1.3 Topological bands with time-reversal symmetry:

The quantum spin Hall effect

We seek models with

* Lattice models
* Band insulator (non-interacting)
* Time-reversal symmetric (!)
* Topological band structure (!) $\rightsquigarrow$ We'll need a new top. invariant!

Definition: Topological Insulator:

$$\text{Topological Insulator (TI)} = \left\{ \begin{array}{l} \text{Lattice model} \\ \text{Band insulator} \\ \text{Topological bands} \\ \text{Time-reversal symmetry} \end{array} \right.$$

Careful, there are other definitions of "TI"!

$\boxed{\text{Are there topological insulators?}}$

1.3.1. Construction of the Kane-Mele model

1. Starting point: Low-energy theory of graphene $m = 0 = t$:

$$H(\vec{K}+\vec{k}) = -\frac{\sqrt{3}}{2}\left(k_x\sigma^y - k_y\sigma^x\right)$$

$$H(\vec{K}'+\vec{k}) = -\frac{\sqrt{3}}{2}\left(k_x\sigma^y + k_y\sigma^x\right)$$

Rotation by $\frac{\pi}{2}$: $\quad k_x \mapsto k_y \,,\; k_y \mapsto -k_x$

$$H(\vec{k}) := H(\vec{K}+\vec{k}) = -\frac{\sqrt{3}}{2}\left(k_x\sigma^x + k_y\sigma^y\right)$$

$$H'(\vec{k}) := H(\vec{K}'+\vec{k}) = -\frac{\sqrt{3}}{2}\left(-k_x\sigma^x + k_y\sigma^y\right)$$

$\rightarrow \quad \tilde{H}_0(\vec{k}) := H(\vec{k}) \oplus H'(\vec{k})$

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

$$= v_F \left(\sigma^x \otimes \tau^z k_x + \sigma^y \otimes \mathbb{1}_\tau k_y \right)$$

$$= v_F \left(\sigma^x \tau^z k_x + \sigma^y k_y \right)$$

σ^i: band DOF (mixes upper/lower bands)

τ^i: valley DOF (mixes modes between $\vec{K}, \vec{K}'$)

$v_F = -\frac{\sqrt{3}}{2}$: Fermi velocity

Time reversal symmetry: $\vec{k}+\vec{u} \to -\vec{k}-\vec{u} = \vec{k}'-\vec{u}$

$$\tilde{T}_0 := \mathbb{1}_\sigma \otimes \tau^x \mathcal{K} \to \tilde{T}_0^2 = +\mathbb{1}$$

$$\to \quad \tilde{T}_0 \tilde{H}_0(\vec{u}) \tilde{T}_0^{-1} = \tilde{H}_0(-\vec{u})$$

2. Add spin-$\frac{1}{2}$: Pauli matrice μ^i, $i = x, y, z$

$$\tilde{H}_{\frac{1}{2}}(\vec{u}) = v_F \left(\sigma^x \otimes \mathbb{1}_\mu \otimes \tau^z u_x + \sigma^y \otimes \mathbb{1}_\mu \otimes \mathbb{1}_\tau u_y \right)$$

$$= v_F \left(\sigma^x \tau^z u_x + \sigma^y u_y \right)$$

$\to$ Bloch space $\mathcal{H}(\vec{u}) \simeq \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \simeq \mathbb{C}^8$

$\to$ Time reversal: $\boxed{\tilde{T}_{\frac{1}{2}} = \mathbb{1}_\sigma \otimes \mu^y \otimes \tau^x K \quad \text{with} \quad \tilde{T}_{\frac{1}{2}}^2 = -\mathbb{1}}$

$$\to \quad \tilde{T}_{\frac{1}{2}} H_{\frac{1}{2}}(\vec{u}) \tilde{T}_{\frac{1}{2}}^{-1} = \tilde{H}_{\frac{1}{2}}(-\vec{u})$$

3. <u>Goal:</u> Open topological gap by adding terms to $\tilde{H}_{\frac{1}{2}}(\vec{k})$:

a) Observation I: Must contain σ^z!

Otherwise we only shift the Dirac points:

$$\tilde{H}(\vec{k}) = v_F(\sigma^x\tau^z k_x + \sigma^y k_y) + v_F(\delta_x \sigma^x\tau^z + \delta_y\sigma^y)$$

$$= v_F\left[\sigma^x\tau^z(k_x+\delta_x) + \sigma^y(k_y+\delta_y)\right]$$

$$= H(\underbrace{\vec{k}+\vec{\delta}}_{\vec{k}_\delta}+\vec{q}) \oplus H(\underbrace{\vec{k}'+\vec{\delta}}_{\vec{k}_\delta'}+\vec{q}')$$

$\delta = (\delta_x, \delta_x)^T$

b) <u>Trivial mass term:</u> $\delta\tilde{H}_m(\vec{k}) = m\sigma^z$

* TRI: $\tilde{T}_{\frac{1}{2}}\,\delta\tilde{H}_m(\vec{k})\,\tilde{T}_{\frac{1}{2}}^{-1} = \delta\tilde{H}_m(\vec{k})$
* Opens gap of $2m$

* **But:** Bands are topologically trivial !

c) **Haldane mass term** $\left(\varphi = -\frac{\pi}{2}\right)$

$$\delta \tilde{H}_H(\vec{k}) = \tau^z \sigma^z \, 3\sqrt{3}\, t$$

$\rightarrow$ $\tilde{H}_H := \tilde{H}_{\frac{1}{2}} + \delta \tilde{H}_m + \delta \tilde{H}_H$ = two independent copies of the Haldane model

$\rightarrow$ Not TRI: $\tilde{T}_{\frac{1}{2}} \, \delta \tilde{H}_H(\vec{k}) \, \tilde{T}_{\frac{1}{2}}^{-1} \neq \delta \tilde{H}_H(-\vec{k})$

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

$\rightarrow$ $$\boxed{\delta \tilde{H}_{KM}(\vec{k}) := \lambda_{SO} \, \sigma^z \otimes \underbrace{\mu^z \otimes \tau^z}_{\text{Spin orbit coupling}} \rightarrow \text{TRI} \checkmark}$$

$\rightarrow$ Kane-Mele mass term

4. Kane-Mele model

Low energy description: $\tilde{H}'_{KM}(\vec{u}') := \tilde{H}_{\frac{1}{2}}(\vec{u}') + \delta\tilde{H}_{m}(\vec{u}') + \delta\tilde{H}_{KM}(\vec{u}')$

→ Full lattice model:

$$\boxed{\hat{H}'_{KM} = \underbrace{\sum_{\substack{\langle i,j\rangle,\alpha \\ (\text{spin } \uparrow,\downarrow)}}' c^{\dagger}_{i\alpha} c_{j\alpha}}_{\text{Spinful graphene}} + \underbrace{m \sum_{i,\alpha} \varepsilon_i c^{\dagger}_{i\alpha} c_{i\alpha}}_{\text{Staggered potential}} + \underbrace{\lambda_{SO} \sum_{\langle\langle i,j\rangle\rangle,\alpha,\beta} i\eta_{ji}\, c^{\dagger}_{i\alpha} \mu^{z}_{\alpha\beta} c_{j\beta}}_{\substack{\text{Complex NNN hopping} \\ \text{with SO coupling}}}}$$

5. Observation III: $[\hat{H}'_{KM}, N_\alpha] = 0$ with $N_\alpha := \sum_i c^{\dagger}_{i\alpha} c_{i\alpha}$

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

→ Not generic

→ Add term that breaks the unitary symmetry generated by N_α

6. Rashba term:

$$\delta \tilde{H}_R(\vec{u}) := \lambda_R \left[\sigma^x \mu^y \tau^z - \sigma^y \mu^x \right]$$

$$\rightarrow \tilde{T}_{\frac{1}{2}} \, \delta \tilde{H}_R(\vec{u}) \, \tilde{T}_{\frac{1}{2}}^{-1} = \delta H_R(-\vec{u})$$

$$\rightarrow \quad \hat{H}_{KM} := \hat{H}'_{KM} + \lambda_R \sum_{\langle i,j \rangle, \alpha, \beta} c^{\dagger}_{i\alpha} R^{\alpha\beta}_{ij} c_{j\beta}$$

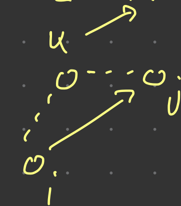
with

$$R^{\alpha\beta}_{ij} \hat{=} i \left[\left(\vec{\mu} \times \underbrace{\vec{d}_{ij}}_{\text{vector from site } i \text{ to site } j} \right) \cdot \overbrace{\hat{e}_z}^{\text{unit vector in } z \text{ direction}} \right]_{\alpha\beta}$$

$$\rightarrow \left[\hat{H}_{KM}, N_\alpha \right] \neq 0$$

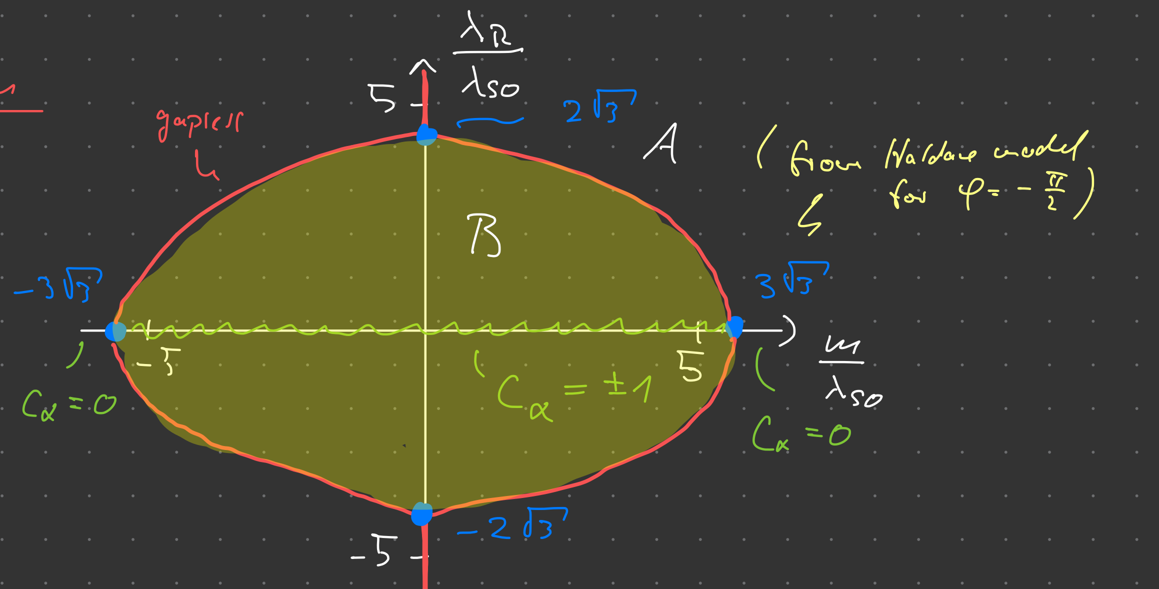
Note: Kane-Mele term: $\sum_{\langle\langle i,j\rangle\rangle,\alpha,\beta} c^\dagger_{i\alpha} H^{\alpha\beta}_{ij} c_{j\beta}$

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



1.3.2. Phase diagram

1. Gap closing:



2. $\measuredangle\ \lambda_R = 0 \rightarrow$ Spin-sectors decouple

$\rightarrow$ Chern number C_α of spin-polarized sub-bands well defined

$\rightarrow$
$$I^* := \frac{C_\uparrow - C_\downarrow}{2} \bmod 2 = \begin{cases} 1 & \text{in phase B} \\ 0 & \text{in phase A} \end{cases}$$

$$C_\uparrow + C_\downarrow \overset{\text{TRI}}{=} 0$$

$\rightarrow$ Suggests that phase B topological (Phase A is trivial.)

$\rightarrow$ Not characterized by I^*

$\rightarrow$ What characterizes phase B?

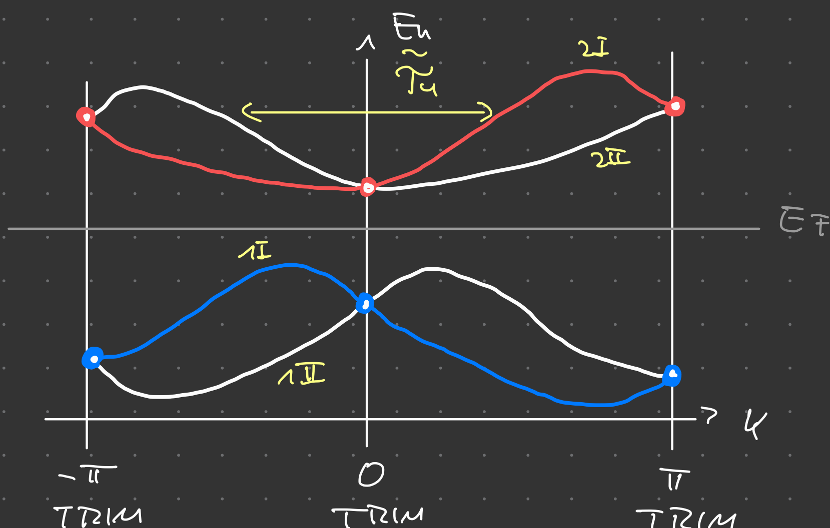
1.3.3 Vorticity of the Pfaffian and the $\mathbb{Z}_2$ index

1. $\exists$ TRI system with $\tilde{T}_u^2 = -\mathbb{1}$ $\rightarrow$ Band crossings at TRIMs

TRIM = Time-reversal invariant momentum

$\vec{k}^* \in T^2$ TRIM $\Leftrightarrow$ $-\vec{k}^* = \vec{k}^* + \vec{G}$, $\vec{G}$: reciprocal lattice vector

$\rightarrow$ Generic bandstructure of TRI system in 1D:



Note:

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

$\tilde{T}_u H(k^*) \tilde{T}_u^{-1} = H(-k^*)$

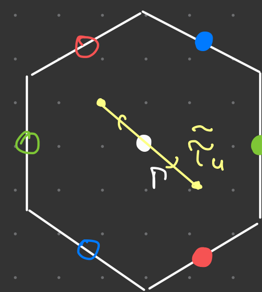
$= H(k^* + G)$

$= H(k^*)$

$\longrightarrow$ $\exists$ Gapped system

$\rightarrow$ Even number $2n$ of filled bands

Four TRIMs of hexagonal lattice:



$\rightsquigarrow$ 4 TRIMs

2. & Matrix of $\tilde{T}_u$ on occupied Bloch space $\mathcal{H}^{\text{filled}}_{\vec{k}'} = \text{span}\{ |u_i(\vec{k}')\rangle \}_{j}$

$i = 1 \dots 2n$

$$\mathcal{M}_{ij}(\vec{k}') := \langle u_i(\vec{k}') | \tilde{T}_u | u_j(\vec{k}') \rangle$$

depends on basis of $\mathcal{H}_u^{\text{filled}}$

$\hookrightarrow$

$U^T = -U$, $\tilde{T}_u^2 = -1$

$$= \langle u_i(k) | U | u_j^*(k) \rangle$$

$$= - \langle U^* u_i(k) | u_j^*(k) \rangle$$

$$= - \langle u_j(k) | U u_i^*(k) \rangle$$

$$= - \langle u_j(k) | \tilde{T}_u | u_i(k) \rangle$$

$$= - \mathcal{M}_{ij}^T(k)$$

* Gauge dependent

* $\mathcal{M}(k)$ skew-symmetric matrix of even dimension $(2n \times 2n)$

Def. Pfaffian

M : $2n \times 2n$ skew-symmetric matrix

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

* $\left(\mathrm{Pf}[M]\right)^2 = \det(M)$
* $\mathrm{Pf}[BAB^T] = \det(B) \cdot \mathrm{Pf}[A]$

B: arbitrary matrix

$\rightarrow$ $P : T^2 \rightarrow \mathbb{R}$, $\quad P(\vec{k}) = \mathrm{Pf}[M(\vec{k})]$

Wave-Model: $\quad P(\vec{k}) = M_{12}(\vec{k}) = \langle u_1(\vec{k}) | \tilde{T}_{\frac{1}{2}} | u_2(\vec{k}) \rangle$

3. Properties of $\mathcal{P}(\vec{u})$:

* Not gauge invariant: $\measuredangle\ U \in U(24)$ and $|u_i'(u)\rangle := U_{ij}|u_j(u)\rangle$

Basis transformation on $\mathcal{H}_u^{\text{filled}}$

$U = e^{i\phi}\tilde{U}$ with $\tilde{U} \in SU(24)$:

$$\mathcal{P}'(u) = \mathrm{Pf}\left[\left(\langle u_i'(u)|\tilde{T}_u|u_j'(u)\rangle\right)_{ij}\right]$$

$$= \mathrm{Pf}\left[\left(U_{ii'}^* \langle u_{i'}(u)|\tilde{T}_u|u_{j'}(u)\rangle U_{jj'}^*\right)_{ij}\right]$$

$$= \mathrm{Pf}\left[U^* \left(\langle u_{i'}(u)|\tilde{T}_u|u_{j'}(u)\rangle\right)_{i'j'} (U^*)^T\right]$$

$$= \det(U^*)\,\mathcal{P}(u)$$

$$= e^{-i24\phi}\,\mathcal{P}(u)$$

$\to$ $|\mathcal{P}(u)|$ is gauge invariant

Note:

$$|\Psi_0'\rangle = \prod_k \prod_i c'^{\dagger}_{k,i}|0\rangle = \prod_k \prod_i U_{ij}\, c^{\dagger}_{k,j}|0\rangle$$

$\{c^{\dagger}_{ki}, c^{\dagger}_{kj}\}=0$

$$= \prod_k \det(U) \prod_i c^{\dagger}_{k,i}|0\rangle = e^{i\chi} \prod_k \prod_i c^{\dagger}_{ki}|0\rangle = e^{i\chi}|\Psi_0\rangle$$

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* TRS

→ Chern number of the valence bundle $\mathcal{H}_k^{\text{filled}}$ vanishes

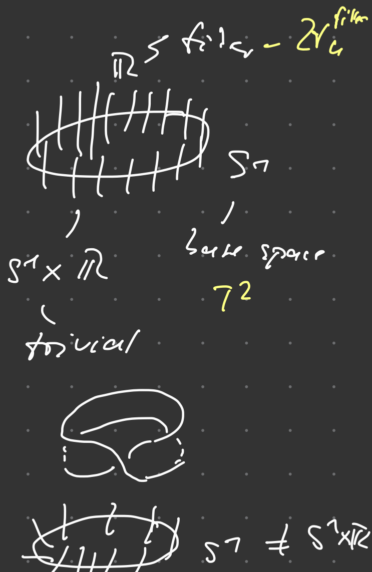
→ $\mathcal{H}_k^{\text{filled}}$ = trivial vector bundle

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

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

* $|e_i(k)\rangle$: globally continuous basis (e.g. not eigenbasis of $H(k)$)

* $|u_i(k)\rangle$: eigenbasis of $H(k)$ (not nec. continuous on T^2)



* $\exists$ Two subspaces of Bloch Hamiltonians:

- $\mathcal{H}_u^{\text{filled}}$ even $:\Leftrightarrow$ $\tilde{T}_u \mathcal{H}_u^{\text{filled}} = \mathcal{H}_u^{\text{filled}}$

$\rightarrow$ $|P(u)| = |\mathrm{Pf}[M(u)]| = \sqrt{|\det(M(u))|} \underline{\underline{= 1}}$

unitary $M \neq 0$

$\tilde{T}_u |u_i(u)\rangle = M_{ij} |u_j(u)\rangle$

- $\mathcal{H}_u^{\text{filled}}$ odd $:\Leftrightarrow$ $\tilde{T}_u \mathcal{H}_u^{\text{filled}} \perp \mathcal{H}_u^{\text{filled}}$

$\rightarrow$ $|P(u)| = |\mathrm{Pf}[M(u)]| \underline{\underline{= 0}}$

$\langle u_j(u) | \tilde{T}_u | u_i(u) \rangle = M_{ij} = 0$

Remember: $\mathcal{H}_u = \mathcal{H}_u^{\text{filled}} \oplus \mathcal{H}_u^{\text{empty}}$

* <u>Observation:</u> K^* TRIM $\rightarrow$ $\mathcal{H}_{K^*}^{\text{filled}}$ is even since

$$\tilde{T}_u H(u^*) \tilde{T}_u^{-1} = H(u^*)$$

$$\boxed{\rightarrow |P(u^*)| = 1 \text{ at all TRIMS } K^*}$$

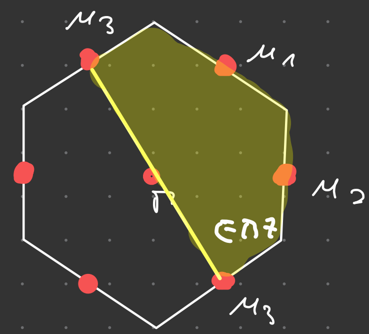
* <u>Effective Brillouin Zone = EBZ</u>

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

→ Defining $H(k)$ on <u>half</u> the BZ is sufficient

→ EBZ = subset T^2 such that it never contains k and $-k$ (except for the boundaries)

<u>Example:</u>



* EBZ not unique

* Topology of a cylinder

→ Consequence for $P(k)$:

$$\tilde{T}_u H(k) \tilde{T}_u^{-1} = H(-k) \Rightarrow \tilde{T}_u \mathcal{H}_k^{\text{filled}} = \mathcal{H}_{-k}^{\text{filled}}$$

$$\Rightarrow |e_i(-k)\rangle = w_{ij}^*(k) \cdot \tilde{T}_u |e_j(k)\rangle$$

$\omega_{ij}(k) = \langle e_i(-k) | \tilde{T}_k | e_j(k) \rangle$: unitary sewing matrix

$\rightarrow$

$$\underline{P(-k)} = \mathrm{Pf}[\mathcal{M}(-k)]$$

$$= \mathrm{Pf}\left[\left(\langle e_i(-k) | \tilde{T}_k | e_j(-k) \rangle\right)_{ij}\right]$$

$$= \mathrm{Pf}\left[\left(\omega_{ii'}(k) \langle \tilde{T}_k e_{i'}(k) | \underbrace{\tilde{T}_k \, \tilde{T}_k}_{-1} e_{j'}(k) \rangle \, \omega_{jj'}(k)\right)_{ij}\right]$$

$$= (-1)^k \, \mathrm{Pf}\left[\left(\omega_{jj'}(k) \langle e_{j'}(k) | \tilde{T}_k | e_{i'}(k) \rangle^* \, \omega_{ii'}(k)\right)_{ij}\right]$$

$$= (-1)^k \, \mathrm{Pf}\left[\omega(k) \mathcal{M}^*(k) \, \omega^T(k)\right]$$

$$= (-1)^k \underbrace{\overset{\neq 0}{\det(\omega(k))}}_{\text{phase since } \omega\omega^\dagger = \mathbb{1}} \underline{[P(k)]^*}$$

→ <u>Two conclusions:</u>

- $P(u') = 0 \iff P(-u') = 0$

- The vorticities ν around u' and $-u'$ have opposite signs:

$$\boxed{\nu[u'] = \frac{1}{2\pi i} \oint_{\partial u'} \nabla \log[P(u)] \cdot d\vec{u} = -\nu[-u'] \quad \in \mathbb{Z}}$$

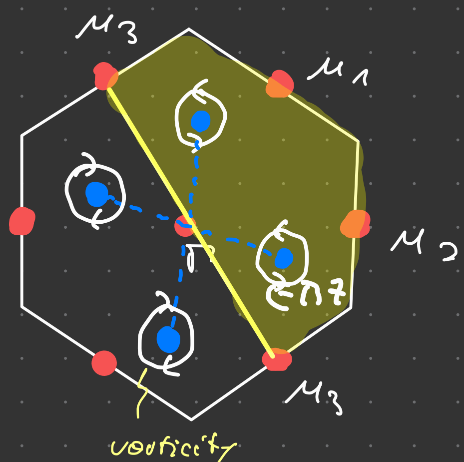
→ Vortices come in pairs of opposite vorticity

* <u>Observation:</u> Zeros of $P(u)$ with $\nu[u']$ are topologically stable

→ Generic picture:

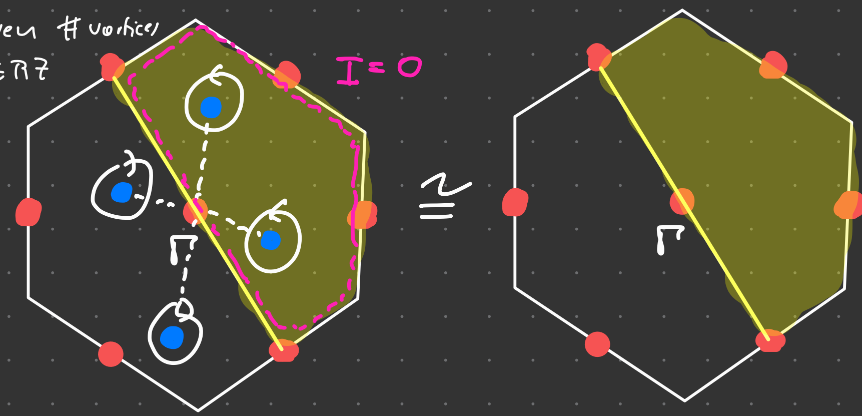
● $|P(\psi)| = 1$

● $|P(\psi)| = 0$

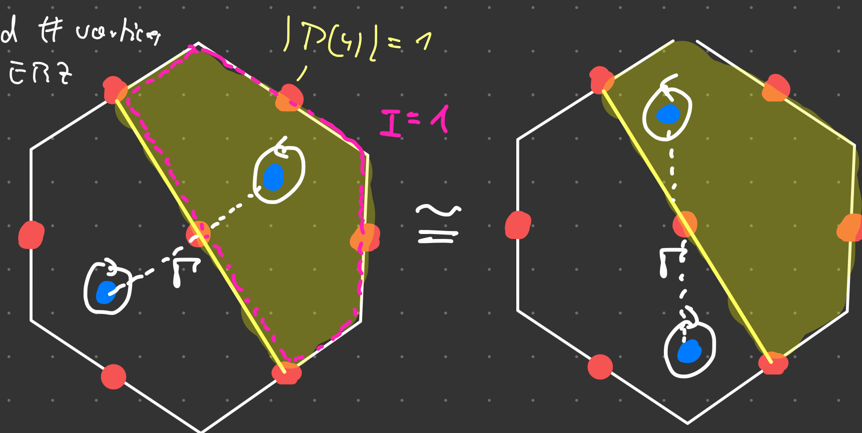


4. Two situations:

* Even # vortices in ERZ



* Odd # vortices in ERZ



→ Two cases are topologically distinct (as long as TRS is not broken)

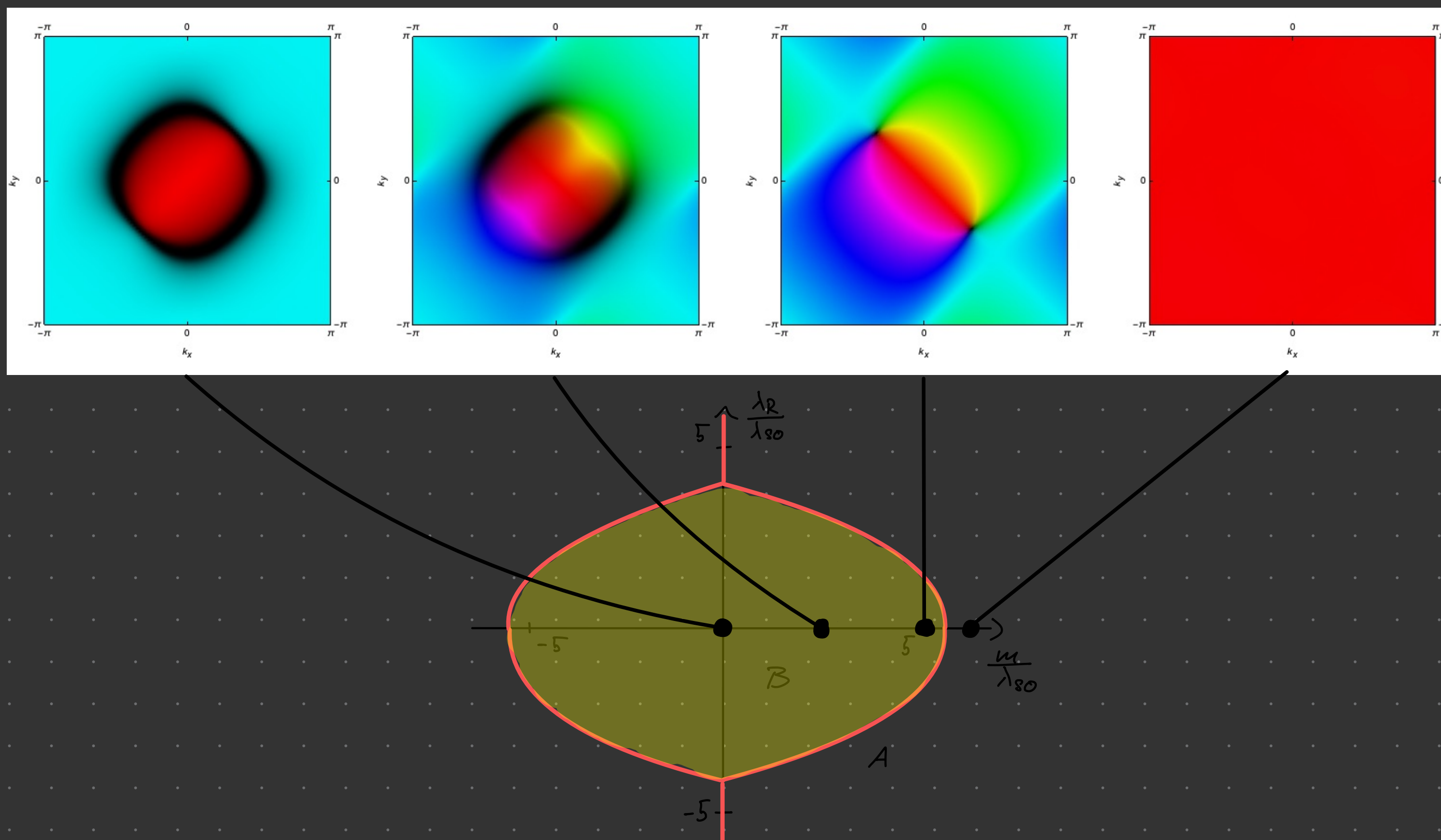
→ Odd number of vortices = Topological phase B protected by TRS

5. Def. Topological $\mathbb{Z}_2$ index:

$$\boxed{\begin{aligned} I &= \frac{1}{2\pi i} \oint_{\partial EBZ} \nabla \log\left[P(\vec{k})\right] d\vec{k} \mod 2 \\ &= \frac{1}{2\pi i} \oint_{\underbrace{\partial EBZ}_{\text{closed path that encircles an EBZ}}} d \log\left[P(\vec{k})\right] \mod 2 \end{aligned}}$$

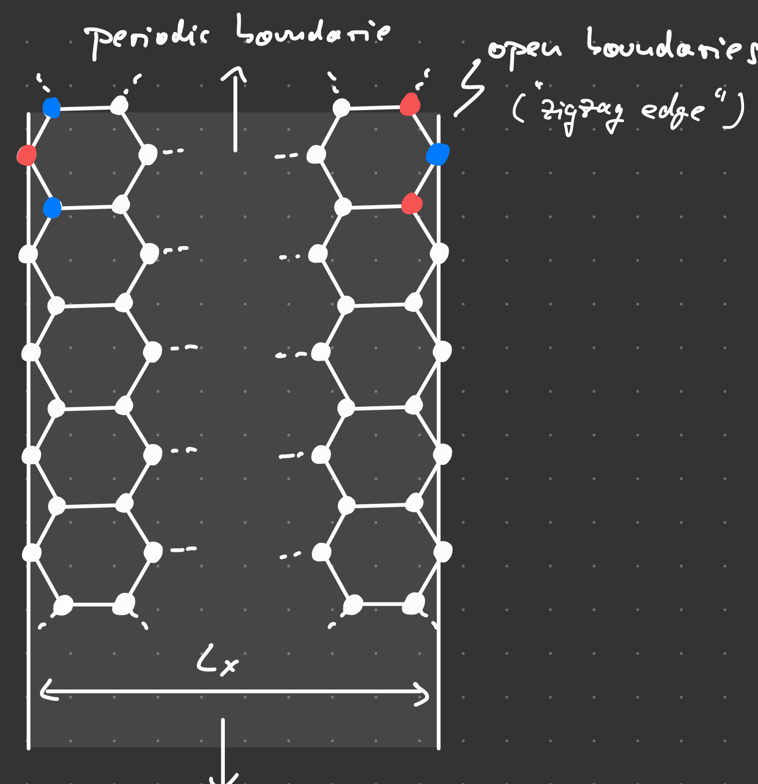
<u>Note</u>: I is gauge invariant under globally continuous gauge transformations

6. Example: Kane-Mele model

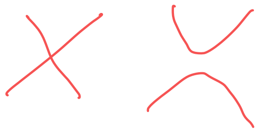


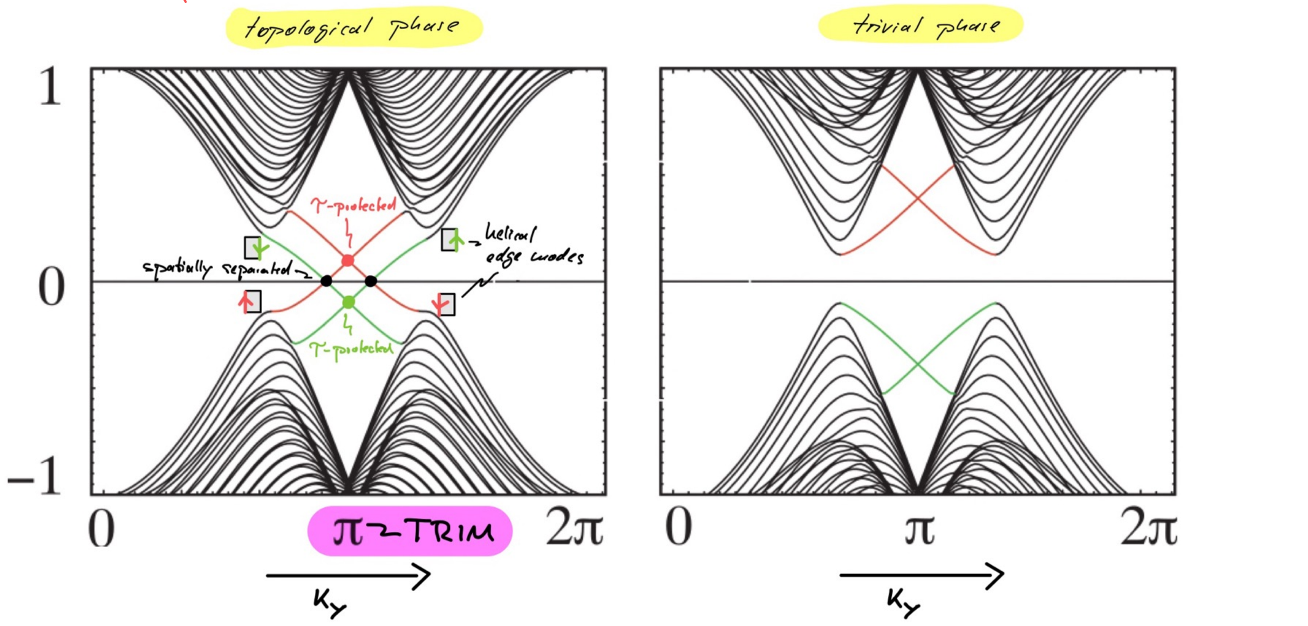
1.3.4 Edge modes

1. $\hat{H}_{HM}$ on a cylinder:



2. Edge modes:





topological phase
trivial phase
1
0
−1
T-protected
T-protected
spatially separated
helical edge modes
0
π ≈ TRIM
2π
0
π
2π
k_y
k_y

* <u>Topological:</u> Gapless edge modes (2 per edge)
* <u>Trivial:</u> No edge modes

$\boxed{\text{Kane-Mele model realizes the Quantum Spin Hall Effect.}}$