3. Topological Bands with Time-Reversal Symmetry: The Topological Insulator

This section is based on various sources. A detailed account can be found in Bernevig's textbook [1]. However, also the original papers by KANE and MELE [111,112] and FU and KANE [98,113] are accessible and worthwhile to read. The concept of vector bundles is discussed by CARPENTIER [114,115] from a physicists perspective; a more mathematical account is given by WEHEFRITZ-KAUFMANN [116]. The mathematical foundations underlying topological band theory (in particular the concepts of vector bundles and their characterization) are covered in the textbooks by NASH and SEN [117] and NAKAHARA [13].

We seek for models with the following properties:

- Lattice model
- Band insulator
- Time-reversal symmetric (!)
- Topological band structure (!)
  ¡! We do not call for *Chern bands* as we known that this is impossible without breaking time-reversal symmetry. So we need to look for another topological invariant …

Before we proceed, let us fix the nomenclature:

⁂ Definition: Topological insulator

$$\text{Topological insulator (TI)} := \begin{cases} \text{Lattice model} \\ \text{Band insulator} \\ \text{Topological band structure} \\ \text{Time-reversal symmetric} \end{cases} \tag{3.1}$$

Prototype: Kane-Mele model

With this definition, the question we want to answer is:

Are there topological insulators?

The term "topological insulator" is not used consistently in the literature. In particular, the above definition is only one of at least three:

- Sometimes "TI" refers specifically to the Kane-Mele model. This is usually the case when people talk about *the* topological insulator.

- Sometimes "TI" is used to denote the class of gapped free fermion theories with time-reversal symmetry, particle number conservation (to distinguish them from superconductors, → *later*) and topological bands. This is essentially our definition above.
- Sometimes "TI" refers to arbitrary band insulators with topological bands (then including also Chern insulators). This is how the term is used when referring to the class of *topological insulators & superconductors*. I.e., there the term "insulator" distinguishes models from "superconductors" (which violate particle number conservation) without referring to time-reversal symmetry.

So be aware of this when you study other sources.

3.1. Construction of the Kane-Mele model

1 | Starting point: ◁ Low-energy theory of ← *graphene*:

Recall that this is just the ← *Haldane model* for $m = 0 = t$ [Eq. (2.58)]:

$$H(\boldsymbol{K} + \boldsymbol{k}) = -\frac{\sqrt{3}}{2}(k_x\sigma^y - k_y\sigma^x) \tag{3.2a}$$

$$H(\boldsymbol{K}' + \boldsymbol{k}) = -\frac{\sqrt{3}}{2}(k_x\sigma^y + k_y\sigma^x) \tag{3.2b}$$

To translate into the conventions used in the original papers, we rotate in momentum space by $\pi/2$ so that $k_x \mapsto k_y$ and $k_y \mapsto -k_x$:

$$H(\boldsymbol{k}) := H(\boldsymbol{K} + \boldsymbol{k}) = -\frac{\sqrt{3}}{2}(k_x\sigma^x + k_y\sigma^y) \tag{3.3a}$$

$$H'(\boldsymbol{k}) := H(\boldsymbol{K}' + \boldsymbol{k}) = -\frac{\sqrt{3}}{2}(-k_x\sigma^x + k_y\sigma^y) \tag{3.3b}$$

2 | The low-energy physics is determined by momentum modes in the vicinity of $\boldsymbol{K}$ and $\boldsymbol{K}'$. We can therefore combine the two Bloch Hamiltonians by a direct sum (corresponding to the direct sum of low-energy single-particle momentum modes): →

$$\tilde{H}_0(\boldsymbol{k}) := H(\boldsymbol{k}) \oplus H'(\boldsymbol{k}) \tag{3.4a}$$

$$= v_F \begin{pmatrix} k_x\sigma^x + k_y\sigma^y & 0 \\ 0 & -k_x\sigma^x + k_y\sigma^y \end{pmatrix} \tag{3.4b}$$

$$= v_F(\sigma^x \otimes \tau^z\, k_x + \sigma^y \otimes \mathbb{1}\, k_y) \tag{3.4c}$$

$$\equiv v_F(\sigma^x\tau^z k_x + \sigma^y k_y) \tag{3.4d}$$

- σ^i: band DOF (mixes modes of upper/lower bands)
- τ^i: valley DOF (mixes modes between valleys $\boldsymbol{K}/\boldsymbol{K}'$)
- $v_F = -\sqrt{3}/2$: Fermi velocity

3 | Time-reversal:

Note that under time-reversal we have $\boldsymbol{K} + \boldsymbol{k} \mapsto -\boldsymbol{K} - \boldsymbol{k} = \boldsymbol{K}' - \boldsymbol{k}$ so that in the low-energy description time-reversal flips the valley DOF; this can be achieved by τ^x:

$$\tilde{T}_0 := \mathbb{1}_\sigma \otimes \tau^x\, \mathcal{K} \quad \text{with} \quad \tilde{T}_0^2 = +\mathbb{1} \tag{3.5}$$

$$\to \tilde{T}_0 \tilde{H}_0(\boldsymbol{k}) \tilde{T}_0^{-1} = \tilde{H}_0(-\boldsymbol{k})$$

The time-reversal operator of spinless graphene is simply $T_0 = \mathcal{K}$ (all terms in the Hamiltonian are real). The τ^x in Eq. (3.5) is a consequence of our low-energy description at the two Dirac points.

4 | Add Spin-$\frac{1}{2}$: Pauli matrices μ^i with $i = x, y, z$

This gives us more possibilities to add gap-opening terms to $\tilde{H}_0$. It is also physically motivated: electrons *do have* spin!

$$\tilde{H}_{\frac{1}{2}}(\boldsymbol{k}) := v_F(\sigma^x \otimes \mathbb{1}_\mu \otimes \tau^z k_x + \sigma^y \otimes \mathbb{1}_\mu \otimes \mathbb{1}_\tau k_y) \tag{3.6a}$$

$$\equiv v_F(\sigma^x \tau^z k_x + \sigma^y k_y) \tag{3.6b}$$

→ Bloch space $\mathcal{H}(\boldsymbol{k}) \simeq \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \simeq \mathbb{C}^8$

→ Time-reversal:

$$\tilde{T}_{\frac{1}{2}} := \mathbb{1}_\sigma \otimes \mu^y \otimes \tau^x \mathcal{K} \quad \text{with} \quad \tilde{T}_{\frac{1}{2}}^2 = -\mathbb{1} \tag{3.7}$$

→ $\tilde{T}_{\frac{1}{2}} \tilde{H}_{\frac{1}{2}}(\boldsymbol{k}) \tilde{T}_{\frac{1}{2}}^{-1} = \tilde{H}_{\frac{1}{2}}(-\boldsymbol{k})$

Note that this model is perfectly spin-degenerate: we "copied" the 4-band model $\tilde{H}_0$ to represent spin *up* and *down*, but didn't add any coupling between the two copies yet!

5 | Goal: Open topological gap by adding terms to $\tilde{H}_{\frac{1}{2}}(\boldsymbol{k})$:

At this point it is unclear what we mean by a "topological gap" (→ *below*).

The rationale is to use the linearized Bloch Hamiltonian for this construction because it is simpler. We can then later reconstruct a *lattice* model from the low-energy (= small momentum) Hamiltonian as we did for the QWZ model. The 8 bands of $\tilde{H}_{\frac{1}{2}}$ will therefore reduce again to 4 bands since the valley Hilbert space $\mathbb{C}^2$ does not exist for a true lattice model.

i | Observation I: Must contain σ^z!

Because otherwise we only shift the position of the Dirac points:

$$\tilde{H}(\boldsymbol{k}) = v_F[\sigma^x \tau^z k_x + \sigma^y k_y] + v_F(\delta_x \sigma^x \tau^z + \delta_y \sigma^y) \tag{3.8a}$$

$$= v_F[\sigma^x \tau^z (k_x + \delta_x) + \sigma^y (k_y + \delta_y)] \tag{3.8b}$$

$$= H(\underbrace{\boldsymbol{K} + \boldsymbol{\delta}}_{\boldsymbol{K}_\delta} + \boldsymbol{k}) \oplus H(\underbrace{\boldsymbol{K}' + \boldsymbol{\delta}}_{\boldsymbol{K}'_\delta} + \boldsymbol{k}) \tag{3.8c}$$

with $\boldsymbol{\delta} = (\delta_x, \delta_y)^T$. You can think of δ_x and δ_y as operators (products of Pauli matrices) that do not contain any σ^i matrices. Then Eq. (3.8a) is the most general modification *without* using σ^z. The argument that the cones are shifted but not gapped then applies within the eigenspaces of the operators δ_x and δ_y.

ii | We know already the Trivial mass term: [*cf.* Eq. (2.58) for $t = 0$]

$$\delta\tilde{H}_m(\boldsymbol{k}) = m\sigma^z \tag{3.9}$$

→

- ✓ Time-reversal invariant [since $\tilde{T}_{\frac{1}{2}} \delta\tilde{H}_m(\boldsymbol{k}) \tilde{T}_{\frac{1}{2}}^{-1} = \delta\tilde{H}_m(-\boldsymbol{k})$]
- ✓ Opens a gap of $2m$
- ✗ *But:* Bands are topologically trivial ☹

  They are "topologically trivial" because their Chern number vanishes. However, below we will derive a new topological invariant distinct from the Chern number, so that this statement seems short-sighted. The true argument is therefore that for $m \to \infty$ the

system is clearly a trivial band insulator where one sublattice is empty and the other completely filled; this phase is "trivial" in the original sense of being a product state. Then, no matter which topological invariant we cook up, to comply with our physically motivated notion of "trivial", it *must* vanish in the gapped phase dominated by $\delta\tilde{H}_m$.

→ So we should look for other gap opening terms …

iii | We also know the Haldane mass term:

$$\text{Eq. (2.58)} \quad \xrightarrow[m=0]{\varphi=-\pi/2} \quad \delta\tilde{H}_{\text{H}}(\boldsymbol{k}) = \tau^z\sigma^z\, 3\sqrt{3}\,t \tag{3.10}$$

Because of the valley encoding, we can now combine both Hamiltonians in Eq. (2.58) into a single expression with τ^z.

→ $\tilde{H}_{\text{H}} := \tilde{H}_{\frac{1}{2}} + \delta\tilde{H}_m + \delta\tilde{H}_{\text{H}}$ = two independent copies of the Haldane model (one for spin *up*, one for spin *down*)

→ Not TRI:

$$\tilde{T}_{\frac{1}{2}}\,\delta\tilde{H}_{\text{H}}(\boldsymbol{k})\tilde{T}_{\frac{1}{2}}^{-1} \neq \delta\tilde{H}_{\text{H}}(-\boldsymbol{k}) \quad ☹ \tag{3.11}$$

Of course you do not have to check this. Since the two copies of the Haldane model are independent, we can consider them separately. But each allows for bands with non-zero Chern numbers (this was the point!). But then the model must *break* TRS because we know that this is a necessary condition for non-zero Chern numbers in the first place (← Section 2.1.2).

iv | Observation II: Must contain spin-coupling that *anticommutes* with $\tilde{T}_{\frac{1}{2}}$!

→

$$\delta\tilde{H}_{\text{KM}}(\boldsymbol{k}) := \lambda_{\text{SO}}\,\sigma^z \otimes \mathbb{1}_\mu \otimes \tau^z \qquad \propto \delta\tilde{H}_{\text{H}} \quad \to \text{Not TRI} \quad ✗ \tag{3.12a}$$

$$\delta\tilde{H}_{\text{KM}}(\boldsymbol{k}) := \lambda_{\text{SO}}\,\sigma^z \otimes \mu^{\{x,y,z\}} \otimes \mathbb{1}_\tau \qquad \to \text{Not TRI} \quad ✗ \tag{3.12b}$$

$$\delta\tilde{H}_{\text{KM}}(\boldsymbol{k}) := \lambda_{\text{SO}}\,\sigma^z \otimes \mu^{\{x,y,z\}} \otimes \tau^z \qquad \to \text{TRI} \quad ✓ \tag{3.12c}$$

→ ⁂ *Kane-Mele mass term*

- Couples "orbital" DOFs (τ^z) with spin DOFs (μ^z)

  → Discrete version of ↓ *Spin-orbit coupling (SO)*
- $\delta\tilde{H}_{\text{KM}}(\boldsymbol{k})$ is just Haldane's TRS breaking term $\tau^z\sigma^z\, 3\sqrt{3}t\,\sin(\varphi)$ augmented by spin-orbit coupling to "recover" time-reversal symmetry.
- The choice of μ^z is arbitrary since all μ^i anticommute with $\tilde{T}_{\frac{1}{2}}$. It is just conventional to think in the z-basis for spin (*i.e.*, spin "up" and "down" now have conjugate imaginary hopping phases). Note also that on its own, μ^z is interchangeable with the other Pauli matrices by permutations (or spin rotations) without changing the spin-algebra.

6 | Kane-Mele model:

Low-energy description:

$$\tilde{H}'_{\text{KM}}(\boldsymbol{k}) := \tilde{H}_{\frac{1}{2}}(\boldsymbol{k}) + \delta\tilde{H}_m(\boldsymbol{k}) + \delta\tilde{H}_{\text{KM}}(\boldsymbol{k}) \tag{3.13}$$

$\overset{\circ}{\rightarrow}$ Reconstruction of the Full lattice model:

$$\hat{H}'_{\mathrm{KM}} = \overbrace{\sum_{\langle i,j\rangle,\alpha} c^\dagger_{i\alpha} c_{j\alpha}}^{\triangleq \tilde{H}_{\frac{1}{2}}(\boldsymbol{k})} + \overbrace{m \sum_{i,\alpha} \epsilon_i c^\dagger_{i\alpha} c_{i\alpha}}^{\triangleq \delta\tilde{H}_m(\boldsymbol{k})} + \overbrace{\lambda_{\mathrm{SO}} \sum_{\langle\langle i,j\rangle\rangle,\alpha,\beta} i\eta_{ji}\, c^\dagger_{i\alpha} \mu^z_{\alpha\beta} c_{j\beta}}^{\triangleq \delta\tilde{H}_{\mathrm{KM}}(\boldsymbol{k})} \tag{3.14}$$

Spinful graphene | Staggered potential | Complex NNN hopping *with SO coupling*

$c^\dagger_{i\alpha}$: Creates fermion with spin $\alpha \in \{\uparrow, \downarrow\}$ on site i

- Note that the phase in the Kane-Mele term is the phase $e^{i\eta_{ij}\varphi}$ of the Haldane term for $\varphi = -\pi/2$.
- If you don't believe this, you can retrace our path to derive the Dirac Hamiltonian for the Haldane model again for the Kane-Mele model to derive $\tilde{H}'_{\mathrm{KM}}(\boldsymbol{k})$ in Eq. (3.13) from Eq. (3.14).
- The model (3.14) (together with the Rashba term → *below*) was introduced by C. L. KANE and E. J. MELE in 2005 [111, 112] under the name *Quantum spin Hall effect* as a time-symmetric generalization of Haldane's ← *Chern insulator* discussed in Chapter 2 (the designation "Quantum spin Hall effect" is a bit misleading and subtle, see comments at the end of Section 3.4).

7 | Observation III: $\hat{H}'_{\mathrm{KM}}$ does *not* mix spin:

$$\left[\hat{H}'_{\mathrm{KM}}, N_\alpha\right] = 0 \quad \text{with} \quad N_\alpha := \sum_i c^\dagger_{i\alpha} c_{i\alpha} \tag{3.15}$$

→ $\hat{H}'_{\mathrm{KM}}$ = two *decoupled* copies of the Haldane model with opposite complex phases

Note that this rather trivial construction already fixed the breaking of time-reversal symmetry because the two copies map onto each other under time reversal. However …

→ Not generic

Mixing of up and down spins can happen, *e.g.*, by applying an electric field perpendicular to the plane. The conservation of spin should not be necessary for the system to be time-reversal symmetric. That is, the model H'_{KM} is a bit too symmetric …

→ Add term that *breaks* the unitary symmetry generated by N_α (but preserves TRS)

8 | Rashba term:

There is indeed another SO coupling term that does not break TRS known as
⁂ *Rashba spin-orbit coupling*:

$$\delta\tilde{H}_{\mathrm{R}}(\boldsymbol{k}) := \lambda_R \left[\sigma^x \mu^y \tau^z - \sigma^y \mu^x\right] \tag{3.16}$$

→ $\tilde{T}_{\frac{1}{2}} \delta\tilde{H}_{\mathrm{R}}(\boldsymbol{k}) \tilde{T}^{-1}_{\frac{1}{2}} = \delta\tilde{H}_{\mathrm{R}}(-\boldsymbol{k})$

- Does not open a gap (missing σ^z) …
- … but *modifies* the gap generated by the Kane-Mele term.
- *Breaks* spin conservation (the ↑ and ↓ sectors no longer decouple)

This type of SO coupling in 2D systems was first studied by Y. A. BYCHKOV and E. I. RASHBA in 1984 [118], *i.e.*, long before the discovery of the Kane-Mele model.

$\overset{\circ}{\rightarrow}$ We make the KM model more generic by adding the Rashba term:

$$\hat{H}_{\mathrm{KM}} := \hat{H}'_{\mathrm{KM}} + \overbrace{\underbrace{\lambda_R \sum_{\langle i,j\rangle,\alpha,\beta} c^\dagger_{i\alpha} R^{\alpha\beta}_{ij} c_{j\beta}}_{\text{NN hopping with Rashba SO coupling}}}^{\triangleq \delta \tilde{H}_R(\boldsymbol{k})} \tag{3.17}$$

with

$$R^{\alpha\beta}_{ij} \triangleq i \left[(\vec{\mu} \times \vec{d}_{ij}) \cdot \hat{e}_z \right]_{\alpha\beta} \tag{3.18}$$

$\vec{d}_{ij}$: vector from site i to site j (in the x-y-pane)

$\vec{\mu} = (\mu^x, \mu^y, \mu^z)$: vector of spin matrices

$\hat{e}_z$: unit vector in z-direction

- Note that $(\vec{\mu} \times \vec{d}_{ij})_z = \mu^x d^y_{ij} - \mu^y d^x_{ij}$ is a Hermitian 2×2 matrix.
- Because of the μ^x and μ^y in the Rashba term, it is now $[\hat{H}_{\mathrm{KM}}, N_\alpha] \neq 0$ so that $\hat{H}_{\mathrm{KM}}$ can no longer be interpreted as a sum of two independent Haldane models.
- The direction-dependent phase and spin-coupling of the *Kane-Mele term* can be encoded in a similar form (for the fixed hopping phase $\varphi = -\pi/2$):

$$H^{\alpha\beta}_{ij} := e^{\eta_{ij} i\varphi} \mu^z_{\alpha\beta} = -i\eta_{ij} \mu^z_{\alpha\beta} \triangleq i\, 2\sqrt{3} \left[(\vec{d}_{ik} \times \vec{d}_{kj}) \cdot \vec{\mu} \right]_{\alpha\beta} \tag{3.19}$$

  where k denotes the site that is *skipped* when jumping from i to the next-nearest neighbour j.
- You can think of the Rashba term being induced by an *electric* field perpendicular to the 2D system. Then electrons hopping from one site to another experience an *in-plane magnetic field* (remember you course on ↓ *electrodynamics*) which couples to the magnetic moment induced by the spin via μ^x- and μ^y-components. The direction of the magnetic field depends on the direction the electron hops, which explains the directional dependence in Eq. (3.18).

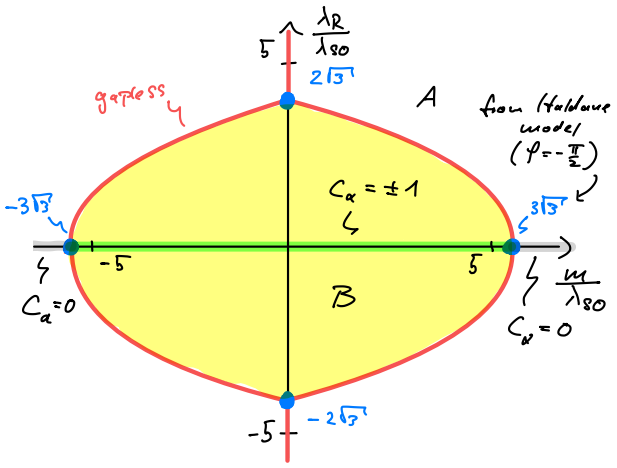
3.2. Phase diagram

We are now ready to sketch the phase diagram of $\hat{H}_{\mathrm{KM}}$ by identifying the *gapped phases* in parameter space and the *gapless phase transitions* that separate them:

1 | Gap closings:

We have three parameters (in units of the graphene hopping strength). For simplicity, we fix the Kane-Mele term λ_{SO} and plot the gap closings in the λ_R-m-plane:

$\prec 0 < \lambda_{SO} = \text{const} \ll 1$:



- The gapless values on the m-axis follow directly from our discussion of the Haldane model with $\varphi = -\pi/2$.
- Note that there are two gapless lines emanating from region B along the λ_R-axis. These divide region A, which must be the trivial phase (because it contains the limit $m \to \pm\infty$ in which the system is clearly in a product state). As before, one can connect these two halves of region A without crossing the gapless line on the γ_R-axis by extending the Hamiltonian appropriately, *i.e.*, there is only *one* (trivial) phase A.
- To derive the full plot, you must Fourier transform $\hat{H}_{\text{KM}}$ on a periodic lattice to derive the 4×4-Bloch Hamiltonian,

$$\tilde{H}_{\text{KM}}(\boldsymbol{k}) = \sum_{i=1}^{5} d_i(\boldsymbol{k})\Gamma_i + \sum_{i<j=1}^{5} d_{ij}(\boldsymbol{k})\Gamma_{ij} \tag{3.20}$$

  which is generated by (at most) 15 terms which take the place of the three-component Bloch vector $\vec{d}(\boldsymbol{k})$ for models with two bands. Recall that $n \times n$ Hamiltonians (with vanishing trace) generate unitaries in the group $\text{SU}(n)$ which has $n^2 - 1$ generators; *e.g.*, 3 Pauli matrices for $n = 2$ or 15 Γ-matrices for $n = 4$. The generators for $n = 4$ satisfy $\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}$ and $\Gamma_{ij} = 1/2i\,[\Gamma_i, \Gamma_j]$ with $i, j \in \{1, \ldots, 5\}$. See [112] for the expressions for d_i and d_{ij}.

2 | $\prec \underline{\lambda_R = 0}$ (m-axis in the above plot)

→ Spin-sectors decouple

→ Chern number C_α of spin-polarized sub-bands well-defined →

$$I^* := \frac{C_\uparrow - C_\downarrow}{2} \mod 2 = \begin{cases} 1 & \text{topologial phase of Haldane model(s)} \\ 0 & \text{trivial phase of Haldane model(s)} \end{cases} \tag{3.21}$$

Note that the *sum* $C_\uparrow + C_\downarrow = 0$ of the filled bands is zero everywhere because of TRS!

→ *Suggests* that Phase B is in some sense topological. (Phase A is a trivial insulator.)

→ *Not* characterized by I^* since I^* requires spin-conservation, whereas the phase is stable against perturbations that violate spin-conservation (like the Rashba term).

→ What characterizes Phase B?

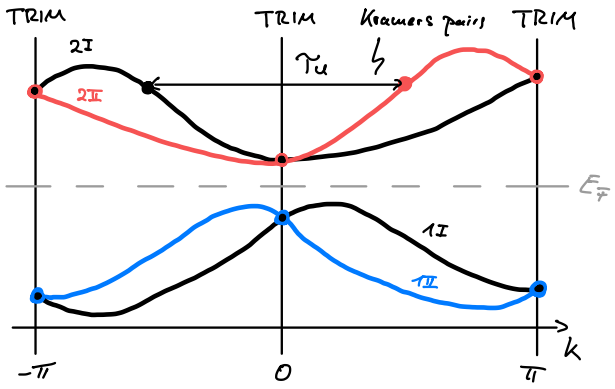
3.3. Vorticity of the Pfaffian and the $\mathbb{Z}_2$-Index

So what is the label that distinguishes the two phases of the Kane-Mele model?
We need a *new topological index* that replaces the Chern number …

3 | ◁ TRI system with $\tilde{T}_U^2 = -\mathbb{1}$ → Band crossings at TRIMs
TRIM ≡ ⁂ *Time-reversal invariant momentum*

$$\boldsymbol{K}^* \in T^2 \,:\, \text{TRIM} \;\Leftrightarrow\; -\boldsymbol{K}^* = \boldsymbol{K}^* + \boldsymbol{G}\,,\quad \boldsymbol{G}\,:\,\text{reciprocal lattice vector} \tag{3.22}$$

→ Generic bandstructure of TRI System in 1D with $\tilde{T}_U^2 = -\mathbb{1}$:

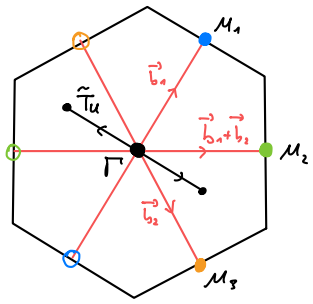


◁ Gapped system → *Even* number $2n$ of filled bands

- Note that time-reversal symmetry (irrespective of $T_U^2 = \pm\mathbb{1}$) implies the $\boldsymbol{k} \leftrightarrow -\boldsymbol{k}$ symmetry of the spectrum [← Eq. (2.33)]. However, this does *not* imply a degeneracy at the TRIMs! (Think of free fermions on a lattice.)
- If $T_U^2 = -\mathbb{1} \;\Leftrightarrow\; \tilde{T}_U^2 = -\mathbb{1}$, ← *Kramers theorem* (← Section 2.1.2, ➲ Problemset 6) applies to the single-particle Hamiltonian, $T_U\, H\, T_U^{-1} = H$, and demands a two-fold degeneracy for *every* eigenenergy. At the TRIMs, this necessitates a crossing band; hence all bands come in pairs!
- For the Bloch Hamiltonians $H(\boldsymbol{k})$, Kramers theorem does *not* apply in general, since TRI requires $\tilde{T}_U\, H(\boldsymbol{k}) \tilde{T}_U^{-1} = H(-\boldsymbol{k})$ which is *not* a symmetry of $H(\boldsymbol{k})$. Only at the TRIMs we have $\tilde{T}_U\, H(\boldsymbol{K}^*) \tilde{T}_U^{-1} = H(-\boldsymbol{K}^*) = H(\boldsymbol{K}^* + \boldsymbol{G}) = H(\boldsymbol{K}^*)$ so that Kramers theorem implies a two-fold degeneracy *in the Bloch space* of a TRIM $\boldsymbol{K}^*$. This is another perspective on the band crossings at the TRIMs.
- Note that the Kamers pairs of bands (I and II) *can* be degenerate everywhere in the BZ (for the Kane-Mele model they are perfectly degenerate for $\lambda_R = 0 = m$). TRI only requires this degeneracy at the TRIMs but does not exlude it elsewhere.

In particular, there are …

Four TRIMs for the hexagonal lattice:



4 | ◁ Matrix of $\tilde{T}_U$ on occupied Bloch space $\mathcal{H}_{\boldsymbol{k}}^{\text{filled}} := \text{span}\,\{|u_i(\boldsymbol{k})\rangle\}_{i=1\ldots 2n}$

Here, i, j run over the occupied bands. For the 4-band Kane-Mele model, this means $i, j \in \{1, 2\}$ which correspond to the filled lower bands of the spin-up and -down copy of the Haldane model (for $\lambda_R = 0$).

$$\begin{aligned} M_{ij}(\boldsymbol{k}) &:= \langle u_i(\boldsymbol{k})|\tilde{T}_U|u_j(\boldsymbol{k})\rangle && \text{(3.23a)}\\ &= \langle u_i(\boldsymbol{k})|U u_j^*(\boldsymbol{k})\rangle && \text{(3.23b)}\\ &= -\langle U^* u_i(\boldsymbol{k})|u_j^*(\boldsymbol{k})\rangle && \text{(3.23c)}\\ &= -\langle u_j(\boldsymbol{k})|U u_i^*(\boldsymbol{k})\rangle && \text{(3.23d)}\\ &= -\langle u_j(\boldsymbol{k})|\tilde{T}_U|u_i(\boldsymbol{k})\rangle && \text{(3.23e)}\\ &\overset{\circ}{=} -M_{ij}^T(\boldsymbol{k}) && \text{(3.23f)} \end{aligned}$$

Here we used $U^\dagger = (U^*)^T$ and $U^T = -U$ since $\tilde{T}_U^2 = \tilde{T}_{\frac{1}{2}}^2 = -\mathbb{1}$ with $\tilde{T}_{\frac{1}{2}} = \mathbb{1}_\sigma \otimes \mu^y\, \mathcal{K}$.

- The matrix $M(\boldsymbol{k})$ is Gauge-dependent (= depends on chosen basis of $\mathcal{H}_{\boldsymbol{k}}^{\text{filled}}$)
- For every $\boldsymbol{k} \in T^2$, $M(\boldsymbol{k})$ is a Skew-symmetric matrix of even dimensions

  (Remember that TRI demands an even number of filled bands.)

↓ **Lecture 12** [23.05.25]

5 | → ◁ Pfaffian:

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

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

Cf. the ↓ *Leibniz formula* for determinants:

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

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

- $(\text{Pf}[M])^2 = \det(M)$, *i.e.*, the Pfaffian contains the same information as the determinant (but with an additional sign that is lost when considering the determinant).
- $\text{Pf}\left[BAB^T\right] = \det(B)\,\text{Pf}[A]$ 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!).