What is the topological invariant for $\lambda_R = 0$

$$\boxed{\nu_2 \equiv \frac{1}{2} \left| Ch_\uparrow - Ch_\downarrow \right|} \quad (308)$$

but what for $\lambda_R \neq 0$?

7. $\mathbb{Z}_2$ topological invariant for TR symmetric bandstructures

7.1 Kramers doublet

For a many body (lattice) Hamiltonian with TR invariance

$$(309) \qquad [\hat{T}, \hat{H}] = 0$$

$\Rightarrow$ common eigenbasis

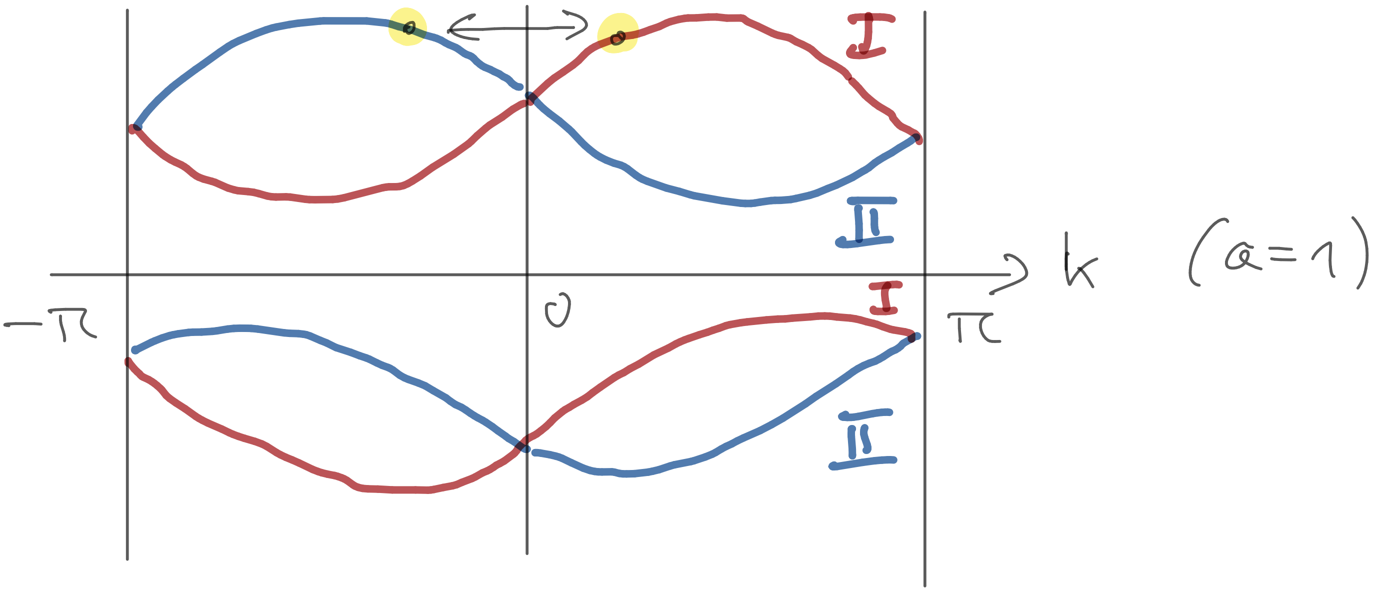
$$|u(\vec{k})\rangle \quad \text{and} \quad \hat{T}|u(\vec{k})\rangle$$

are eigenstates with the same energy

$$(310) \qquad \boxed{|u_{II}(-\vec{k})\rangle = e^{i\chi(\vec{k})} \hat{T} |u_I(\vec{k})\rangle}$$

This is the so-called Kramers doublett

energy bands come in pairs



- at TR symmetric momenta $\vec{k} = 0, \pm\pi$ bands must be degenerate due to (3.10), i.e. TR symmetry
- there is no coupling (avoided crossing) at the TR invariant momenta due to TR symmetry if the perturbation does not destroy TR symmetry

proof: perturbation H_1 $\quad T = UK$

$T^2 = -1$ (fermions) i.e. $\Rightarrow U^T = -U$

$$\langle T\phi | T\psi\rangle = \langle \psi | \phi\rangle \qquad \text{(anti-unitary)}$$

choose $T|\psi\rangle \overset{!}{=} H_1|\phi\rangle$

- $$T^2|\psi\rangle = -|\psi\rangle = TH_1|\phi\rangle$$

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

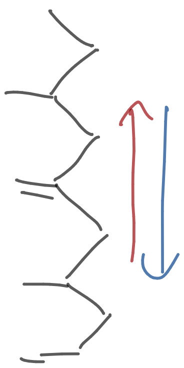
- $$\langle\psi| = -\langle T\phi|H_1$$

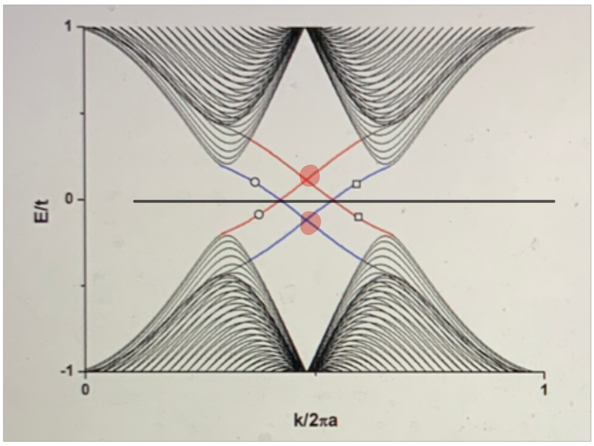
$$\Rightarrow \quad \langle T\phi|H_1|\phi\rangle = -\langle\psi|\phi\rangle$$

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

$$\Rightarrow \quad \boxed{\langle T\phi|H_1|\phi\rangle = 0} \quad \forall H_1 \text{ with } TH_1T^{-1} = H_1 \tag{311}$$

Topological protection of edge modes





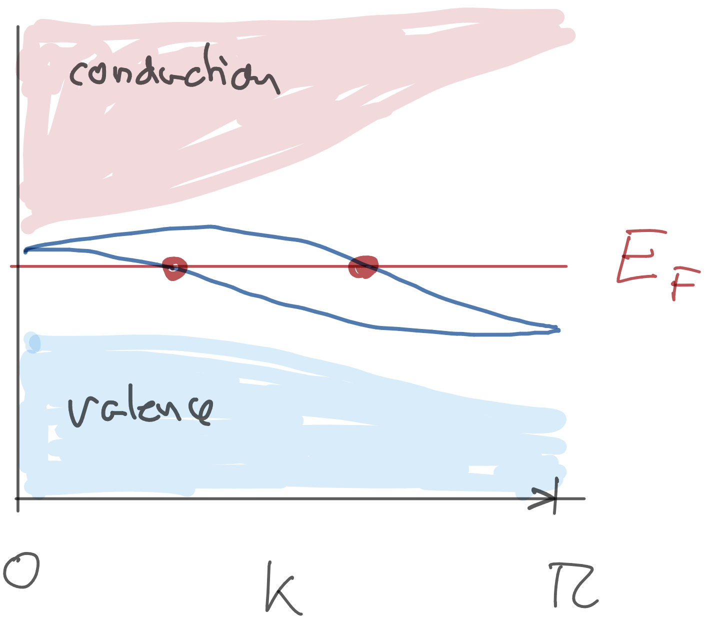
there are crossings of edge modes at the same side. Crossings are protected by TR symmetry

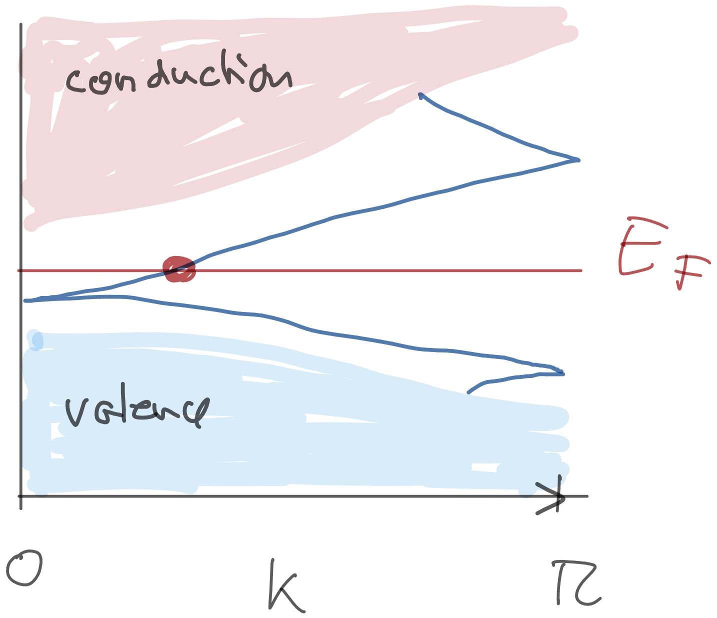
The above argument can be extended to multiple Kramers doubletts, if the number of doubletts is odd. If the number of Kramers doubletts is even than a coupling can exist!

Kramers doublets

even — no protected edge modes — **simple insulator**

odd — edge modes protected by TR symmetry — **$\mathbb{Z}_2$ topological insulator**





(mirror image in $[-\pi, 0]$)

7.2 Kane-Mele invariant

In the QSH phase of the Kane Mele model is NOT characterized by a quantized spin-Hall conductivity due to Rashba SOC! $\Rightarrow$ need different measure

The first $\mathbb{Z}_2$ invariant proposed in the original paper by Kane and Mele PRL 95 146802 (2005) is based on the

time reversal matrix

(312) $$\boxed{M_{ij}(\vec{k}) \equiv \langle u_i(\vec{k})|T|u_j(\vec{k})\rangle}$$

M_{ij} is anti-symmetric

(313) $$M_{ij}(\vec{k}) = -M_{ji}(\vec{k})$$

proof:

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

since $T^2=-1 \Rightarrow U^T = -U$

$$\Rightarrow M_{ij} = \sum_{m,n} u_i(\vec{k})^*_m U_{mn} u_j(\vec{k})^*_n$$
$$= -\sum_{mn} u_j(\vec{k})^*_n U_{nm} u_i(\vec{k})^*_m = -M_{ji}$$

Pfaffian of M_{ij}

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

Pfaffian

$M = -M^T$ $n \times n$ matrix

(3.15)

$n = 2m+1$ $\quad Pf(M) = 0$

$n = 2m$ $\quad Pf(M)$ number

Def: π set of all partitions of $(1,2,3,\dots,2m)$ into pairs (e.g. $(1,2);(3,4),\dots$). total number $(2m-1)!!$

(3.16) $$M_\alpha \equiv \mathrm{sgn}(\alpha)\, M_{i_1 k_1} M_{i_2 k_2} \cdots M_{i_m k_m}$$

with $\alpha \in \pi$: $\{(i_1 k_1); (i_2 k_2); \dots; (i_m k_m)\}$

$\mathrm{sgn}(\alpha) = (-1)^p$ $\quad p$ # of permutations needed for

$$\begin{matrix} 1\,2 & 3\,4 & 5\,6 & \cdots & 2m \\ i_1 k_1 & i_2 k_2 & \cdots & \cdots & k_m \end{matrix}$$

(3.17) $$\boxed{Pf(M) = \sum_{\alpha \in \pi} M_\alpha}$$

Without further discussion and proofs: One can introduce a gauge invariant quantity

$$\boxed{\nu_2 = \#\text{ of zeroth of } P(\vec{k}) \text{ in half the Brillouin zone modulo } 2}$$

$\mathbb{Z}_2$ topological invariant

problem: not very intuitive; how to measure?

7.3 Spin Chern number

A more intuitive $\mathbb{Z}_2$ invariant was proposed by Haldane et al. in Sheng PRL 97, 036808 (2006)

They considered the Chern matrix (here in a modified form)

(3.18)
$$\boxed{C^{\alpha\beta} = \frac{i}{4\pi} \oint dk_x dk_y \left[\left\langle \frac{\partial \psi}{\partial k_x^\alpha} \middle| \frac{\partial \psi}{\partial k_y^\beta} \right\rangle - \left\langle \frac{\partial \psi}{\partial k_y^\beta} \middle| \frac{\partial \psi}{\partial k_x^\alpha} \right\rangle \right] \qquad \alpha, \beta = \uparrow, \downarrow}$$

where $|\psi\rangle$ is the many-body ground state and $\frac{\partial}{\partial k_x^\alpha}$ means that only the momentum k_x of spin component α

(3.19)
$$\boxed{\nu_2^H = \frac{1}{2} \left| \sum_{\alpha,\beta} \alpha C^{\alpha\beta} \right|}$$

here $\alpha, \beta = \pm 1$

ν_2^H reduces to $\frac{1}{2}|C_\uparrow - C_\downarrow|$ in the case without Rashba SOC. That it is still a good quantum number in the presence of Rashba SOC is surprising.

But: It may be restricted to phases which can be smoothly connected to a phase with spin conservation without closing of a gap.

7.4 Time reversal polarization

A more general concept is the time-reversal polarization by Fu and Kane PRB 74, 195312 (2006)

(A) 1D lattice with TR symmetry

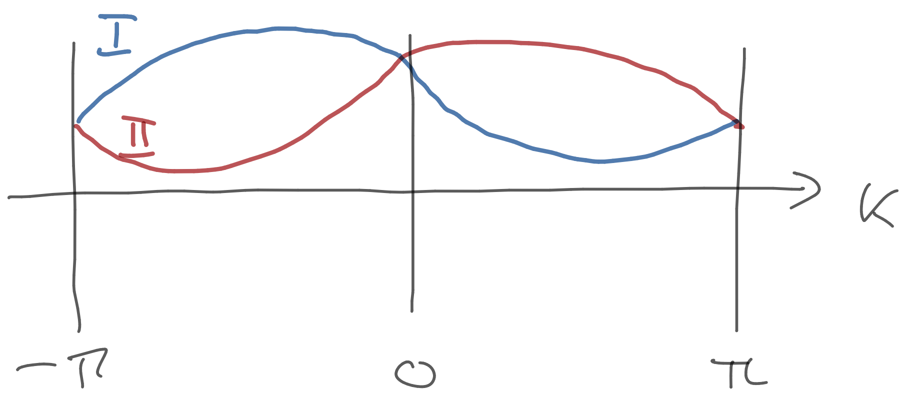
We first consider 1D models and extend this then to 2D

Spinless fermions $\qquad \hat{T} = K$

Kramers pairs

$$|u_{II}(-k)\rangle = e^{i\chi(k)}\, T\, |u_{I}(k)\rangle \qquad (320)$$

$\Rightarrow$ use Kramers pairs instead of $|\uparrow\rangle$ and $|\downarrow\rangle$ as basis



polarization (Zak phase) of one of the Kramers partners

(320)
$$\boxed{P^s = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk \sum_{\mu}' \langle u_\mu^s(k) | \partial_k u_\mu^s(k) \rangle}$$

μ orbital bands $\qquad s = \mathrm{I}, \mathrm{II}$

then the difference is called time-reversal polarization

(321)
$$\boxed{P_\theta = P^{\mathrm{I}} - P^{\mathrm{II}}}$$

For time dependent Hamiltonians with periodic time dependence and TR invariance ($t \to -t$)

$$H(t+T) = H(t) \qquad T H(t) T^{-1} = H(-t)$$

one can define a $\mathbb{Z}_2$ invariant

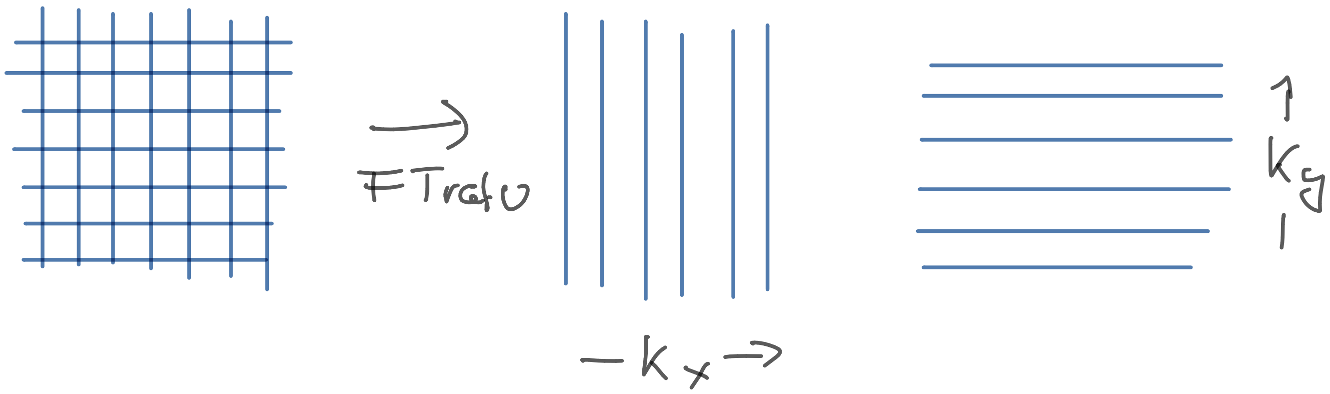
(322)
$$\boxed{\nu_2 = P_\theta\left(\frac{T}{2}\right) - P_\theta(0) \mod 2}$$

At $t=0$ and $t=\frac{T}{2}$ Kramers partners become degenerate due to TR symmetry.

(323)
$$T H\left(\frac{T}{2}\right) T^{-1} = H\left(-\frac{T}{2}\right) = H\left(-\frac{T}{2}+T\right) = H\left(\frac{T}{2}\right)$$

(B) 2D band structures

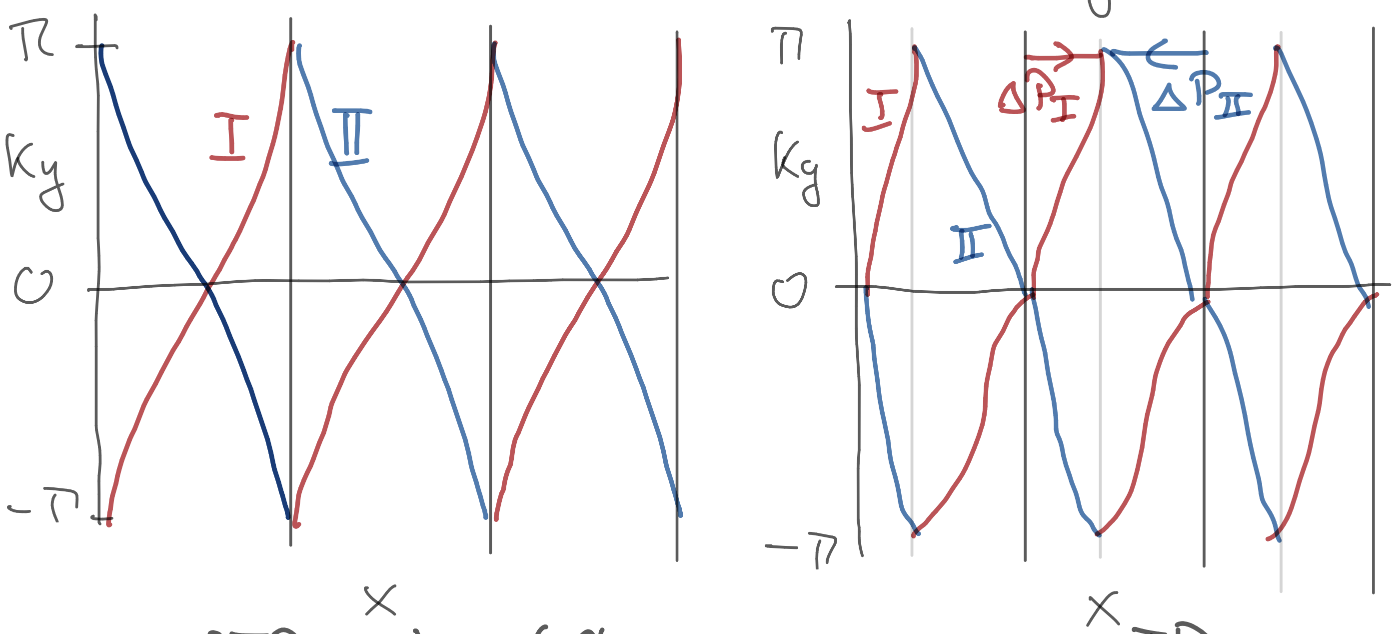
For generalization to 2D we follow the common approach



$$P_\theta(t) \longrightarrow P_\theta^x(k_y) \text{ or } P_\theta^y(k_x)$$

(324) $$\boxed{\nu_2 = P_\theta^x(k_y = 0) - P_\theta^x(k_y = -\pi)}$$

or y and k_x



2TR copies of Chern

$Ch_I = -Ch_{II} = 1$

general TR

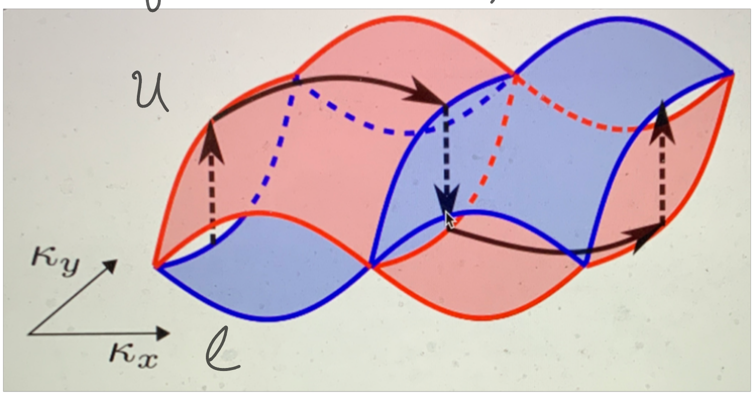
$\Delta P_I - \Delta P_{II} = 1$

(c) continuous TR polarization

A disadvantage of (324) is that it requires calculating P_θ at two points where one has to make sure that the same gauge was used! It would be more convenient to formulate ν_2 as a winding.

The problem is that $P_\theta^x(k_y)$ is not smooth in k_y

$\Rightarrow$ continuous TR polarization



(325)
$$\boxed{\tilde{P}_\theta = \frac{i}{2\pi}\left[\int_{-\pi}^{0} dk_x \langle u^u(k_x)|\partial_{k_x} u^u(k_x)\rangle + \int_{0}^{\pi} dk_x \langle u^e(k_x)|\partial_{k_x} u^e(k_x)\rangle\right]}$$

(326)
$$\boxed{\nu_2 = P_\theta^x(k_y=\pi) - P_\theta^x(k_y=0) = \int_{-\pi}^{0} dk_y \frac{\partial \tilde{P}_\theta^x(k_y)}{\partial k_y}}$$