{-\pi}^{\pi} \text{d} k \, A(k) - \int_{-\pi}^{\pi} \text{d} k \, \frac{\text{Pf} (B(k))}{\text{Pf} (B(0))} \right\}
\]

is a good invariant \( \mathbb{Z}_2 \).

One can show

\[
\int_{-\pi}^{\pi} \text{d} k \, A(k) - \int_{-\pi}^{\pi} \text{d} k \, A(k) = \frac{1}{i} \int_{-\pi}^{\pi} \text{d} k \, \text{Tr} \left\{ B^+ \partial_k B \right\}
\]

and due to the block-diagonal form of \( B \) one has moreover

\[
\text{Tr} \left\{ B^+ \partial_k B \right\} = \partial_k \ln \det (B(k))
\]

This then finally yields
\[
\text{(3.10)} \quad P_T = \frac{1}{\pi i} \ln \left[ \frac{\text{Det}[B(r)]}{\text{Pf}(B(\pi))} \frac{\text{Pf}(B(0))}{\sqrt{\text{Det}[B(\alpha)]}} \right]
\]

Since \( \text{Det}[B] = \left(\text{Pf}(B)\right)^2 \) \( \Rightarrow P_T \) is "modulo 2"

\[P_T \text{ is a } \mathbb{Z}_2 \text{ topological invariant}\]

(i) \( \text{Pf}(B(\pi)) \) and \( \text{Pf}(B(0)) \) have same sign

\[P_T = 0 \quad \text{mod } 2\]

(ii) \( \text{Pf}(B(\pi)) \) and \( \text{Pf}(B(0)) \) have different sign

\[P_T = 1 \quad \text{mod } 2\]

- In case (i) there must be an even number of zeros of \( \text{Pf}(B(\pi)) \) in the half \( \text{BZ} \)

- In case (ii) there must be an odd number of zeros of \( \text{Pf}(B(\pi)) \) in the half \( \text{BZ} \)
The previous discussion was for 1D systems with
\( B_2 \text{ k e } [-\pi, \pi] \rightarrow 2D \text{ lattice models } \)

Generalization to 2D lattice models

\( \Gamma \)-trafo in one direction say \( y \quad P_T \rightarrow P_T [k_y] \)

\[ \Delta P_T = P_T (k_y, \gamma_1) - P_T (k_y, \gamma_2) \] (3.11)

2 TR topics aka Chern insulator with

\( \text{Ch}_I = - \text{Ch}_\Pi = 1 \)

\( \Delta P_I - \Delta P_\Pi = 1 \)

(e.g. trivial QSHE) Exchange of TR partners of \( k_y = 0 \)

\[ I = \prod \frac{\text{Det } B[b_j]}{\text{Pf } B(b_j)} \] (3.12)

\( \tilde{b}_j \) are TR invariant momenta