8. $\mathbb{Z}_2$ topological invariant

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

8.1 Kramers doublett of edge modes

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

let $\quad \underline{\psi}_1(x, k_y) \quad$ be 1-particle edgemode (function of k_y) with energy $E_0(k_y)$ in band gap

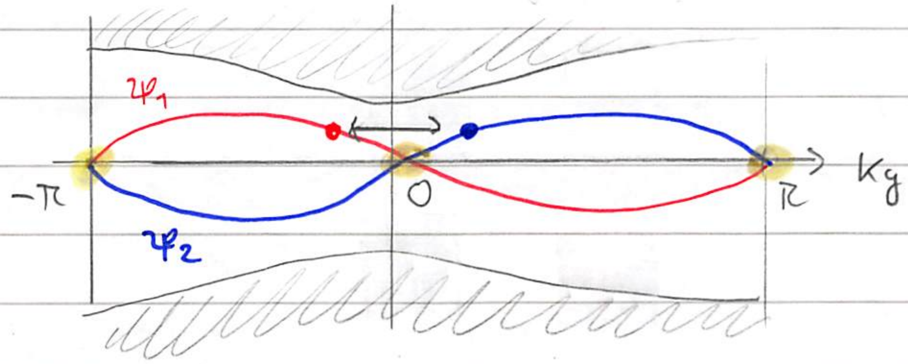
Kramers theorem (p. 81) + TR invariance

$$\exists \quad \underline{\psi}_2(x, k_y) \text{ with } \underline{\psi}_2(x, -k_y) = T\underline{\psi}_1(x, k_y)$$

with energy $E_0(k_y)$

Kramers doublett of edge modes

Kramers doublett



What happens at degeneracy points $k_y = 0, \pm\pi$?
Can ψ_1 scatter into ψ_2 ? I.e. is there an avoided crossing in the presence of a perturbation ?

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

<u>Proof</u>: perturbation H_1 $\qquad T = UK \qquad T^2 = -1$ (fermions)

$$\Rightarrow U^T = -U$$

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

$$= \sum_{mpr} U_{pm}^+ U_{mr} \psi_r^* \phi_p = \langle \psi | \phi\rangle$$

choose $\quad |T\psi\rangle = H_1 |\phi\rangle \qquad$ ($|T\psi\rangle$ and $|\phi\rangle$ have same unperturbed energies)

$$T^2|\psi\rangle = -|\psi\rangle = TH_1|\phi\rangle = \underbrace{TH_1T^{-1}}_{=H_1 \text{ iff } H_1 \text{ is TR invariant}} T|\phi\rangle = H_1 T|\phi\rangle$$

$$\langle\psi| = -\langle T\phi| H_1 \Rightarrow \langle T\phi | H_1 | \phi\rangle = -\langle \psi|\phi\rangle$$
$$= -\langle T\phi | H_1 | \phi\rangle$$

(276) $\quad \boxed{\langle T\phi | H_1 | \phi\rangle = 0} \qquad \forall H_1 \text{ with } THT^{-1} = H_1$

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

\# Kramers doubletts

- even
  - no protected edge modes
    - $\boxed{\text{simple insulator}}$
- odd
  - edge modes by TR symmetry protected
    - $\boxed{\mathbb{Z}_2 \text{ topological insulator}}$

8.2 $\mathbb{Z}_2$ invariant: zeroth of the Pfaffian *

(A) Pfaffian of an anti-symmetric matrix

let $\quad M_{jk} = - M_{kj} \quad$ be a $n \times n$ matrix

$n = 2m+1 \quad \boxed{Pf(\underline{M}) \doteq 0} \qquad (277)$

$n = 2m \quad$ Pf is a number

Def: Π set of all partitions of $(1,2,3,\dots,2m)$ into pairs (e.g. $(1,2);(3,4);\cdots$). 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 $i_n < k_n$ and $i_1 < i_2 < i_3 < \cdots$

(278) Def: $$M_\alpha \equiv \mathrm{sgn}(\alpha)\, M_{i_1k_1} M_{i_2k_2} \cdots M_{i_mk_m}$$

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

$$\begin{matrix} 1 & 2 & 3 & 4 & \cdots & 2m \\ & & & \downarrow & & \\ i_1 & k_1 & i_2 & k_2 & & k_m \end{matrix}$$

Thm (279) $$\boxed{\mathrm{Pf}(\underline{\underline{M}}) = \sum_{\alpha \in \Pi} M_\alpha}$$

properties:

(280) $$[\mathrm{Pf}(\underline{\underline{M}})]^2 = \mathrm{Det}(\underline{\underline{M}})$$

(281) $$\mathrm{Pf}(\underline{\underline{B}}\,\underline{\underline{M}}\,\underline{\underline{B}}^T) = \mathrm{Det}(\underline{\underline{B}})\,\mathrm{Pf}(\underline{\underline{M}})$$

(282) $$\mathrm{Pf}(\lambda \underline{\underline{M}}) = \lambda^m\, \mathrm{Pf}(\underline{\underline{M}})$$

(283) $$\mathrm{Pf}(\underline{\underline{M}}^T) = (-1)^m\, \mathrm{Pf}(\underline{\underline{M}})$$

example: $\underline{\underline{M}} = \begin{pmatrix} \emptyset & a \\ -a & \emptyset \end{pmatrix}$ $\quad \mathrm{Pf}(\underline{\underline{M}}) = a$

$$\underline{\underline{M}} = \begin{pmatrix} 0 & \lambda_1 & & & \\ -\lambda_1 & 0 & & & \\ & & 0 & \lambda_2 & \\ & & -\lambda_2 & 0 & \\ & & & & \ddots \end{pmatrix} \Rightarrow \mathrm{Pf}(\underline{\underline{M}}) = \lambda_1 \cdot \lambda_2 \cdots \lambda_m$$

(B) Zeroth of the Pfaffian of time-reversal matrix

Let $\{|u_i(\bar{k})\rangle\}$ be a Bloch eigenbasis of a TR invariant Hamiltonian. To characterize the effect of time reversal on these states consider the matrix

(284) $$\boxed{M_{ij}(\bar{k}) \equiv \langle u_i(\bar{k})| T |u_j(\bar{k})\rangle}$$ time-reversal matrix

- $M_{ij}(\bar{k})$ is anti-symmetric

(285) $$M_{ij}(\bar{k}) = -M_{ji}(\bar{k})$$

proof: $M_{ij}(\bar{k}) = \langle u_i | T | u_j \rangle = \langle u_i | UK | u_j \rangle$

$T = UK$ since $T^2 = -1 \rightsquigarrow U^T = -U \quad (U^\dagger = U^{-1})$

$$\Rightarrow \quad M_{ij} = (u_i(\bar{k})^*)_m \, U_{mn} \, (u_j(\bar{k})^*)_n$$
$$= -u_j(\bar{k})^*_n \, U_{nm} \, (u_i(\bar{k})^*)_m$$
$$= -\langle u_j(\bar{k})| T |u_i(\bar{k})\rangle = -M_{ji}(\bar{k}) \quad \square$$

Def: $\{|u_i(\bar{k})\rangle\}_o$ set of all eigenstates of H which are odd under TR

$\{|u_i(\bar{k})\rangle\}_e$ set of all eigenstates of H which are even under TR

(286) $T|u_i(\bar{k})\rangle_o \perp \{|u_i(\bar{k})\rangle\}_o \qquad T|u_i(\bar{k})\rangle_e \in \{|u_i(\bar{k})\rangle\}_e$

Pfaffian of time reversal matrix

(287) $$\boxed{P(\bar{k}) \equiv \mathrm{Pf}\left[\underline{\underline{M}}(\bar{k})\right]}$$

(*) $P' = \mathrm{Pf}\left[\langle u_i' | T | u_j' \rangle\right]$
$= \mathrm{Pf}\left[\langle u_m | R^*_{im} \, T \, R_{jn} | u_n \rangle\right]$
$= \mathrm{Pf}\left[R^*_{im} \langle u_m | T | u_n \rangle R^*_{jn}\right]$
$= \mathrm{Pf}\left[R^*_{im} \langle u_m | T | u_n \rangle (R^{*T})_{nj}\right]$

- $P(\bar{k})$ is not gauge invariant as
$|u_j(\bar{k})\rangle \rightarrow |u_j'(\bar{k})\rangle = R_{je} |u_e(\bar{k})\rangle$

$$P(\bar{k}) \rightarrow P'(\bar{k}) \overset{(*)}{=} \mathrm{Pf}\left[\underline{\underline{R}}^* \underline{\underline{M}} \, \underline{\underline{R}}^{*T}\right] = \det(\underline{\underline{R}}^*) \, P(\bar{k})$$

but $\boxed{|P(\bar{k})| \text{ is gauge invariant}}$

- consider two bands i.e. $(i,j) \in (1,2)$

$\mathcal{H}_o$ | (288) $$\boxed{|P(\bar{k})| = 0 \quad \text{for all } |u_{1,2}(\bar{k})\rangle \in \mathcal{H}_o}$$

trivial since $\underline{\underline{M}} = 0$

$\mathcal{H}_e$ | only $M_{12} \neq 0$ $\quad M_{12} = \langle \psi_1(k) | T | \psi_2(k) \rangle$

$T|\psi_2\rangle$ has full overlap with $|\psi_1\rangle$

since $\langle \psi_2(k) | T | \psi_2(k) \rangle = 0 \Rightarrow |M_{12}| = 1$

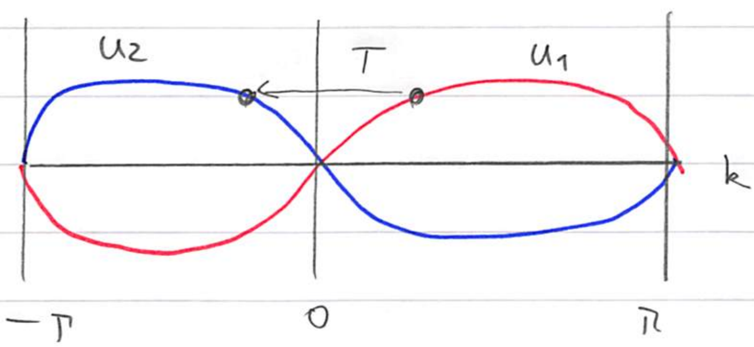
(289) $$\boxed{|P(\bar{k})| = 1 \quad \text{for all } |u_i(\bar{k})\rangle \in \mathcal{H}_e}$$

- 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) $$|u_j(-\vec{k})\rangle = B_{ji}(\vec{k})\, T\, |u_i(\vec{k})\rangle$$

where $B_{ji}(\vec{k})$ is a unitary matrix, the sewing matrix



Thus

$$P(-\vec{k}) = Pf\left[\langle u_i(-\vec{k})|\, T\, |u_j(-\vec{k})\rangle\right]$$

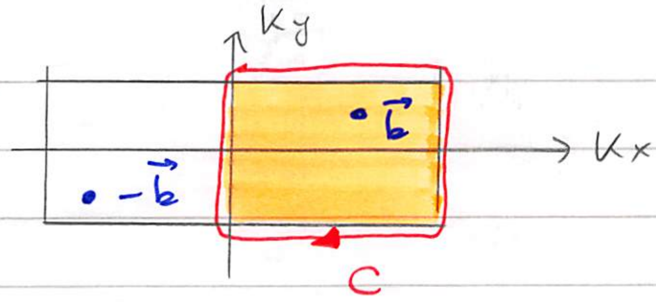
$$= Det\left[B^*\right] Pf\left[\langle u_m(k)|\, T\, |u_n(\vec{k})\rangle\right]^*$$

(291) $$P(-\vec{k}) = Det\left[B^*\right] P(\vec{k})^*$$

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

(292) $$\nu = \frac{1}{2\pi i}\int_C d\vec{k}\; \vec{\nabla}\log(P(\vec{k}))$$

- it is sufficient to consider half BZ
- an even number of vortices in half the BZ can be removed without closing of a band gap



$\mathbb{Z}_2$ topological invariant (without further proof)

I = # of zeroth of $P(\vec{k})$ in the half Brillouin zone modulo 2

(293) $$\boxed{I = \frac{1}{2\pi i} \oint_C d\vec{k} \cdot \vec{\nabla} \ln (P(\vec{k})) \mod 2}$$

problem: this has no intuitive interpretation. How to measure I ?

8.3 TR polarization

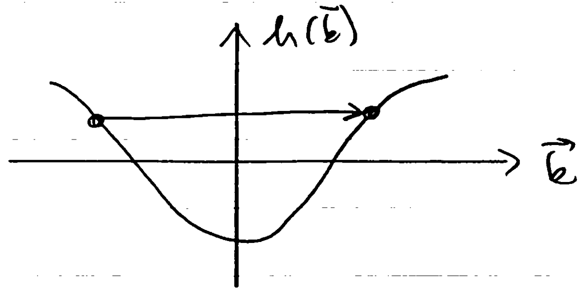
For the trivial QSHE we have seen that $Ch_\uparrow - Ch_\downarrow$ is a topolog. invariant. $Ch_\uparrow$ characterizes the winding of $P_\uparrow$ in a closed parameter loop. We now want to generalize this to coupled spins

(A) 1D lattice with TR invariance

- spinless particle $\quad T = K$
  1 band

$$THT^{-1} = H \quad \Rightarrow \quad T h(k) T^{-1} = h(-k)$$

(294) $$\boxed{T h(k) T^{-1} = h^*(k) = h(k) = h(-k)}$$



- spin 1/2 particle $\qquad T = -i s_y K$

1 band

(295) $$\boxed{\underline{\underline{h}}(k) = i\underline{\underline{\sigma}}_y^T \, \underline{\underline{h}}(-k)^* \, i\underline{\underline{\sigma}}_y}$$

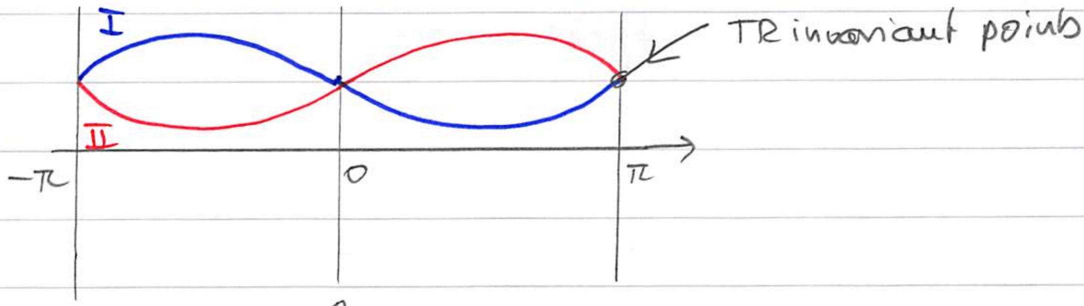
$$\underline{\underline{h}}(k) = \begin{bmatrix} h_{11}(k) & h_{12}(k) \\ h_{21}(k) & h_{22}(k) \end{bmatrix} \overset{!}{=} \begin{bmatrix} h_{22}^*(-k) & -h_{21}^*(-k) \\ -h_{12}^*(-k) & h_{11}^*(-k) \end{bmatrix}$$

(296) $$= \begin{bmatrix} h_{22}(-k) & -h_{12}(-k) \\ -h_{21}(-k) & h_{11}(-k) \end{bmatrix}$$

(297) $$\varepsilon_\pm(k) = \frac{1}{2}\left(h_{11} + h_{22} \pm \sqrt{h_{11}^2 + 4|h_{12}|^2 - 2h_{11}h_{22} + h_{22}^2}\right)_k$$

$$\varepsilon_\pm(-k) = \frac{1}{2}\left(h_{22} + h_{11} \pm \sqrt{h_{22}^2 + 4|h_{12}|^2 - 2h_{11}h_{22} + h_{22}^2}\right)_k$$

$$= \varepsilon_\pm(k)$$



Kramers pairs

(298) $$\boxed{|u^{I}(-k)\rangle = e^{i\chi_k}\,\mathcal{T}\,|u^{II}(k)\rangle}$$

use Kramers pairs instead of $|\uparrow\rangle$ and $|\downarrow\rangle$ as in the trivial QSHE !

→ polarization of one of the two solutions in whole BZ

→ better: consider both solutions but only in half BZ

Polarization (Zak phase) of one of the Kramers pairs

(299) $$\boxed{P^{s} \equiv \frac{i}{2\pi}\int_{-\pi}^{\pi} dk \sum_{a}{}' \langle u_a^{s}(k)|\frac{\partial}{\partial k}|u_a^{s}(k)\rangle \qquad s = I, II}$$

sum over occupied bands a

Berry connection of Kramers pair

$$(300)\qquad A^{s}(k) = i \sum_a \langle u_a^{s}(k) | \frac{\partial}{\partial k} | u_a^{s}(k) \rangle \qquad s = \mathrm{I}, \mathrm{II}$$

We can write ($s = \mathrm{I}$)

$$P^{\mathrm{I}} = \frac{1}{2\pi} \int_0^{\pi} dk \, \left(A^{\mathrm{I}}(k) + A^{\mathrm{I}}(-k) \right)$$

<u>relation between $A^{\mathrm{I}}(-k)$ and $A^{\mathrm{II}}(k)$</u>

$$A^{\mathrm{I}}(-k) = -i \sum_a \langle u_a^{\mathrm{I}}(-k) | \partial_k | u_a^{\mathrm{I}}(-k) \rangle \qquad \partial_{-k} = -\partial_k$$

$$= -i \sum_a \langle T u_a^{\mathrm{II}}(k) | \partial_k | T u_a^{\mathrm{II}}(k) \rangle$$

$$- i \sum_a i \, \partial_k \chi_{ka} \underbrace{\langle T u_a^{\mathrm{II}}(k) | T u_a^{\mathrm{II}}(k) \rangle}_{=1}$$

now $\quad T = UK \qquad U^* = (U^+)^T \qquad$ (drop band index a)

$$\langle T u^{\mathrm{II}}(k) | \partial_k | T u^{\mathrm{II}}(k) \rangle = \left(U_{mn} u_n^{\mathrm{II}}(k)^* \right)^* \partial_k \, U_{mp} u_p^{\mathrm{II}*}(k)$$

$$= \underbrace{U^+_{nm} U_{mp}}_{\delta_{np}} u_n^{\mathrm{II}}(k) \, \partial_k u_p^{\mathrm{II}}(k)^* = u_n^{\mathrm{II}}(k) \, \partial_k u_n^{\mathrm{II}}(k)^*$$

$$\underset{\text{part. integration}}{=} - u_n^{\mathrm{II}*}(k) \, \partial_k u_n^{\mathrm{II}}(k) = - \langle u^{\mathrm{II}}(k) | \partial_k | u^{\mathrm{II}}(k) \rangle$$

(sum convention!)

$\Rightarrow$

$$(301)\qquad A^{\mathrm{I}}(-k) = A^{\mathrm{II}}(k) + \sum_a \partial_k \chi_{ka}$$

$$P\mathcal{I} = \frac{1}{2\pi}\int_0^\pi dk\,\left(A^{I}(k) + A^{II}(k)\right) + \frac{1}{2\pi}\int_0^\pi dk \sum_a \partial_k \chi_{ka}$$

$$P\mathcal{I} = \frac{1}{2\pi}\int_0^\pi dk\,\left(A^{I}(k) + A^{II}(k)\right) + \sum_a \left(\chi_{\pi a} - \chi_{0,a}\right) \tag{302}$$

We now want to express the last term in terms of the sewing matrix (290)

$$\boxed{B_{ji}(\bar{k}) \equiv \langle u_j(-\bar{k})|T|u_i(\bar{k})\rangle} \tag{303}$$

$2n\times 2n$ matrix "2" because of Kramers pairs

Due to TR invariance

(i) $$|u^{I}_a(-k)\rangle = e^{i\chi_{ka}}T|u^{II}_a(k)\rangle$$

$$T\,|u^{I}_a(-k)\rangle = Te^{i\chi_{ka}}T^{-1}\underbrace{T^2}_{=-1}|u^{II}_a(k)\rangle$$

$$= -e^{-i\chi_{ka}}|u^{II}_a(k)\rangle$$

$\Rightarrow$

(ii) $$|u^{II}_a(-k)\rangle = -e^{i\chi_{-k,a}}|u^{I}_a(k)\rangle$$

$\Rightarrow$ $$B^{II,I}_{mn}(k) \equiv \langle u^{II}_m(-k)|T|u^{I}_n(k)\rangle = -\delta_{mn}e^{-i\chi_{-kn}}$$

$$B^{I,II}_{mn}(k) = -B^{II,I}_{mn}(-k)$$

$\Rightarrow$ B is block diagonal

$$(304)\quad B_{m,n}(k) = \begin{bmatrix} \ddots & & \\ & \begin{array}{cc} \begin{bmatrix} 0 & e^{i\chi_{kn}} \\ -e^{-i\chi_{kn}} & 0 \end{bmatrix} & \begin{array}{c} \mathrm{I} \\ \mathrm{II} \end{array} \end{array} & \\ & & \ddots \end{bmatrix}$$

Thus $\mathrm{Pf}[B(k)] = \prod_n e^{i\chi_{kn}}$

$$(305) \Rightarrow \quad \sum_a \left[\chi_{\pi a} - \chi_{0a}\right] = i \ln \frac{\mathrm{Pf}(B(\pi))}{\mathrm{Pf}(B(0))}$$

This yields eventually

$$(306)\quad \boxed{P^{\mathrm{I}} = \frac{1}{2\pi} \int_0^{\pi} dk \, \underbrace{\left(A^{\mathrm{I}}(k) + A^{\mathrm{II}}(k)\right)}_{= A(k) \text{ total Berry connection}} + i \ln \frac{\mathrm{Pf}(B(\pi))}{\mathrm{Pf}(B(0))}}$$

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

$$(307)\quad P^{\mathrm{I}} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \, A^{\mathrm{I}}(k)$$

Analogously one finds

$$(308)\quad \boxed{P^{\mathrm{II}} = \frac{1}{2\pi} \int_{-\pi}^{0} dk \left(A^{\mathrm{I}}(k) + A^{\mathrm{II}}(k)\right) - i \ln \frac{\mathrm{Pf}(B(\pi))}{\mathrm{Pf}(B(0))}}$$

the total polarization $P = P^{I} + P^{II}$ reads

$$P = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \, (A^{I} + A^{II})$$

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

However: the difference, called TR-polarization

(309) $$\boxed{\begin{aligned} P_T &= P^{I} - P^{II} \\ &= \frac{1}{2\pi} \left\{ \int_0^{\pi} dk \, A(k) - \int_{-\pi}^{0} dk \, A(k) + 2i \ln \frac{Pf(B(\pi))}{Pf(B(0))} \right\} \end{aligned}}$$

is a good invariant $\mathbb{Z}_2$

One can show

$$\int_0^{\pi} dk \, A(k) - \int_{-\pi}^{0} dk \, A(k) = \frac{1}{i} \int_0^{\pi} dk \, Tr\{B^{+} \partial_k B\}$$

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

$$Tr\{B^{+} \partial_k B\} = \partial_k \ln \det(B(k))$$

This then finally yields

(310) $$\boxed{P_T = \frac{1}{\pi i} \ln \left[\frac{\sqrt{\mathrm{Det}[B(\pi)]}}{\mathrm{Pf}(B(\pi))} \frac{\mathrm{Pf}(B(0))}{\sqrt{\mathrm{Det}[B(0)]}} \right]}$$

Since $\mathrm{Det}[B] = (\mathrm{Pf}(B))^2 \Rightarrow P_T$ is "modulo 2"

P_T is a <u>$\mathbb{Z}_2$ topological invariant</u>

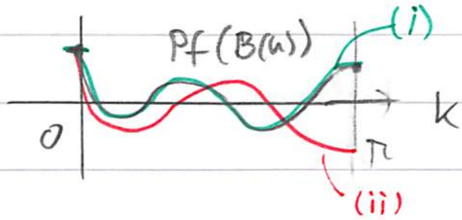
(i) $\mathrm{Pf}(B(\pi))$ and $\mathrm{Pf}(B(0))$ have same sign

$$\boxed{P_T = 0} \quad \mathrm{mod}\ 2$$

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

$$\boxed{P_T = 1} \quad \mathrm{mod}\ 2$$

- In case (i) there must be an <u>even</u> number of zeroth of $\mathrm{Pf}(B(k))$ in the half BZ



trivial case

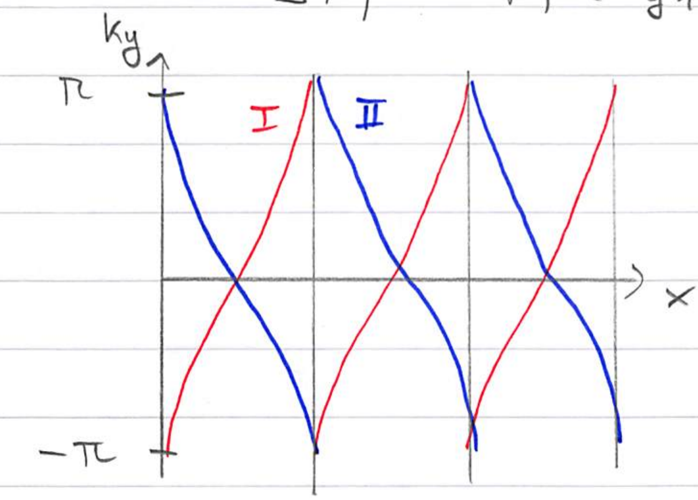
- In case (ii) there must be an <u>odd</u> number of zeroth of $\mathrm{Pf}(B(k))$ in the half BZ

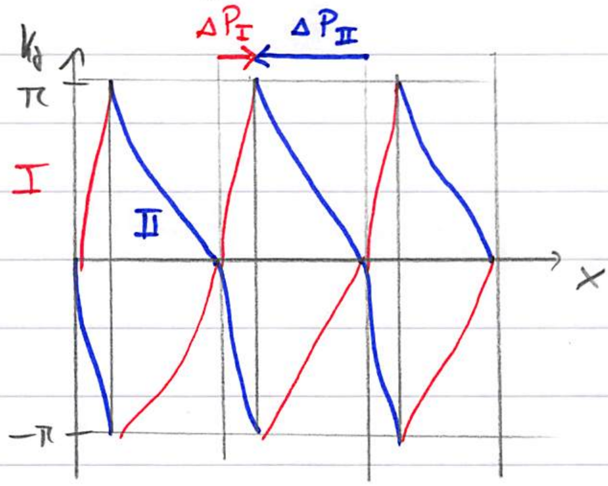
The previous discussion was for 1D systems with
BZ $k \in [-\pi, \pi]$ $\rightarrow$ 2D lattice models

<u>generalization to 2D lattice models</u>

F-trafo in one direction say y $\quad P_T \rightarrow P_T[k_y]$

(311) $$\Delta P_T \equiv P_T(k_{y1}) - P_T(k_{y2})$$





2 TR copies of a Chern insulator with

$$Ch_I = -Ch_{II} = 1$$

(e.g. trivial QSHE)

general TR invariant topolog. insulator with

$$\Delta P_I - \Delta P_{II} = 1$$

exchange of TR partners at $k_y = 0$

(312) $$\boxed{I = \prod_j \frac{\sqrt{\mathrm{Det}\, B[\bar{k}_j]}}{\mathrm{Pf}\, B(\bar{k}_j)}}$$

$\bar{k}_j$ are TR invariant momenta