↓ **Lecture 12** [23.05.25]

5 | → ◁ Pfaffian:

Definition: For M a skew-symmetric $2n \times 2n$-matrix, the Pfaffian is defined as

$$\mathrm{Pf}[M] := \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} (-1)^\sigma \prod_{i=1}^{n} M_{\sigma(2i-1),\sigma(2i)} \tag{3.24}$$

Cf. the ↓ *Leibniz formula* for determinants:

$$\det(M) = \sum_{\sigma \in S_{2n}} (-1)^\sigma \prod_{i=1}^{2n} M_{i\sigma(i)} \tag{3.25}$$

$\overset{\circ}{\rightarrow}$ It follows:

- $(\mathrm{Pf}[M])^2 = \det(M)$, i.e., the Pfaffian contains the same information as the determinant (but with an additional sign that is lost when considering the determinant).
- $\mathrm{Pf}\left[BAB^T\right] = \det(B)\,\mathrm{Pf}[A]$ for an arbitrary $2n \times 2n$-matrix B
- For skew-symmetric matrices of even dimension, the Pfaffian is a "more natural" object than the determinant (it contains at least as much information!).

This motivates the definition of the following function:

$$P : T^2 \to \mathbb{C} \qquad P(\boldsymbol{k}) := \mathrm{Pf}[M(\boldsymbol{k})] \tag{3.26}$$

Kane-Mele model: $P(\boldsymbol{k}) = M_{12}(\boldsymbol{k}) = \langle u_1(\boldsymbol{k})|\tilde{T}_U|u_2(\boldsymbol{k})\rangle$

→ $P(\boldsymbol{k})$ is a complex-valued function on the BZ that depends (continuously) on the Hamiltonian.

The idea is now to identify topologically robust properties of this function to distinguish the two phases of the Kane-Mele model …

6 | Properties of $P(\boldsymbol{k})$:

Next, we carefully study the properties of $P(\boldsymbol{k})$ to lay the foundations for a new topological index defined → *below*:

i | Not gauge invariant: ◁ $U \in \mathrm{U}(2n)$ and $|u_i'(\boldsymbol{k})\rangle := U_{ij}|u_j(\boldsymbol{k})\rangle$

This gauge transformation mixes the $2n$ filled bands!

w.l.o.g. $U = e^{i\phi}\tilde{U}$ with $\tilde{U} \in \mathrm{SU}(2n)$ →

$$P'(\boldsymbol{k}) = \mathrm{Pf}\left[\left(\langle u_i'(\boldsymbol{k})|\tilde{T}_U|u_j'(\boldsymbol{k})\rangle\right)_{ij}\right] \tag{3.27a}$$

$$= \mathrm{Pf}\left[\left(U_{ii'}^*\langle u_{i'}(\boldsymbol{k})|\tilde{T}_U|u_{j'}(\boldsymbol{k})\rangle U_{jj'}^*\right)_{ij}\right] \tag{3.27b}$$

$$= \mathrm{Pf}\left[U^*\left(\langle u_{i'}(\boldsymbol{k})|\tilde{T}_U|u_{j'}(\boldsymbol{k})\rangle\right)_{i'j'}(U^*)^T\right] \tag{3.27c}$$

$$= \det(U^*)P(\boldsymbol{k}) \tag{3.27d}$$

$$= e^{-i2n\phi}P(\boldsymbol{k}) \tag{3.27e}$$

Here we used that $\det(\tilde{U}) = 1$.

→ $|P(\boldsymbol{k})|$ is gauge invariant

Note: We can consider even unitary transformations *between* filled bands (for a fixed $\boldsymbol{k}$) although these states are not energetically degenerate (strictly speaking, they do not even have to be energy eigenstates to begin with, → *below*) because such transformations do *not* alter the many-body ground state (namely the Fermi sea or the Slater determinant):

$$|\Psi_0'\rangle = \prod_{\boldsymbol{k}}\prod_i c'^{\dagger}_{\boldsymbol{k},i}|0\rangle = \prod_{\boldsymbol{k}}\prod_i U_{ij}c^{\dagger}_{\boldsymbol{k},j}|0\rangle \tag{3.28a}$$

$$\hat{=} \prod_{\boldsymbol{k}}\det(U)\prod_i c^{\dagger}_{\boldsymbol{k},i}|0\rangle = e^{i\chi}\prod_{\boldsymbol{k}}\prod_i c^{\dagger}_{\boldsymbol{k},i}|0\rangle = e^{i\chi}|\Psi_0\rangle\,. \tag{3.28b}$$

Here, $c^{\dagger}_{\boldsymbol{k},i}$ creates a fermion in mode $|u_i(\boldsymbol{k})\rangle$ and $e^{i\chi}$ is some *global* (and therefore unphysical) phase determined by (powers of) $\det(U)$. The determinant arises due to the anticommutation relations $\{c^{\dagger}_{\boldsymbol{k},i}, c^{\dagger}_{\boldsymbol{k},j}\} = 0$; have a look at the concepts of ↑ *alternating multilinear forms* and the ↑ *exterior algebra* if so don't believe this (or prove it by hand).

ii | Time-reversal symmetry (TRS/TRI)

→ Chern numbers of "valence bundle" $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}} = \text{span}\,\{|u_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ vanish

→ $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ = ↑ *Trivial vector bundle*

→ ∃ Continuous basis $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ of $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ on T^2

It is $|e_i(\boldsymbol{k})\rangle = U_{ij}(\boldsymbol{k})|u_j(\boldsymbol{k})\rangle$ a (potentially discontinuous) gauge transformation.

Remember that we showed in Section 1.3.1 (for the speciall case of a single band) that a non-zero Chern number implies that a globally continuous Bloch basis does *not* exists. Here we use the inverse claim (without proof).

→ $P(\boldsymbol{k})$ continuous on T^2 if defined by $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$

This follows from the fact that the Chern number(s) of the filled Bands (mathematically speaking, the filled ↑ *Bloch bundle* or ↑ *valence bundle*) vanish. Thus there is no obstruction in choosing a globally defined, continuous basis $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ of the filled band fiber $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ at every $\boldsymbol{k}$. Mathematically, this means that the Bloch bundle of filled bands can be ↑ *trivialized*. Because there is a continuous basis choice $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ for the filled bands, the matrix of $\tilde{T}_U$, and subsequently the Pfaffian $P(\boldsymbol{k})$, are continuous on T^2 if defined with this basis choice.

Note that in general the continuous basis $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ is *not* necessarily an eigenbasis of the Bloch Hamiltonian! This is why we changed the notation from $u_i(\boldsymbol{k})$ to $e_i(\boldsymbol{k})$; in the following, $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ always denotes a globally continuous basis whereas $\{|u_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ is a (potentially discontinuous) *eigen*basis of the Bloch Hamiltonian.

iii | ⋖ Two special subspaces of Bloch states:

- $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ is ⁂ *even* $\;:\Leftrightarrow\;$ $\tilde{T}_U\mathcal{H}^{\text{filled}}_{\boldsymbol{k}} = \mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$

  This means that $\tilde{T}_U|u_i(\boldsymbol{k})\rangle = M_{ij}|u_j(\boldsymbol{k})\rangle$ with a *unitary* matrix $M \neq 0$.

  → $|P(\boldsymbol{k})| = |\,\text{Pf}\,[M(\boldsymbol{k})]\,| = \sqrt{|\det M(\boldsymbol{k})|} = 1$

  To show that $M(\boldsymbol{k})$ is unitary, evaluate $(M^{\dagger}M)_{ij}$ using the definition in Eq. (3.23) and use that the projector $P_{\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}} = \sum_{k=1}^{2n}|u_k(\boldsymbol{k})\rangle\langle u_k(\boldsymbol{k})|$ acts as the idenity on $\tilde{T}_U|u_j(\boldsymbol{k})\rangle$ since $\tilde{T}_U\mathcal{H}^{\text{filled}}_{\boldsymbol{k}} = \mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ by assumption. Remember that $\tilde{T}_U = U\mathcal{K}$ with $U^{\dagger}U = \mathbb{1}$ and use that $\langle u_i^*(\boldsymbol{k})|u_j^*(\boldsymbol{k})\rangle = \langle u_j(\boldsymbol{k})|u_i(\boldsymbol{k})\rangle = \delta_{ij}$.

- $\mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$ is ⁂ *odd* $\;:\Leftrightarrow\;$ $\tilde{T}_U\mathcal{H}^{\text{filled}}_{\boldsymbol{k}} \perp \mathcal{H}^{\text{filled}}_{\boldsymbol{k}}$

This means that $\langle u_j(\boldsymbol{k})|\tilde{T}_U|u_i(\boldsymbol{k})\rangle = 0 = M_{ij}$. Remember that i runs only over *filled* bands whereas $\tilde{T}_U$ can mix the *whole* fiber $\mathcal{H}_{\boldsymbol{k}} = \mathcal{H}_{\boldsymbol{k}}^{\text{filled}} \oplus \mathcal{H}_{\boldsymbol{k}}^{\text{empty}}$.

$\rightarrow |P(\boldsymbol{k})| = |\,\text{Pf}[M(\boldsymbol{k})]\,| = 0$

These are two *special cases*; $\mathcal{H}_{\boldsymbol{k}}^{\text{filled}}$ can also be *neither* even *nor* odd!

iv | Observation: $\boldsymbol{K}^*$ TRIM $\rightarrow \mathcal{H}_{\boldsymbol{K}^*}^{\text{filled}}$ is *even* since

$$\tilde{T}_U H(\boldsymbol{K}^*)\tilde{T}_U^{-1} = H(\boldsymbol{K}^*) \tag{3.29}$$

This means that $\tilde{T}_U$ can only mix states with the same eigenenergy. In particular, a mixing between valence and conduction bands cannot occur. Note that this argument breaks down at a gapless point!

$\rightarrow |P(\boldsymbol{K}^*)| = 1$ at all TRIMs $\boldsymbol{K}^*$

v | Effective Brillouin Zones:

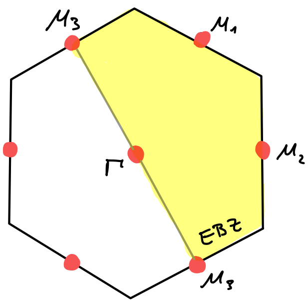
Remember:

$$\text{TRI} \quad \Leftrightarrow \quad \tilde{T}_U H(\boldsymbol{k})\tilde{T}_U^{-1} = H(-\boldsymbol{k}) \tag{3.30}$$

$\rightarrow$ Defining $H(\boldsymbol{k})$ on *half* the BZ is sufficient!
The other half can then be reconstructed via Eq. (3.30).

$\rightarrow$ Define an ⁂ *Effective Brillouin Zone* (EBZ) as any subset of T^2 that does not contain both $\boldsymbol{k}$ and $-\boldsymbol{k}$ (except for the boundaries which connect pairs of TRIMs).

Example on the hexagonal lattice:



- The EBZ has the topology of a cylinder (and not a torus).
- Note that the choice of an EBZ is not unique [113].
- The concept of an EBZ was originally introduced by MOORE and BALENTS in 2007 [100]. See also Ref. [113] for an accessible introduction.

The concept of an EBZ will become important → *below*.

vi | Consequences for $P(\boldsymbol{k})$ from TRI:
(Remember the TRI band structure with Kramers pairs above!)

$$\tilde{T}_U H(\boldsymbol{k})\tilde{T}_U^{-1} = H(-\boldsymbol{k}) \quad \Rightarrow \quad \tilde{T}_U \mathcal{H}_{\boldsymbol{k}}^{\text{filled}} = \mathcal{H}_{-\boldsymbol{k}}^{\text{filled}} \tag{3.31a}$$

$$\Rightarrow \quad |e_i(-\boldsymbol{k})\rangle = w_{ij}^*(\boldsymbol{k})\tilde{T}_U|e_j(\boldsymbol{k})\rangle \tag{3.31b}$$

$w_{ij}(\boldsymbol{k}) := \langle e_i(-\boldsymbol{k})|\tilde{T}_U|e_j(\boldsymbol{k})\rangle$: unitary ⁂ *Sewing matrix*

$|e_i(\boldsymbol{k})\rangle$ denotes the globally continuous basis of the valence bundle $\mathcal{H}_{\boldsymbol{k}}^{\text{filled}}$ defined ← *above*.

The sewing matrix was originally introduced by FU and KANE in 2006 [112]. See also FRUCHART and CARPENTIER [113] and ➲ Problemset 6.

→ With this we can evaluate the Pfaffian at $-\boldsymbol{k}$:

$$\begin{aligned}
P(-\boldsymbol{k}) &= \mathrm{Pf}[M(-\boldsymbol{k})] && (3.32a)\\
&= \mathrm{Pf}\Big[\big(\langle e_i(-\boldsymbol{k})|\tilde{T}_U|e_j(-\boldsymbol{k})\rangle\big)_{ij}\Big] && (3.32b)\\
&= \mathrm{Pf}\Big[\big(w_{ii'}(\boldsymbol{k})\,\langle \tilde{T}_U e_{i'}(\boldsymbol{k})|\tilde{T}_U|\tilde{T}_U e_{j'}(\boldsymbol{k})\rangle\, w_{jj'}(\boldsymbol{k})\big)_{ij}\Big] && (3.32c)\\
&= (-1)^n\,\mathrm{Pf}\Big[\big(w_{jj'}(\boldsymbol{k})\,\langle e_{j'}(\boldsymbol{k})|\tilde{T}_U|e_{i'}(\boldsymbol{k})\rangle^*\, w_{ii'}(\boldsymbol{k})\big)_{ij}\Big] && (3.32d)\\
&\stackrel{\circ}{=} (-1)^n\,\mathrm{Pf}\Big[w(\boldsymbol{k})\,M^*(\boldsymbol{k})\,w^T(\boldsymbol{k})\Big] && (3.32e)\\
&= (-1)^n\,\det[w(\boldsymbol{k})]\,[P(\boldsymbol{k})]^* && (3.32f)
\end{aligned}$$

Here we used $\tilde{T}_U^2 = -1$, $\mathrm{Pf}[\lambda A] = \lambda^n\,\mathrm{Pf}[A]$ and that $\tilde{T}_U$ is antiunitary.

→ Two conclusions:

- $P(\boldsymbol{k}') = 0 \;\Leftrightarrow\; P(-\boldsymbol{k}') = 0$

  Note that $w^\dagger(\boldsymbol{k})w(\boldsymbol{k}) = \mathbb{1}$ so that $\det[w(\boldsymbol{k})] \neq 0$ for all $\boldsymbol{k} \in T^2$.

- The ⁂ *vorticities* ν around $\boldsymbol{k}'$ and $-\boldsymbol{k}'$ have opposite signs:

$$\nu[\boldsymbol{k}'] := \frac{1}{2\pi i}\oint_{\partial\boldsymbol{k}'} \nabla\log[P(\boldsymbol{k})]\cdot\mathrm{d}\boldsymbol{k} = -\nu[-\boldsymbol{k}'] \quad \in \mathbb{Z} \qquad (3.33)$$

  $\partial\boldsymbol{k}'$: loop around $\boldsymbol{k}'$

  - The vorticity $\nu[\boldsymbol{k}']$ measures the *complex phase* accumulated when travelling around the zero of $P(\boldsymbol{k})$ at $\boldsymbol{k}'$. Since $P(\boldsymbol{k})$ is continuous, this can only be integer multiples of 2π.
  - Since $w(\boldsymbol{k})$ is continuous and unitary, the vorticity of $\det[w(\boldsymbol{k})] \neq 0$ must vanish everywhere, so that the vorticity of the expression in Eq. (3.32f) is completely determined by $[P(\boldsymbol{k})]^*$ [which has the negative vorticity of $P(\boldsymbol{k})$].
  - Let $P(\boldsymbol{k}) = |P(\boldsymbol{k})|e^{i\arg P(\boldsymbol{k})}$ so that $\log[P(\boldsymbol{k})] = \ln|P(\boldsymbol{k})| + i\arg P(\boldsymbol{k})$.

    Then we have

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_{\partial\boldsymbol{k}'} \nabla\log[P(\boldsymbol{k})]\cdot\mathrm{d}\boldsymbol{k} && (3.34a)\\
&= \underbrace{\frac{1}{2\pi i}\oint_{\partial\boldsymbol{k}'} \nabla\ln|P(\boldsymbol{k})|\cdot\mathrm{d}\boldsymbol{k}}_{=0} + \frac{1}{2\pi}\underbrace{\oint_{\partial\boldsymbol{k}'} \nabla\arg P(\boldsymbol{k})\cdot\mathrm{d}\boldsymbol{k}}_{\in 2\pi\mathbb{Z}} && (3.34b)
\end{aligned}$$

    where we used that $|P(\boldsymbol{k})| \neq 0$ is continuous everywhere along the contour $\partial\boldsymbol{k}'$; in particular, the argument $\arg P(\boldsymbol{k})$ can only change by multiples of 2π. This shows that the expression (3.33) measures the phase winding of $P(\boldsymbol{k})$ along the contour $\partial\boldsymbol{k}'$, i.e., its *vorticity*.

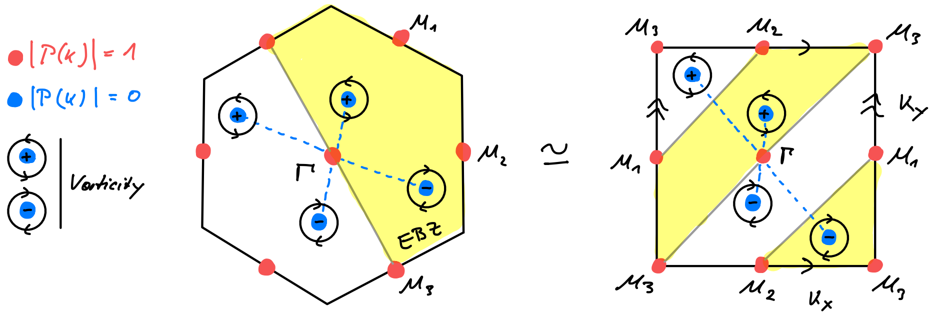
→ Phase vortices of $P(\boldsymbol{k})$ on the BZ T^2 come in pairs of opposite vorticity

vii | Observation: Zeros of $P(\boldsymbol{k})$ with $\nu[\boldsymbol{k}'] \neq 0$ are topologically stable

This is intuitively clear: If one makes the function non-zero at the vortex, it becomes discontinuous at this point due to the winding phase. Furthermore, the winding phase cannot be smoothly removed without discontinuous deformations of the function as well.

7 | If we combine all the above facts, we arrive at the following ...

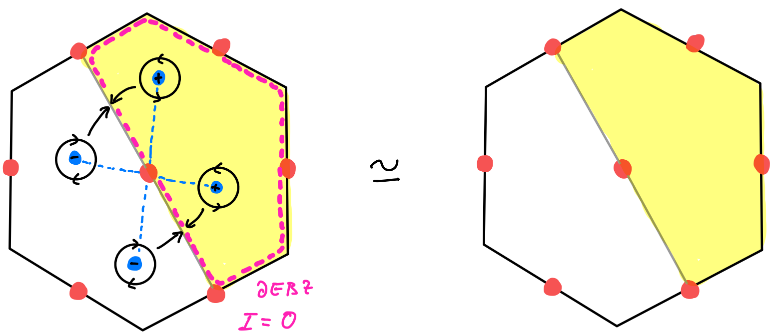
→ Generic picture:



- Without additional symmetries, the zeros of $|P(\boldsymbol{k})|$ occur at *points* in the BZ.
  This is true for the Kane-Mele model if $m \neq 0$.
- With additional symmetries, the zeros can form *lines* that avoid the TRIMs.
  In the Kane-Mele model, this happens for $m = 0$, ↑ Ref. [111] and → *below*.
- Zeros with vanishing vorticity are not stable and therefore not "generic" but "fine-tuned."
- On the TRIMs, $|P(\boldsymbol{k})|$ is pinned to 1, so that zeros (vortices) *cannot* occupy these positions.
- In the following, we focus on the least symmetric (and therefore most generic) case with point-like zeros. Without loss of generality, we assume a vorticity of ± 1 per vortex (a vortex with vorticity $|\nu| > 1$ can be continuously split into $|\nu|$ vortices of vorticity ± 1). Furthermore, we assume that all vortices in the EBZ have the same vorticity (vortices of opposite vorticity in the EBZ can be pairwise annihilated).

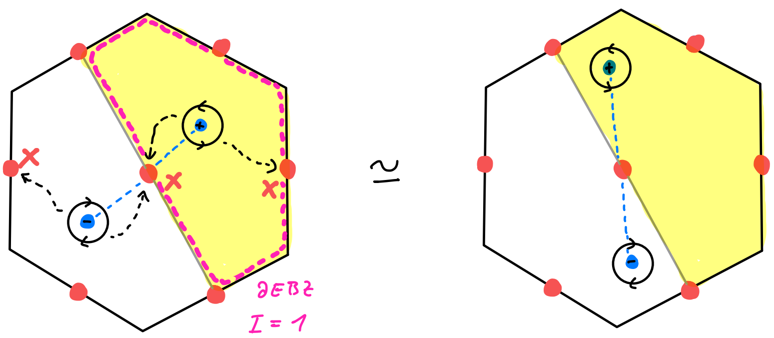
8 | Two situations:

- ⊲ Even number of vortices in EBZ:



→ All vortices can be continuously removed

- ⊲ Odd number of vortices in EBZ:



- To remove the last vortex pair, the partners must meet at one of the TRIMs.
- But this is *impossible* because of TRS which demands $|P(\boldsymbol{K}^*)| = 1$ [← Eq. (3.29)].

→ A single pair of vortices cannot be continuously removed

→ The two situations are Topologically distinct (as long as TRS is not broken)

→ Odd number of vortices = Topological phase protected by time-reversal symmetry

This is our first example of a true ← *symmetry-protected topological* (SPT) phase.

9 | This distinction is quantified by the ⁂ *Topological/Pfaffian* $\mathbb{Z}_2$ *index* …

$$I := \frac{1}{2\pi i}\oint_{\partial\mathrm{EBZ}} \nabla \log[P(\boldsymbol{k})]\cdot \mathrm{d}\boldsymbol{k} \mod 2 = \frac{1}{2\pi i}\oint_{\partial\mathrm{EBZ}} \mathrm{d}\log[P(\boldsymbol{k})] \mod 2 \tag{3.35}$$

∂EBZ: Closed path that encircles an EBZ

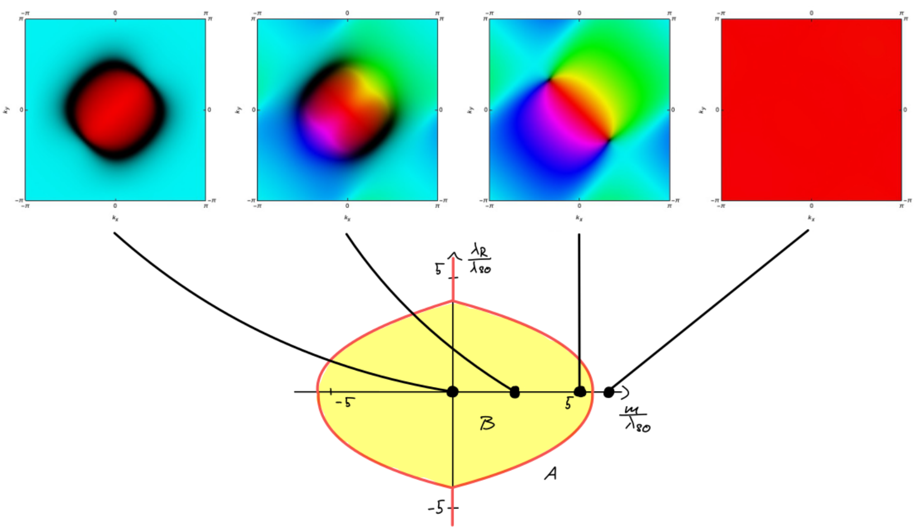
…which measures the parity of the total vorticity in half the Brillouin zone.

- The choice of a EZB is constrained by the vortices. It should be chosen such that the vortices stay away from the boundary ∂EBZ. For example, see Ref. [111, Fig. 2].
- $I \in \mathbb{Z}_2$ is gauge invariant because a gauge transformation that is continuous everywhere cannot change the vorticity of $P(\boldsymbol{k})$ [← Eq. (3.27)].
- There is an alternative way to compute the topological $\mathbb{Z}_2$ index I by evaluating the ← *sewing matrix* $w(\boldsymbol{k})$ at the TRIMs:

$$(-1)^I \overset{*}{=} \prod_{\boldsymbol{K}^*\ \mathrm{TRIM}} \frac{\mathrm{Pf}[w(\boldsymbol{K}^*)]}{\sqrt{\det w(\boldsymbol{K}^*)}}\,. \tag{3.36}$$

This assumes that the sewing matrix $w_{ij}(\boldsymbol{k}) = \langle e_i(-\boldsymbol{k})|\tilde{T}_U|e_j(\boldsymbol{k})\rangle$ is calculated from a globally continuous basis $|e_i(\boldsymbol{k})\rangle$. You show the equivalence of Eq. (3.35) and Eq. (3.36) on ➔ Problemset 6. This alternative form of the $\mathbb{Z}_2$ index is important because it naturally generalizes to three dimensions and paves the way to ↑ *3D topological insulators* and ↑ *weak topological insulators* [96].

10 | Example: Kane-Mele model:



- In the color plots, the BZ is deformed to a square. The color denotes the phase (red = $+1$, turquoise = -1) and the lightness the absolute value (black = 0) of the Pfaffian computed from a family of global sections of the valence bundle.
- Note that in the topological phase (for $m \neq 0$) there is a single vortex in each EBZ and the phase winds once around each vortex so that $I = 1$. For this result, it is crucial that the Pfaffian is computed from a *globally continuous basis* $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ (= a family of global sections of the valence bundle that form a basis at every point), otherwise the vorticity can be changed by integers (even if the Pfaffian is continuous!) and I cannot distinguish the phases. Note that these global sections are typically not eigenstates of the Bloch Hamiltonian; their existence, however, is guaranteed by time-reversal symmetry (because then all Chern numbers of the rank-2 valence bundle vanish).
- Here you can download the `Mathematica` notebook that I used to create the plots above:

Download `Mathematica` notebook

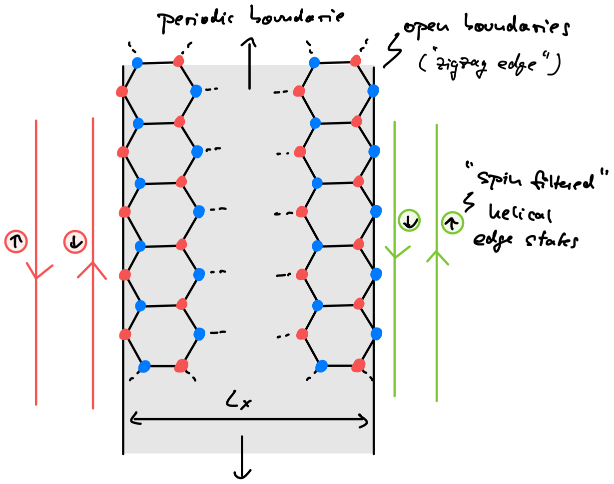
- The enhanced symmetry for $m = 0$ make the zeros form a line that circles the central TRIM (and therefore cannot be contracted without breaking TRS). In this situation, the Pfaffian can be gauged real (as already mentioned by Kane an Mele [111]). Continuously breaking the "ring of zeros" is only possible if a pair of vortices is introduced that makes the phase wind around the two islands of zeros that result from such a procedure.

3.4. Edge modes

A particularly intriguing feature of phases with topological bands is the emergence of robust *edge modes* (the analogs of the chiral edge modes we encountered in quantum Hall systems, ← Section 1.6):

11 | ◁ $\hat{H}_{\text{KM}}$ on a cylinder:

The system is therefore periodic in y-direction but has *boundaries* in x-direction.



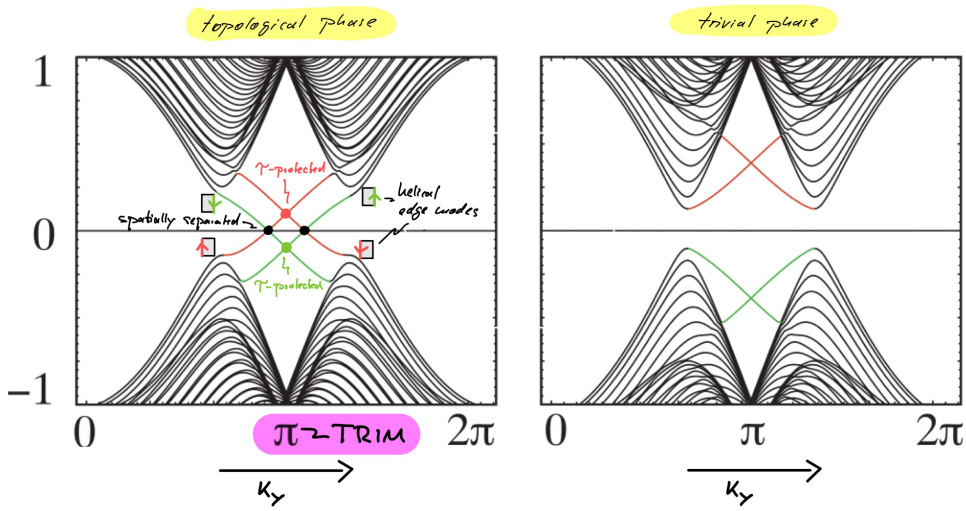
The type of boundary ("zigzag" vs. "armchair") has no effect on the existence of the edge states but the spectrum below looks different for armchair boundaries.

→ Interpret strip as a 1D system with large, L_x-dependent unit cell

→ Fourier transform $\hat{H}_{\text{KM}}$ only in y-direction

→ 1D spectrum with $\mathcal{O}(L_x)$ bands labeled by y-momentum k_y

12 | Numerics → Edge modes:



This figure is taken from KANE and MELE's original work [111].

- Topological phase → Gapless edge modes
  - Robust (= no backscattering / gap opening) to TRS perturbations
  - The four band crossings of the edge modes are protected for two different reasons:
    - Black crossings: The crossing modes are localized on *opposite* edges of the strip. Gapping them out is therefore exponentially suppressed with the width L_x of the strip (gapped bulk!).
    - Colored crossings: The crossing modes live on the *same* edge of the sample (with opposite group velocity). Gapping them out is forbidden by *time-reversal symmetry* as these crossings happen at a TRIM ($k_y = \pi$) and are enforced by Kramers degeneracy. This is why the Kane-Mele topological insulator is an SPT phase: Disorder that *breaks* TRS can hybridize these edge modes and destroy the topological phase.
  - On each edge there is a right-propagating mode for one spin polarization and a left-propagating mode for the opposite spin polarization (for $\lambda_R = 0$, if spin is conserved).

    In the original plots above, it is actually $\lambda_R = 0.05 \neq 0$ so that spin conservation is broken. The breaking of spin-conservation is responsible for the ↓ *avoided crossings* that fuse the edge modes into the bulk bands (for $\lambda_R = 0$ the edge modes would *cross* the bulk modes, ➔ Problemset 6).
  - The edge modes are *helical* (not *chiral*) since the product of spin and momentum is constant on each edge.
- Trivial phase → No gapless edge modes

Details: ➔ Problemset 5

Notes:

- The two "stalactite-stalagmite" pairs in the above spectrum correspond to the 1D projections of the two (gapped) Dirac cones around K and K'. The tips of these bulk bands are connected by the edge modes.
- For $\lambda_R = 0$ you can extract the edge modes of the ← *Haldane Chern insulator* by just looking at one of the two spin sectors (up or down, which determines the sign of the complex NNN

hopping phase). Thus in the topological phase, the Haldane model supports *one* (then *chiral* [since spin does not exist]) edge mode on each boundary.

13 | Final Note on symmetries and names:

- As discussed, the KM model $\hat{H}_{\text{KM}}$ without Rashba SO coupling ($\lambda_R = 0$) can be thought of as two uncoupled, time-reversed copies of Haldane's Chern insulator. As such, the model features a particle conservation symmetry in each of the two spin sectors, i.e., its total symmetry is $U(1)_\uparrow \times U(1)_\downarrow$. By defining *charge* $n_c = n_\uparrow + n_\downarrow$ and *spin* $n_s = n_\uparrow - n_\downarrow$, one can reinterpret this symmetry as $U(1)_{\text{charge}} \times U(1)_{\text{spin}}$, where total charge (particle) conservation $U(1)_{\text{charge}}$ and total spin conservation $U(1)_{\text{spin}}$ hold separately. One can then introduce the usual charge current $\boldsymbol{J}_c = \boldsymbol{J}_\uparrow + \boldsymbol{J}_\downarrow$ and the ⁂ *spin current* $\boldsymbol{J}_s = (\hbar/2e)\left(\boldsymbol{J}_\uparrow - \boldsymbol{J}_\downarrow\right)$ and ask for the linear response of these quantities when an electric field is applied. This response is quantified by the usual charge Hall conductivity σ^c_{xy} (previously σ_{xy}) and its analogue, the ⁂ *spin Hall conductivity* σ^s_{xy}. Because the ground state of $\hat{H}_{\text{KM}}$ is given by two filled Chern bands with opposite Chern numbers $C = \pm 1$, the charge Hall conductivity vanishes identically: $\sigma^c_{xy} = 0$ (this follows from our general discussion in Section 1.4.2). By contrast, the spin Hall conductivity is non-zero and quantized at $\sigma^s_{xy} = e/2\pi = 2 \times (\hbar/2e) \times e^2/h$ (because there are two counterpropagating edge modes with opposite spin, coming from the two Chern bands with opposite Chern number). The phenomenon of a quantized spin Hall conductivity (and vanishing charge Hall conductivity) is called ⁂ *quantum spin Hall effect (QSHE)* and characterized by the combined symmetry $U(1)_{\text{charge}} \times U(1)_{\text{spin}}$.
- It was a remarkable insight by Kane and Mele [111] that the two phases of the "Quantum Spin Hall effect in Graphene" [110] remained topologically distinct (via the Pfaffian index) *even without spin conservation* ($\lambda_R \neq 0$) – time-reversal symmetry is sufficient! This phase, protected by charge conservation $U(1)_{\text{charge}}$ and time-reversal symmetry $\mathbb{Z}_4^T$ [recall that $\tilde{T}_U^2 = -\mathbb{1}$ is equivalent to $\mathcal{T}_U^2 = (-1)^{\hat{N}_c}$, Section 2.1.2], and characterized by the Paffian $\mathbb{Z}_2$ index, is the *topological insulator (TI)* phase. Since spin conservation $U(1)_{\text{spin}}$ is generally broken in this phase, it is *not* characterized by a quantized spin Hall conductivity (= quantum spin Hall effect). One can indeed check that adding either TRS breaking terms *or* superconducting terms to the KM Hamiltonian $\hat{H}_{\text{KM}}$ on a cylinder *gaps out* the edge modes, indicating that the topological insulator is protected by TRS *and* charge conservation symmetry [94].

Thus, the *topological insulator (TI)* and the *quantum spin Hall (QSH) phase* are *different* symmetry-protected topological phases, and the KM model happens to realize both for $\lambda_R = 0$ [35]. [Remember (Section 0.5) that the classification of SPT phases depends on our choice of protecting symmetry!]

In the context of this (modern) terminology, the title of Kane and Mele's original paper "$\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect" [111] is confusing for two reasons: First, the paper is mostly about the topological insulator phase – and not the quantum spin Hall effect. The authors event point this out explicitly: *"The QSH phase is not generally characterized by a quantized spin Hall conductivity."* In addition, their notion of "topological order" does not match the modern terminology of "long-range entanglement." That is, Kane and Mele's topological insulator is the paradigmatic example of a *topological phase* that is *not* topologically ordered but *symmetry protected*.

3.5. ‡ Experiments

- The possibility to observe the quantum spin Hall effect (via a quantized ← *spin Hall conductance* that requires spin conservation, i.e., $\lambda_R = 0$) was predicted by BERNEVIG *et al.* in 2006 [118] and experimentally confirmed by KÖNIG *et al.* in 2007 [119] in so called ↑ HgTe *quantum wells* (HgTe = Mercury-Telluride).
- The alloy $Bi_{1-x}Sb_x$ (BiSb = Bismuth-Antimony) was predicted to be a (strong) topological insulator (in three dimensions) by FU and KANE in 2007 [97] which was experimentally confirmed by HSIEH *et al.* in 2008 [120].
- Following these first discoveries, many more materials were identified as topological insulators. For an extensive review including experimental results (before 2011) see QI and ZHANG [121].

Closing remarks for Chapters 1 to 3

We have now discussed two topological indices to label topological phases in two dimensions:

- The (first) *Chern number* classifies two-dimensional chiral topological phases (IQHE, QWZ model, Haldane model); we discussed these models in Chapters 1 and 2.
  - The Chern number *cannot* be generalized to three dimensions!
    (There are generalizations to *even* dimensions, though [122].)
  - For non-zero Chern numbers, time-reversal symmetry must be *broken*.
  - Phases of non-interacting fermions in bands with non-zero Chern numbers are examples of the ← *invertible topological orders* introduced in Section 0.5 [35].
- The $\mathbb{Z}_2$ *Pfaffian index* classifies symmetry-protected topological (SPT) phases in two dimensions (Kane-Mele topological insulator); we discussed this model in Chapter 3.
  - The Pfaffian index *can* be generalized to three dimensions and allows for the characterization of three-dimensional topological insulators [96, 100, 123].
  - For the Pfaffian index to be well-defined, time-reversal symmetry must be *preserved*.
  - The Kane-Mele topological insulator is a ← *short-range entangled* phase protected by time-reversal symmetry (and particle number/charge conservation) [35].

  We now turn to topological phases of non-interacting fermions in *one* dimension …