IV. Time-reversal symmetric topological insulator : QSHE and the Kane-Mele model

1) Introduction

2D TRB band insulator $\rightarrow$ 2D bands are classified by a Chern number $C_n \in \mathbb{Z}$

the gap is characterized by $TKNN = \sum_{n \text{ occupied}} C_n \in \mathbb{Z}$

and $\sigma_{xy} = \frac{e^2}{h} \times TKNN$ ie. QHE

no QHE in 3D

2D TRS band insulator $\rightarrow$ we will see that there is a $\mathbb{Z}_2$ invariant (ie. only 2 classes of band insulators)

physically : a quantum spin Hall effect (QSHE)

in 2D and in 3D

2) Kane-Mele model

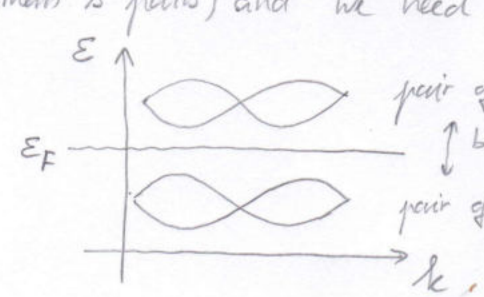
- QHE : experiment in 1980 von Klitzing

  TKNN 1982 : QHE because of a topological invariant, importance of $\vec{B}$ and Landau levels

  Haldane 1988 : no need of Landau levels, no need of homogeneous magnetic field if TRB, bands can have a QHE

  Kane-Mele 2005 : no need of an inhomogeneous magnetic field and of TRB spin-orbit coupling is enough, we can have a topological insulator and TRS : QSHE

- The simplest TRS T.I. has 4 bands because with TRS, bands come in pairs (Kramers's pairs) and we need a band gap $\Rightarrow$



The electron is now spinful (spin 1/2).

2 bands + 2 spin projection $\Rightarrow$ 4 bands

Kane and Mele propose to take 2 copies of the Haldane model but such that TRS is obtained:

$$\text{KM} \sim \underbrace{\text{Haldane with } \varphi \text{ for spin} \uparrow}_{\substack{\text{inhomogeneous} \\ B_z \text{ field} \\ (\varphi = \pi/2)}} + \overbrace{\underbrace{\text{Haldane with } -\varphi \text{ for spin} \downarrow}_{\substack{\text{inhomogeneous} \\ B_z \text{ field with} \\ B_z \to -B_z \quad (-\varphi = -\pi/2)}}}^{\text{TR copy of the first term}}$$

We will use the low-energy effective description with the Dirac equation near the two valleys K and K' at the corner of the hexagonal BZ of the honeycomb lattice:

$$H(\vec{q}) = \tau_z q_x \sigma_x + q_y \sigma_y + \underbrace{m_{SO}\, \sigma_z \tau_z s_z}_{= m_{Haldane}\, \sigma_z \tau_z} \qquad \hbar \equiv 1, \quad v \equiv 1$$

remark: do not mix
$4N \times 4N$: H TB Hamiltonian
4×4: $H(\vec{k})$ Bloch Hamiltonian
8×8: $H(\vec{q})$ low-energy eff. H.

8×8 Hamiltonian: σ_y means $\sigma_y \tau_0 s_0$

3 sets of Pauli matrices:
- $\vec{\sigma}$ sublattice spin $\frac{1}{2}$, $\sigma_z = \pm = A/B$
- $\vec{\tau}$ valley spin $\frac{1}{2}$, $\tau_z = \xi = \pm = K/K'$ (valley index)
- $\vec{s}$ (true) spin $\frac{1}{2}$, $s_z = \pm = \uparrow/\downarrow$ (spin projection)

In order to gap the Dirac cones of graphene, one needs to introduce a finite σ_z term at K/K':

- $M\sigma_z$: Semenoff mass, Boron Nitride, breaks inversion symmetry as $\tau_x \sigma_x H(-\vec{q}) \sigma_x \tau_x \neq H(\vec{q})$
- $m_H \sigma_z \tau_z = 3\sqrt{3}\, t_2 \sin\varphi \cdot \sigma_z \tau_z$: Haldane mass, changes sign with the valley index, breaks TRS as $\tau_x s_y H(-\vec{q})^* s_y \tau_x \neq H(\vec{q})$
- $m_{SO} \sigma_z \tau_z s_z$: Kane-Mele mass, changes sign with both the valley index and the spin projection, respects I and TR as $\tau_x \sigma_x H(-\vec{q}) \sigma_x \tau_x = H(\vec{q})$ and $\tau_x s_y H(-\vec{q})^* s_y \tau_x = H(\vec{q})$

It is also mirror symmetric. On symmetry argument, it should be present.

The term $m_{SO}\, \sigma_z \tau_z s_z$ comes from <u>intrinsic spin-orbit coupling</u> of the material. It is very small in graphene because C is a light element with a small $Z = 6$.

$$[H(\vec{q}), \tau_z] = 0 \quad \text{and} \quad [H(\vec{q}), s_z] = 0$$

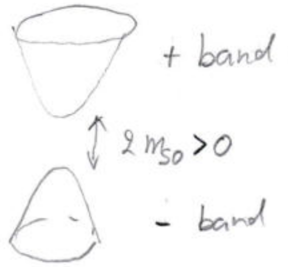
The valley index and the spin projection are conserved. The second property is very particular to this model and not realistic.

$$\underset{\substack{\uparrow \\ (\text{same as } \xi)}}{H_{\tau,s}}(\vec{q}) = \tau q_x \sigma_x + q_y \sigma_y + m_{SO}\, \tau s\, \sigma_z \qquad 2\times 2 \text{ matrix}$$

energy spectrum: $\mathcal{E}_{\pm}(\vec{q}) = \pm\sqrt{q_x^2 + q_y^2 + m_{SO}^2} \qquad \forall\, \tau \text{ and } s$

$\pm$: band index (in the same space as sublattice index)

gapped Dirac cones in 4 copies $(\tau, s) = (\pm, \pm)$



the SOC turns graphene into a band insulator

geometry/topology: 4 copies of a massive 2D Dirac Hamiltonian

$$H_{\tau,s}(\vec{q}) = \underset{\substack{\uparrow \\ \text{chirality} \\ (\text{winding number of} \\ \text{Dirac cone } W_D)}}{\tau} q_x \sigma_x + q_y \sigma_y + \underset{\substack{\uparrow \\ >0}}{m_{SO}}\, \underset{\substack{\uparrow \\ \text{sign}(M_D) \\ \text{sign of the Dirac mass}}}{\underbrace{\tau s}}\, \sigma_z$$

Chern number for the valence band:

$$C_\uparrow = \sum_\tau \frac{1}{2} \times \tau \times \text{sgn}(\tau \underset{\substack{\uparrow \\ +1}}{s}) = \tau^2 = 1$$

$$C_\downarrow = \sum_\tau \frac{1}{2} \times \tau \times \text{sgn}(\tau \underset{\substack{\uparrow \\ -1}}{s}) = -\tau^2 = -1$$

$$\text{TKNN} = \sum_{\substack{-\text{band} \\ s=\pm,\, \tau=\pm}} \text{Chern}_{\text{band, spin, valley}} = 2 \times \frac{1}{2} \times \sum_s s = 0 \quad \text{because of TRS}$$

$$\text{Chern}_{\text{band, spin, valley}} = \frac{1}{2} \times \tau \times \text{sgn}(\tau s) = \frac{1}{2}\, \tau \times \tau s = \frac{1}{2} s$$

But for each spin specie $C_\uparrow \neq 0$, $C_\downarrow \neq 0$

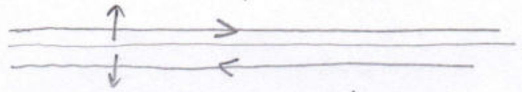
I.e. spin $\uparrow$ is a Chern insulator with $\text{TKNN}_\uparrow = +1$, $\sigma_{xy}^\uparrow = e^2/h$

spin $\downarrow$ ——— $\text{TKNN}_\downarrow = -1$, $\sigma_{xy}^\downarrow = -e^2/h$

As the two spin species are independent (because of S_z conservation) and as a result of bulk-edge correspondance in a Chern insulator, there must be gapless and chiral edge states.

Kane-Mele

$C_\uparrow = 1,\ C_\downarrow = -1$



← interface

boron nitride

$C_\uparrow = 0,\ C_\downarrow = 0$

This is a pair of spin-filtered gapless edge states. The direction of motion (the chirality) is locked to the spin projection (spin-momentum locking). It is called a helical mode. (*)

Such a mode is robust to perturbations that do not act on the spin. So it is robust to non-magnetic elastic disorder that can not backscatter. So this is a symmetry-protected topological insulator (we will see that the symmetry is TRS here).

Is there a corresponding bulk topological invariant?

$$\text{TKNN} = \sum_{\substack{\text{occupied}\\ \text{bands}}} \text{Chern} = C_\uparrow + C_\downarrow = 0 \quad \text{i.e. } \sigma_{xy} = 0$$

but $\underbrace{C_\uparrow - C_\downarrow}_{=2} \neq 0$ a kind of spin Chern number: $C_{spin} = C_\uparrow - C_\downarrow$

There is a quantum spin Hall effect (QSHE) meaning a spin Hall effect in an insulator:

$$\vec{J}_e \equiv e\left(\vec{J}_\uparrow + \vec{J}_\downarrow\right) \quad \text{and} \quad (J_e)_x = \sigma_{xy}\, \mathcal{E}_y \qquad \text{with } \sigma_{xy} = \frac{e^2}{h}\left(C_\uparrow + C_\downarrow\right)$$

$$\vec{J}_S \equiv \frac{\hbar}{2}\left(\vec{J}_\uparrow - \vec{J}_\downarrow\right) \quad \text{and} \quad (J_S)_x = \sigma_{xy}^S\, \mathcal{E}_y$$

Therefore replacing e by $\frac{\hbar}{2}$ i.e. $\frac{e^2}{h}$ by $\frac{e}{4\pi}$

and $C_\uparrow + C_\downarrow$ by $C_\uparrow - C_\downarrow$

$$\sigma_{xy}^{spin} = \frac{e}{4\pi}\left(C_\uparrow - C_\downarrow\right) = \frac{e}{4\pi}\, C_{spin} = \frac{e}{2\pi}$$

The quantized Hall conductivity is an artefact of the model with conserved S_z. And the true topological invariant in the bulk only takes two values: ν_{bulk} = KM index = $C_\uparrow \bmod 2 = \underset{\text{trivial}}{0}$ or $\underset{\text{topo}}{1} \in \mathbb{Z}_2$

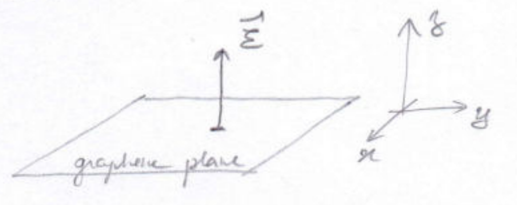
Two subtle things remain to be understood:

- what happens if s_z is not conserved as is the case with true/realistic SOC?
- why does the topological invariant only takes 2 values?

3) Rashba SOC and adiabatic continuity

Applying an electric field $\perp$ to the graphene plane breaks the mirror symmetry $z \to -z$ and introduces a new SOC called Rashba:

$$H_{Rashba}(\vec{q}) = \underset{\substack{\uparrow \\ \propto \mathcal{E}_z \text{ (electric field)}}}{\lambda_R} \left(\tau_z \sigma_x s_y - \sigma_y s_x \right)$$

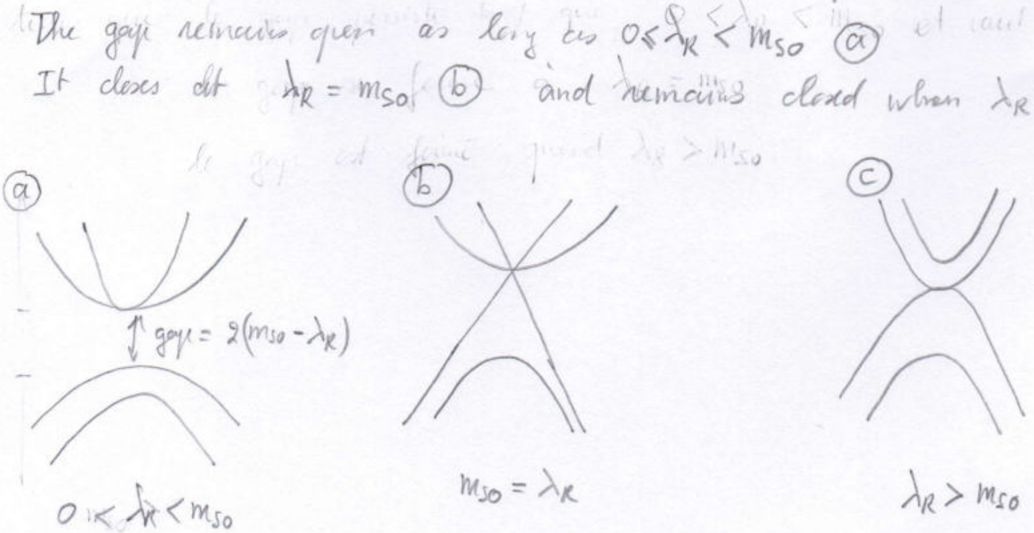


The Rashba term does not open a band gap in graphene (no σ_z), it respects TRS but breaks inversion symmetry and the conservation of s_z:

$$[H_R, s_z] = \lambda_R \tau_z \sigma_x \underbrace{[s_y, s_z]}_{= 2 i s_x} - \lambda_R \sigma_y \underbrace{[s_x, s_z]}_{= -2 i s_y} \neq 0 .$$

$$H(\vec{q}) = \tau_z q_x \sigma_x + q_y \sigma_y + m_{SO} \sigma_z \tau_z s_z + \lambda_R (\tau_z \sigma_x s_y - \sigma_y s_x) \qquad 8 \times 8$$
$$H_\tau(\vec{q}) = \tau q_x \sigma_x + q_y \sigma_y + m_{SO} \tau \sigma_z \tau_z + \lambda_R (\tau \sigma_x s_y - \sigma_y s_x) \qquad 4 \times 4$$

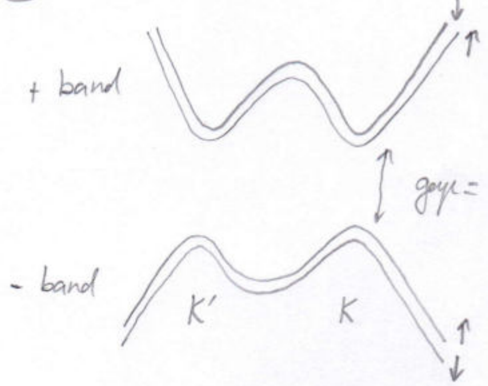
$H_\tau(\vec{q})$ can be diagonalized analytically when $\vec{q} = 0$ and numerically otherwise.
The gap remains open as long as $0 \leqslant \lambda_R < m_{SO}$ ⓐ
It closes at $\lambda_R = m_{SO}$ ⓑ and remains closed when $\lambda_R > m_{SO}$ ⓒ



<u>remark</u>: eigenvalues of $H(\vec{q}=0)$ are $m_{SO}, m_{SO}, -m_{SO} + 2\lambda_R$ and $-m_{SO} - 2\lambda_R$ in both valleys

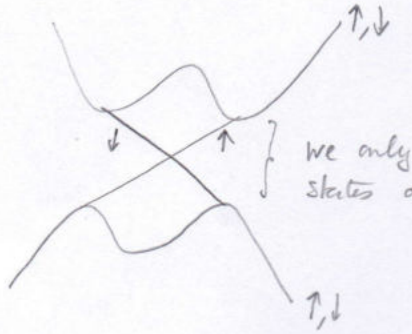
As long as Rashba does not close the gap, it can not change the topological invariant and therefore $\nu_{bulk} = 1 \neq 0$. But the spin Hall effect is no longer quantized and the spin Chern number is no longer well-defined (as the spin projection is no longer a good quantum number that labels the bands).

(*) Kane-Mele at $\lambda_R = 0$

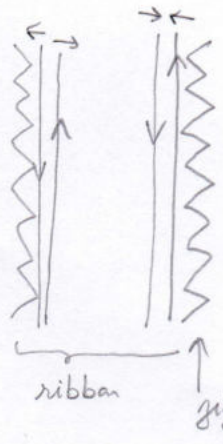


bands are 2-fold spin-degenerate

* From two copies of the Haldane zig-zag ribbon, we know that



we only plot the edge states on one edge



3) TRS and Kramers' theorem

- Time-reversal operation is represented by an <u>anti-unitary operator</u> $T = UK$ where K takes the complex conjugate of everything to its right and U is an unitary operator $U^{\dagger} = U^{-1}$.
- <u>If TR is a symmetry</u> then $\underline{[H, T] = 0}$.
- <u>T^2 can be either $= +1$ or $= -1$</u>. This depends on the total spin of the system being an integer or half-integer. For example a scalar wavefunction is such that $T^2 \psi = \psi$. But for a spinor wavefunction $T^2 \psi = -\psi$.
- Kramers' theorem: <u>if TRS and $T^2 = -1$</u> then <u>each eigenenergy level is at least twofold degenerate</u>.

proof: we assume $[T, H] = 0$ and $T^2 = -1$
and consider $H|\psi\rangle = E|\psi\rangle$

Then $\quad T H|\psi\rangle = H T|\psi\rangle = H|T\psi\rangle = E\,T|\psi\rangle$

i.e. $|T\psi\rangle$ is an eigenvector with energy E.

Let's assume that $|T\psi\rangle = c|\psi\rangle$ with $c \in \mathbb{C}$. T is anti-unitary

Then $\quad T T|\psi\rangle = T^2|\psi\rangle = -|\psi\rangle = T c|\psi\rangle = c^* T|\psi\rangle = c^* c|\psi\rangle = |c|^2|\psi\rangle$

$\Rightarrow |c|^2 = -1 \ \varnothing \ \Rightarrow |T\psi\rangle \perp |\psi\rangle$, i.e. $\deg E \geq 2$.

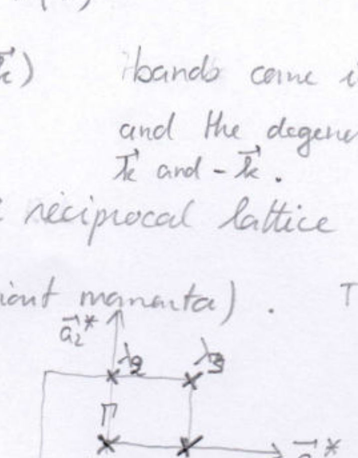
We call $|\psi\rangle$ and $|T\psi\rangle$ a <u>Kramers' pair</u> or <u>Kramers' doublet</u>.

. Now for band structures, $H(\vec{k})$, and TRS with $T^2 = -1$ (because electron) means

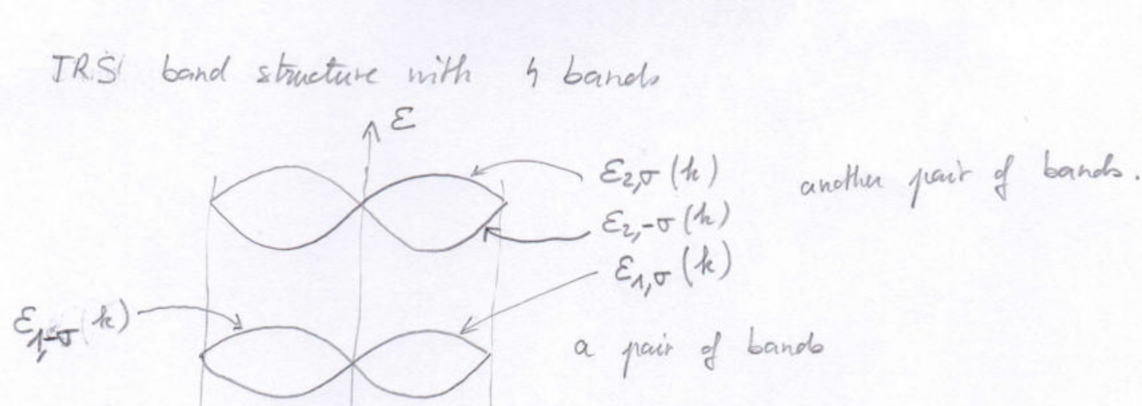
$$T H(-\vec{k}) T^{-1} = H(\vec{k})$$

$\Rightarrow \quad \mathcal{E}_{\sigma}(\vec{k}) = \mathcal{E}_{-\sigma}(-\vec{k}) \quad$ bands come in pairs and the degeneracy is split in $\vec{k}$-space between $\vec{k}$ and $-\vec{k}$.

Unless $\vec{k} \equiv -\vec{k}$ mod. $\vec{G} \in$ reciprocal lattice. These points are called TRIM (Time-reversal invariant momenta). There are 4 such TRIM in a 2D BZ : $\vec{k} = \dfrac{\vec{G}}{2}$



Example: TRS band structure with 4 bands



σ = Kramers' index ("almost the spin index")
despite the bad notation choice, do not mix up with the sublattice Pauli matrices $\sigma_x, \sigma_y, \sigma_z$.

<u>A band crossing at a TRIM is mandatory because of Kramer's theorem:</u>

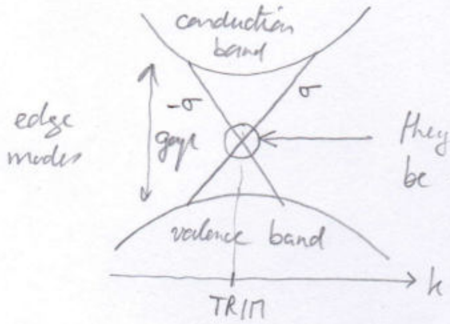
$$\begin{cases} \mathcal{E}_{\sigma}(\vec{k}) = +\mathcal{E}_{-\sigma}(-\vec{k}) \\ \vec{k} \equiv -\vec{k} \text{ mod } \vec{G} \end{cases} \Rightarrow \quad \mathcal{E}_{\sigma}(\vec{k}) = \mathcal{E}_{-\sigma}(\vec{k}) \text{ at a TRIM}$$

In addition, a band crossing at a TRIM is protected, ie. it is robust to any perturbation that respects TRS. Indeed if $[T,V]=0$ (and $T=UK$ and $T^2=-1$) then we can prove that $\langle u(\vec{k})|V|T u(-\vec{k})\rangle = 0$ (see proof in the book by Bernevig page 37).

4) $\mathbb{Z}_2$ invariant, KM index

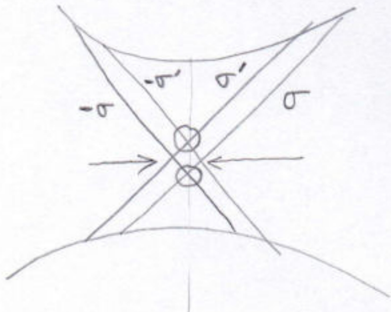
a) robustness of helical modes and edge topological invariant

• 1 helical mode = 1 pair of edge modes

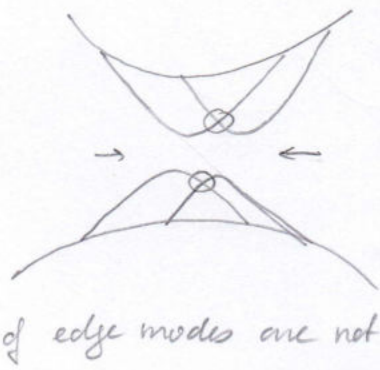


They cross at a TRIM and the degeneracy can not be lifted by any perturbation that respects TRS

• 2 helical modes



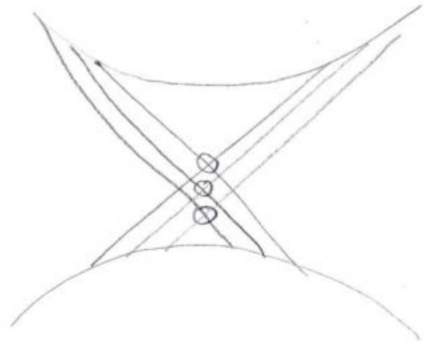
4 crossings:
- 2 at a TRIM → they are protected
- 2 not at a TRIM → the crossing can be avoided due to a perturbation that respects TRS : therefore a gap can open.



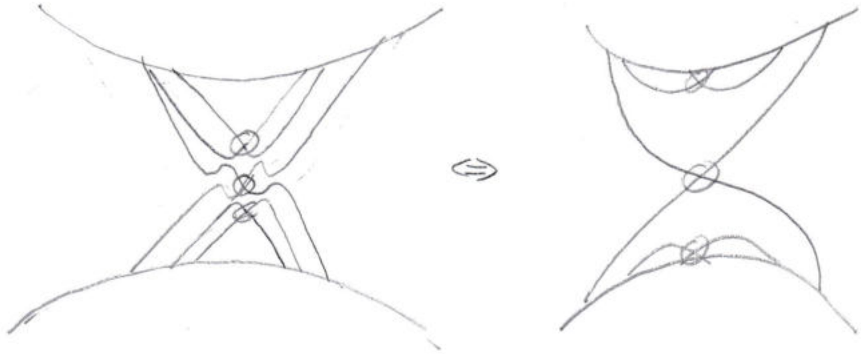
a gap opens in the edge modes

2 pairs of edge modes are not robust and are therefore equivalent to no edge modes: 2 helical modes ≡ 0 helical modes

- 3 helical modes



9 crossings :
- 3 are protected (TRIM)
- 6 are not protected and can be lifted/gapped



remains gapless

3 helical modes ≡ 1 helical mode

etc

$\Rightarrow$ $\boxed{\nu_{edge} \equiv \text{parity of the number of } \underline{\text{helical modes}}}$

↳ Kramers' pair of gapless edge modes with "spin-momentum" locking

i.e. $\underline{\nu_{edge} \in \mathbb{Z}_2 = \{0;1\}}$

b) <u>Bulk topological invariant $\nu_{bulk} \in \mathbb{Z}_2$</u>

(We admit that $BZ = T^2$ can be replaced by S^2 (see Avron, Seiler, B. Simon PRL 1983) here.)

- TRB bands are non-degenerate in general. On a single band there is a scalar wavefunction, ie. a $U(1)$ phase to be placed on each $\vec{k}$ point. We know from Dirac's magnetic monopole that we need two patches and a gluing condition on the boundary between the two patches. The boundary is S^1 and the thing to be glued (the fiber) is also $S^1 = U(1)$ = phase of scalar wf. Therefore $\pi_1(S^1) = \mathbb{Z}$: quantization of the Dirac monopole, ie also Chern number associated to a single band $C_n \in \mathbb{Z}$.

• Now for TRS bands : they come by Kramers pairs. The wf is now a spinor. We still have two patches (why?). And the fiber is $SU(2)$ but as $\vec{k}$ is mapped onto $-\vec{k}$ by TR it is rather $SU(2)/\mathbb{Z}_2 = S^3/\mathbb{Z}_2 = SO(3)$.

Therefore the gluing on the boundary is classified by $\pi_1(SO(3)) = \mathbb{Z}_2$.

$\Rightarrow$ KM index $\nu_{bulk} \in \mathbb{Z}_2$ (see R. Roy, PRB 2009)

is like an S^3 sphere with antipodal points on the surface identified

c) Expression of the bulk invariant ν_{bulk} (KM index)

• TRB : • each band has a Chern number $C_n = \frac{1}{2\pi}\int_{BZ} d^2k\, \Omega_n \in \mathbb{Z}$

(these are the only invariants, see Avron, Seiler and Simon 1983)

• then the gap in an insulator has $\boxed{TKNN = \sum_{n\ occupied} C_n \in \mathbb{Z}}$

• TRS : • bands come in pairs (Kramers) with $C_{n,\sigma} + C_{n,-\sigma} = 0$

pair is characterized by $|C_{n,\sigma}|$. Each band is labelled by (n,σ).

• the gap in an insulator has $\boxed{KM = \sum_{n\ occupied} |C_{n,\sigma}| \mod 2 \in \mathbb{Z}_2}$

no sum over σ
(we only sum over positive Chern numbers)

because we know that only the parity of this number matters for the robustness of the counterpropagating helical edge modes.

(see R. Roy PRB 2009)