7. Topological insulators

(Haldane model of Chern insulator – QHE without net magnetic field;
Kane–Mele model of $\mathbb{Z}_2$ topological insulator, ...)

7.1 Haldane model

We already discussed the Hofstadter problem (square lattice in magnetic field): Chern insulator; e.g., for $n=3$ bands $C_1 = 1$, $C_2 = -2$, $C_3 = 1$ (for any odd n all bands except for the middle one have $C=1$; for even n, two bands in the middle have $C \neq 1$, their Chern numbers are equal; the total Chern number is zero)

When two bands touch, their total Chern number remains a well-defined integer, although individual touching bands may not have their own Chern numbers.

Without breaking TRS all $C_i = 0$ and $\sigma_{xy} = 0$ correspondingly

Haldane: TRS can be broken without net magnetic field, leading to nontrivial Chern bands and to quantization of σ_{xy}

QHE without macroscopic magnetic field (without Landau levels)!

Start with the honeycomb lattice ("graphene") with the nearest-neighbor hopping. Introduce the gap by breaking TRS (spatially variable magnetic Field)

$\rightarrow$ $\pm m\sigma_z$ term in the two Dirac nodes (inversion symmetry is preserved)

Microscopically:

second-neighbor hopping with phases that break TRS, but the total magnetic flux through each hexagon is zero, unlike for the Hofstadter model.

The lower and upper bands have $C=1$ and $C=-1$, respectively $\rightarrow$ IQHE

Compare the two types of gap in graphene: TRS-preserving and TRS-breaking

TRS-preserving:

$$h_{K,K'} = v_G(\pm \sigma_x q_x + \sigma_y q_y) + m\sigma_z$$

The integrated Berry curvatures from the two nodes cancel each other (π, $-\pi$; $\pi + (-\pi) = 0$)

$$C_+ = \frac{1}{2} - \frac{1}{2} = 0, \quad C_- = 0$$

as guaranteed by TRS.

TRS-breaking

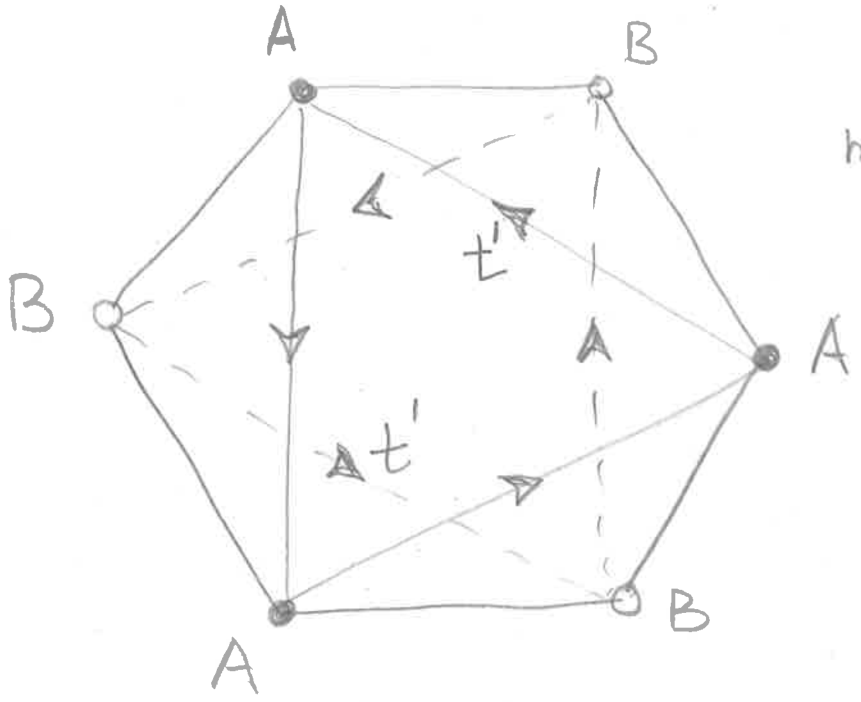
$$h_{K,K'} = v_G(\pm \sigma_x q_x + \sigma_y q_y) \pm m_H \sigma_z$$

or in terms of 4x4 Hamiltonian

$$h = v_G(\tau_z \sigma_x q_x + \sigma_y q_y) + m_H \tau_z \sigma_z$$

where τ-matrices are Pauli matrices in the K, K' space.

The mass term is diagonal in both K, K' and sublattice spaces.



next-to-nearest neighbor hopping operates within one sublattice,

$t' \neq (t')^*$ breaks TRS

choose $t' = i|t'|$ purely imaginary hopping

$$h(\vec{k}) = \begin{pmatrix} |t'|\tilde{f}(\vec{k}) & -tf(\vec{k}) \\ -tf^*(\vec{k}) & -|t'|\tilde{f}(\vec{k}) \end{pmatrix}$$

$$\tilde{f}(\vec{k}) = \sin(\vec{k}\cdot\vec{a}_1) - \sin(\vec{k}\cdot\vec{a}_2) - \sin(\vec{k}(\vec{a}_1 - \vec{a}_2))$$

$\Rightarrow$ reduces to h_K and $h_{K'}$ near Dirac nodes, $m_H = -\frac{3\sqrt{3}}{2}|t'|$ for $|t'| \ll |t|$

The two bands are topologically nontrivial, with $C_\pm = \pm 1$

The net magnetic flux through the hexagon is zero.

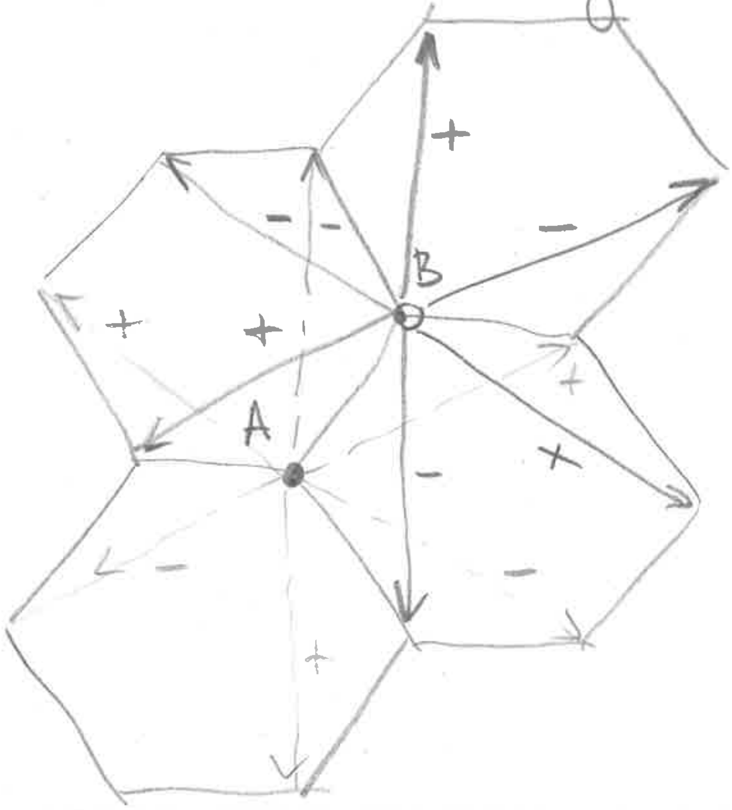
Generalized Haldane's model

$$H = t_1 \sum_{\langle i,j \rangle} c_i^+ c_j + t_2 \sum_{\langle\langle i,j \rangle\rangle} e^{-i \nu_{ij} \varphi} c_i^+ c_j + M \sum_i \epsilon_i c_i^+ c_i$$

$\epsilon_i = \pm 1$ for A and B sites
(TRS-preserving SIS-breaking mass)

$$\nu_{ij} = \text{sign} \left[\vec{\delta} \times \vec{\delta}' \right]_z = \pm 1,$$

where $\vec{\delta}, \vec{\delta}'$ are vectors along the bonds connecting next-nearest neighbors



In this figure, the signs $\pm$ correspond to ν_{ij}

Fourier transformation:

$$h(\vec{k}) = \epsilon(\vec{k}) + \vec{d}(\vec{k}) \cdot \vec{\sigma}$$

Previous consideration: $M=0$, $\varphi = \pm \frac{\pi}{2}$

$$\epsilon(k) = 2t_2 \cos(\varphi)\left[\cos(\vec{k}\vec{a}_1) + \cos(\vec{k}\vec{a}_2) + \cos(\vec{k}(\vec{a}_1 - \vec{a}_2))\right]$$

$$d_x(\vec{k}) = t_1\left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\,\vec{a}_2) + 1\right]$$

$$d_y(\vec{k}) = t_1\left[\sin(\vec{k}\vec{a}_1) + \sin(\vec{k}\cdot\vec{a}_2)\right]$$

$$d_z(\vec{k}) = M + 2t_2 \sin(\varphi)\left[\sin(\vec{k}\cdot\vec{a}_1) - \sin(\vec{k}\vec{a}_2) - \sin(\vec{k}(\vec{a}_1 - \vec{a}_2))\right]$$

TRS:
$$\left.\begin{aligned} \epsilon(\vec{k}) &= \epsilon(-\vec{k}) \\ d_x(\vec{k}) &= d_x(-\vec{k}) \\ d_y(\vec{k}) &= -d_y(-\vec{k}) \end{aligned}\right\} \text{satisfied for all } \varphi$$

$$d_z(\vec{k}) = d_3(-\vec{k})$$ satisfied only for $\varphi = 0, \pi$

SIS (σ_x) around the middle of unit cell

$$\left.\begin{aligned} \epsilon(\vec{k}) &= \epsilon(-\vec{k}) \\ d_x(\vec{k}) &= d_x(-\vec{k}) \\ d_y(\vec{k}) &= -d_y(-\vec{k}) \end{aligned}\right\} \text{Satisfied for all } \varphi$$

$$d_z(\vec{k}) = -d_z(-\vec{k})$$ satisfied only for $M=0$

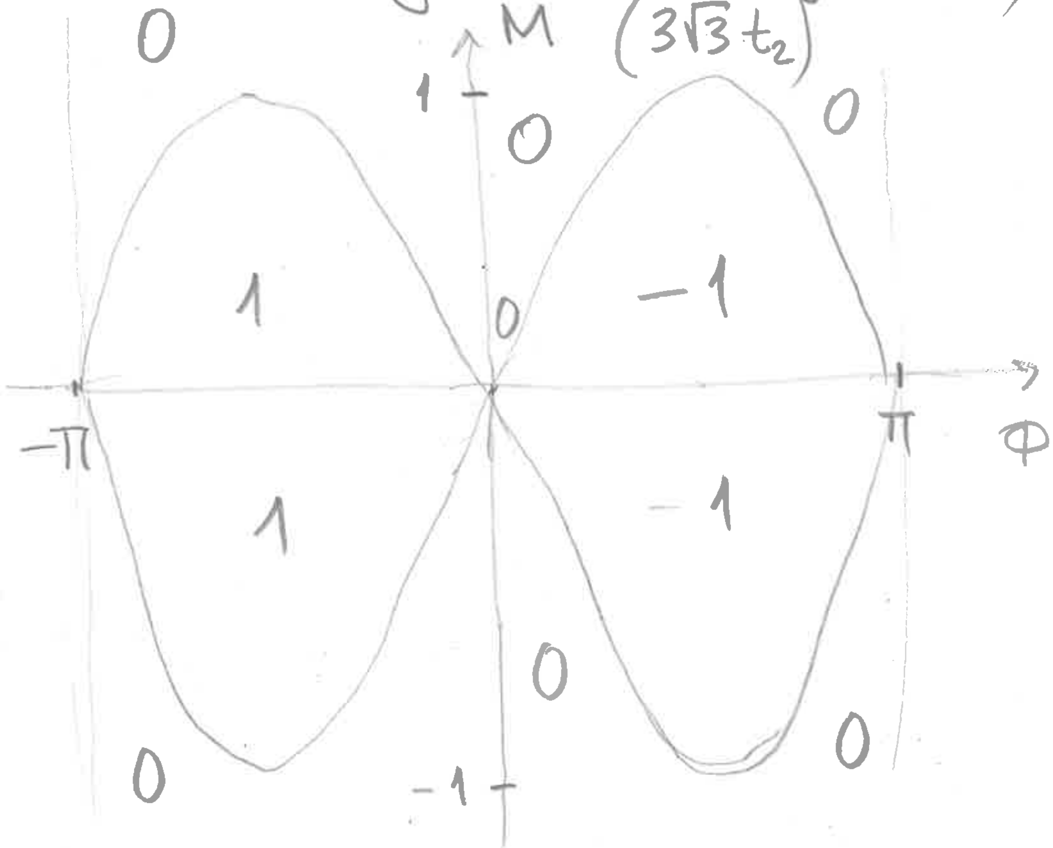
TRS + SIS:

$\varphi = 0$ or $\varphi = \pi$ and $M = 0$

Otherwise, gap opens.

C_3 symmetry is preserved.

Phase diagram: $\sigma_{xy}(M,\varphi)$



QHE transition lines:

$$M = \pm 3\sqrt{3}\, t_2 \sin\varphi$$

$M = +3\sqrt{3}\, t_2 \sin\varphi$: K node experience gap-closing-reopening transition

its Hall conductance changes for $\varphi > 0$ from $\frac{1}{2}\,\mathrm{sign}(M - 3\sqrt{3}\, t_2 \sin\varphi) = \frac{1}{2}$ to $-\frac{1}{2}$, i.e. by -1

$M = -3\sqrt{3}\, t_2 \sin\varphi$: K' node changes σ_{xy} by $+1$.

Edge states in Haldane model.

Return to $M=0$, $\Phi = \frac{\pi}{2}$; set $a=1$

$$d_x = 1+\cos(\sqrt{3}k_y) + \cos\left(\frac{\sqrt{3}}{2}k_y\right)\cos\left(\frac{3}{2}k_x\right) - \sin\left(\frac{\sqrt{3}}{2}k_y\right)\cdot\sin\left(\frac{3}{2}k_x\right)$$

$$d_y = \sin(\sqrt{3}k_y) + \sin\left(\frac{\sqrt{3}}{2}k_y\right)\cos\left(\frac{3}{2}k_x\right) + \cos\left(\frac{\sqrt{3}}{2}k_y\right)\sin\left(\frac{3}{2}k_x\right)$$

$$d_z = 4\sin\left(\frac{\sqrt{3}}{2}k_y\right)\left[\cos\left(\frac{3}{2}k_x\right) - \cos\left(\frac{\sqrt{3}}{2}k_y\right)\right]$$

Fix k_y, consider a semi-infinity system $x \geqslant 0$:

$$k_\perp \equiv k_x, \quad k_\parallel = k_y$$

$$\vec{d}(\vec{k}) = \vec{b}_0 + 2\vec{b}_c\cos\left(\frac{3}{2}k_x\right) + 2\vec{b}_s\sin\left(\frac{3}{2}k_x\right)$$

$$\vec{b}_0 = \left(1+\cos(\sqrt{3}k_y),\ \sin(\sqrt{3}k_y),\ -4\sin\left(\frac{\sqrt{3}}{2}k_y\right)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right)^T$$

$$2\vec{b}_c = \left(\cos\left(\frac{\sqrt{3}}{2}k_y\right),\ \sin\left(\frac{\sqrt{3}}{2}k_y\right),\ 4\sin\left(\frac{\sqrt{3}}{2}k_y\right)\right)^T$$

$$2\vec{b}_s = \left(-\sin\left(\frac{\sqrt{3}}{2}k_y\right),\ \cos\left(\frac{\sqrt{3}}{2}k_y\right),\ 0\right)^T$$

$\vec{b}_0 = \vec{b}_\parallel + \vec{b}_\perp$, where

$$\vec{b}_\parallel = (\hat{b}_c\cdot\vec{b}_0)\hat{b}_c + (\hat{b}_s\cdot\vec{b}_0)\hat{b}_s, \qquad \hat{b}_c = \frac{\vec{b}_c}{|\vec{b}_c|}, \quad \hat{b}_s = \frac{\vec{b}_s}{|\vec{b}_s|}$$

$$\vec{b}_\perp = \vec{b}_0 - \vec{b}_\parallel$$

Condition of existence of edge states:

$$|\vec{b}_\perp| < |2\vec{b}_c|$$

$$\Rightarrow\ 2\left|\cos\left(\frac{\sqrt{3}}{2}k_y\right)\left[1-8\sin^2\left(\frac{\sqrt{3}}{2}k_y\right)\right]\right| < 1+16\sin^2\left(\frac{\sqrt{3}}{2}k_y\right)$$

For such k_y there are edge states with $E_{edge}(k_y) = \pm\ b_\perp(k_\parallel)$

sign depends on edge

$$= \pm 6\,\frac{\sin(\sqrt{3}k_y)}{\sqrt{1+16\sin^2\left(\frac{\sqrt{3}}{2}k_y\right)}}$$

(1 chiral state per edge in a strip)

7.2. Kane-Mele Model

(i) Chern number ($\mathbb{Z}$) exists in insulators when TR symmetry is broken, Hall conductivity is non-zero. Are there topological numbers in the presence of TRS?

(ii) Do topological numbers always form a set $\mathbb{Z}$?

(iii) Do topological numbers exist in metals?

Return to generalized Haldane model

$$H = v(\tau_z \sigma_x p_x + \sigma_y p_y) + M\sigma_z + m_H \tau_z \sigma_z$$

either SIS or TRS is broken or both

Kane-Mele: add real spin and spin-orbit coupling

Simplest mass term: $m_{KM} \tau_z \sigma_z \cdot S_z$

$\vec{S}$ is even under SI (parity) and odd under TR

$\Rightarrow$ Kane-Mele mass term is even under both SI and TR transformations

To generate SIS and TRS gap, take two copies of Haldane's model with <u>opposite</u> next-nearest-neighbor hoppings.

Charge Hall conductance

$\sigma_{xy} = 0$ (canallation between up- and down-spin electrons)

But quantized Spin Hall conductance (difference between spin-up and spin-down Hall conductances)

$\Rightarrow$ "quantum spin Hall state"

two edge modes (spin-up and spin-down) propagating in opposite directions

Thus, there can be topologically nontrivial bands in the presence of TRS.

However, this model is very special: z-component of spin is conserved (not generic, as TRS can be preserved for rotating spin: spin-orbit interaction)

Are gapless "helical" edge states robust when up- and down-spin states are mixed?

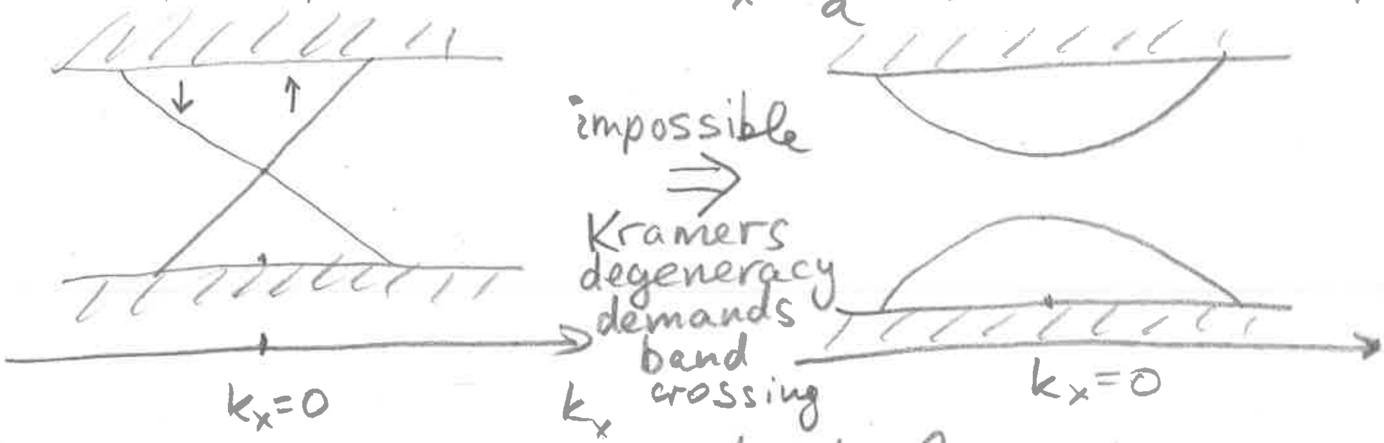
Kane and Mele: Yes!

Kramers' degeneracy

Consider an edge in x-direction, k_x is a good quantum number

TR transformation: $k_x \rightarrow -k_x$

$\Rightarrow$ $k_x = 0$ and $k_x = \frac{\pi}{a}$ are TR invariant



Any TR-invariant potential cannot localize these states:

backscattering is forbidden (requires spin flip)

Kramers' degeneracy:

TR: spin is reversed; for spin-$\frac{1}{2}$:

$$T\vec{\sigma}T^{-1} = -\vec{\sigma} \Rightarrow U_T = e^{i\varphi}\sigma_y$$

with arbitrary phase

$$T^2 = \left(e^{i\varphi}\sigma_y K\right)^2 = -1$$

Assume that TRS is present, and there exists a non-degenerate eigenstate $|\psi\rangle$: $T|\psi\rangle = t|\psi\rangle$ with eigenvalue t, then

$$T^2|\psi\rangle = |t|^2|\psi\rangle, \quad \text{but } T^2 = -1$$

$\Rightarrow$ contradiction $\Rightarrow$ $|\psi\rangle$ is degenerate

Without spin-orbit coupling, Kramers' degeneracy is trivial: each band has two-fold spin degeneracy at every point in the BZ (including $\underbrace{\vec{k} \to -\vec{k}}_{\text{TRS}} + \vec{\sigma} \to -\vec{\sigma}$) TRS with preserved spin

When $\vec{k}$ and $-\vec{k}$ differ by a reciprocal lattice vector, they are equivalent $\longrightarrow$ time-reversal-invariant momenta $\vec{\Lambda}_i$

Qualitatively, two ways to connect the Kramers' pairs at TR-invariant momenta by (non-degenerate) bands

Return to Kane-Mele model, introduce spin rotation

Broken mirror symmetry:
Rashba-type term

$$H_R = \lambda_R \Psi^+ (\sigma_x \tau_z s_y - \sigma_y s_x) \Psi$$

couples to Haldane Hamiltonians

$$h_R(\vec{K}+\vec{q}) \propto \sigma_x s_y - \sigma_y s_x$$

TRS: $h_R(\vec{K}'+\vec{q}) \Rightarrow s_y h_R^*(\vec{K}) s_y \propto -\sigma_x s_y - \sigma_y s_x$

Without $H_{so} = \lambda_{so} \Psi^+ \sigma_z \tau_z s_z \Psi$
(opposite Haldane masses for spin-up and spin-down states)
the Rashba term does not open the gap: at K-point

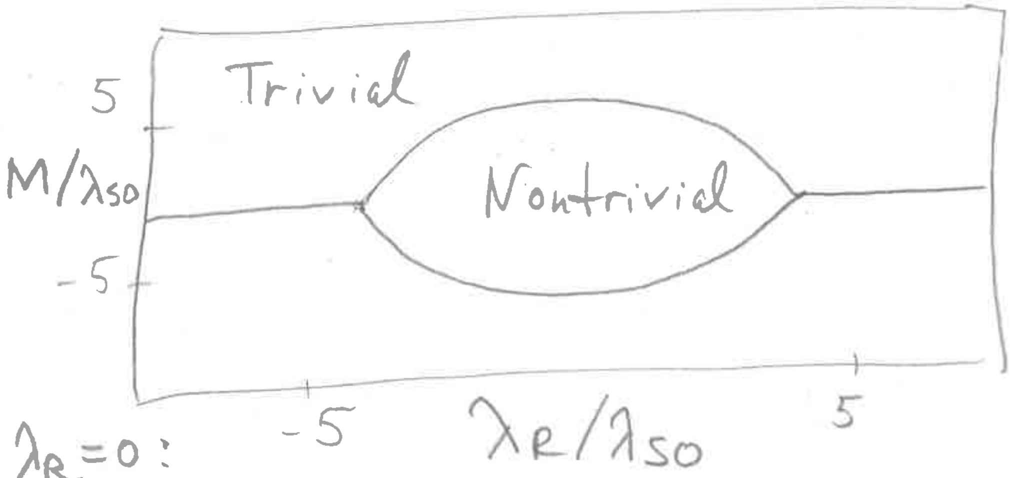
$$E(\vec{K}+\vec{q}) = -\lambda_R \pm \sqrt{v^2 q^2 + \lambda_R^2}$$

and

$$+\lambda_R \pm \sqrt{v^2 q^2 + \lambda_R^2}$$

When λ_{so} is present, λ_R influences the gap (Kane-Mele gap).
Since $\{H_R, H_{so}\} = 0$

Phase diagram for fixed λ_{so}:



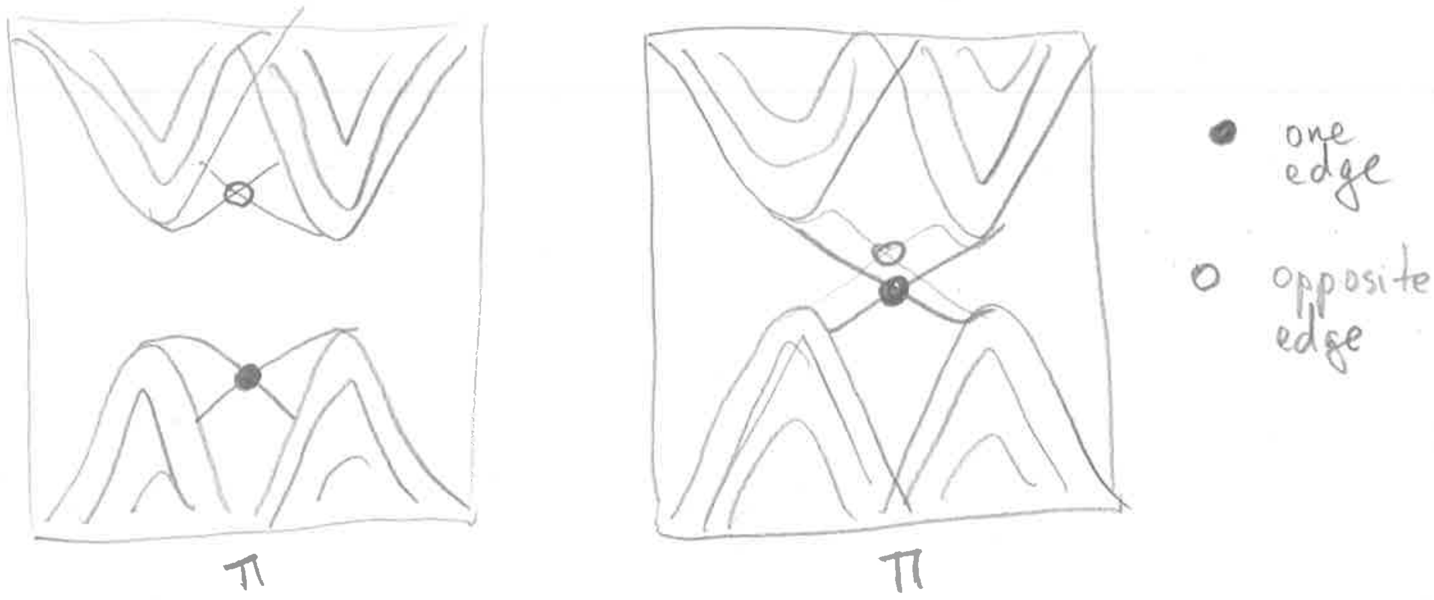
For $\lambda_R = 0$:

$M > 3\sqrt{3}\,\lambda_{so}$: edge states do not cross the bulk gap

$M < 3\sqrt{3}\,\lambda_{so}$: edge states crossing the gap

Here we have S^z conservation

Finite λ_R breaks it but does not change topology as long as the gap does not close (central region in the phase diagram)



7.3. $\mathbb{Z}_2$ characterization of topological insulators

Chern insulator (no TRS):

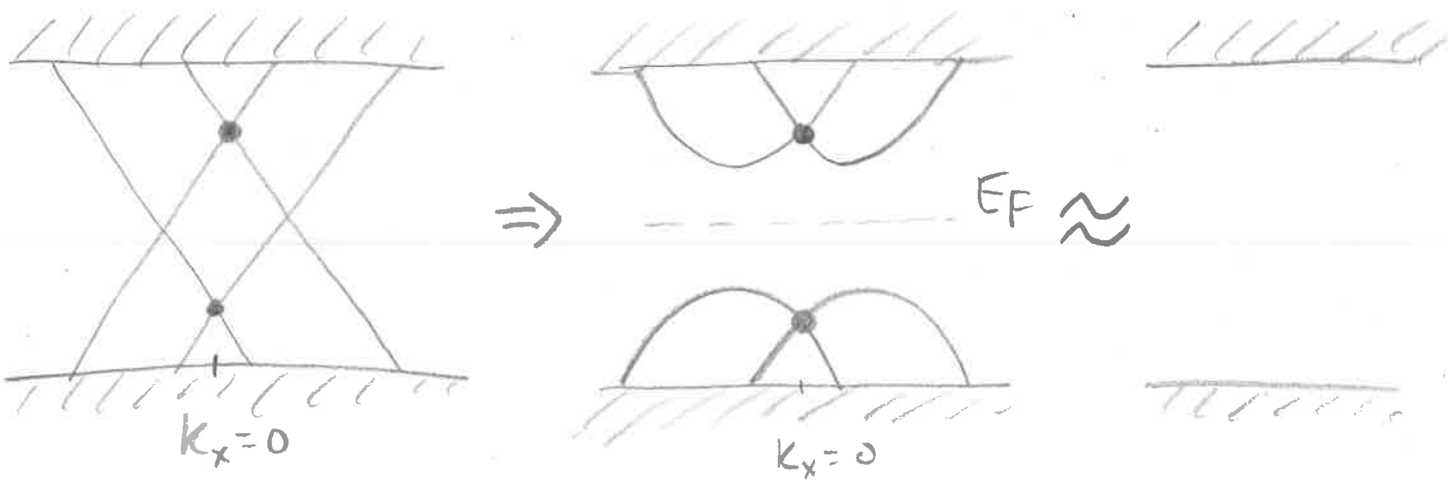
integer Chern number $\rightarrow$ quantized Hall conductance

$C \in \mathbb{Z}$: number of edge modes at each edge
(more precisely - difference of forward- and backward-moving modes).

TRS: counter-propagating edge modes - Kramers' doublets

Natural guess: number of Kramers' doublets is integers, hence again $\mathbb{Z}$-classification. Not true!

Assume that there are 2 pairs:



$k_x=0$: crossing points are still protected by Kramers' degeneracy
other crossings are not protected: gaps may open!

2 pairs of modes $\approx$ 0 pairs

any even number of pairs $\approx$ 0 pairs

any odd number $\approx$ 1 pair

$\Rightarrow$ $\mathbb{Z}_2$ classification (even/odd or 0/1)

$\mathbb{Z}_2$ topological number

Formal definition:

TR-symmetric points ($\vec{k}$ equivalent to $-\vec{k}$)

$$(-1)^{\rho} = \prod_i \mathrm{sign}\left[\mathrm{Pf}\,B(\Lambda_i)\right],$$

where B_{mn} is the matrix representation of the TR operator (sewing matrix)

$$B_{mn}(\vec{k}) = \langle \Psi_m(-\vec{k}) | T | \Psi_n(\vec{k}) \rangle$$

for occupied bands and

Pf stands for the Pfaffian

Even-dimensional skew-symmetric matrices:

$$(\mathrm{Pf}\,T)^2 = \det T$$

$\rho = 0$: trivial insulator

$\rho = 1$: "inverted bands" - topological insulator

Pfaffian

Skew-symmetric (antisymmetric) matrix A:

$$A^T = -A \qquad (a_{ji} = -a_{ij})$$

Recursive definition for $2n \times 2n$ antisymmetric A:

$$Pf(A) = \sum_{j=2}^{2n} (-1)^j a_{1j} \, Pf(A_{\bar{1}\bar{j}}),$$

where $A_{\bar{1}\bar{j}}$ – matrix A with 1st and jth rows and columns removed;

$Pf(0 \times 0) \equiv 1$

$$\boxed{\left(Pf(A)\right)^2 = \det(A)}$$

For n odd, $Pf(A) = 0$

indeed, $\det(A) = \det(-A) = (-1)^n \det(A)$

$\Rightarrow \det(A) = 0 \Rightarrow Pf(A) = 0$

$A = \begin{bmatrix} 0 & a \\ -a & 0 \end{bmatrix}$: $\quad Pf(A) = a$

$A = \begin{bmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{bmatrix}$: $\quad Pf(A) = 0$

$A = \begin{bmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{bmatrix}$: $\quad Pf(A) = af - be + dc$

Properties of Pfaffian:

$$\mathrm{Pf}(A^T) = (-1)^n \mathrm{Pf}(A)$$
$$\mathrm{Pf}(\lambda A) = \lambda^n \mathrm{Pf}(A)$$
$$\mathrm{Pf}(BAB^T) = \det(B)\,\mathrm{Pf}(A)$$
$$\Rightarrow \quad \mathrm{Pf}(A^{2m+1}) = (-1)^{nm}\left[\mathrm{Pf}(A)\right]^{2m+1}$$

$$\frac{1}{\mathrm{Pf}(A)} \frac{\partial\, \mathrm{Pf}(A)}{\partial x} = \frac{1}{2} \operatorname{tr}\left(A^{-1} \frac{\partial A}{\partial x}\right)$$

$$\mathrm{Pf}(A)\,\mathrm{Pf}(B) = \exp\left(\frac{1}{2} \operatorname{tr} \log (A^T B)\right)$$

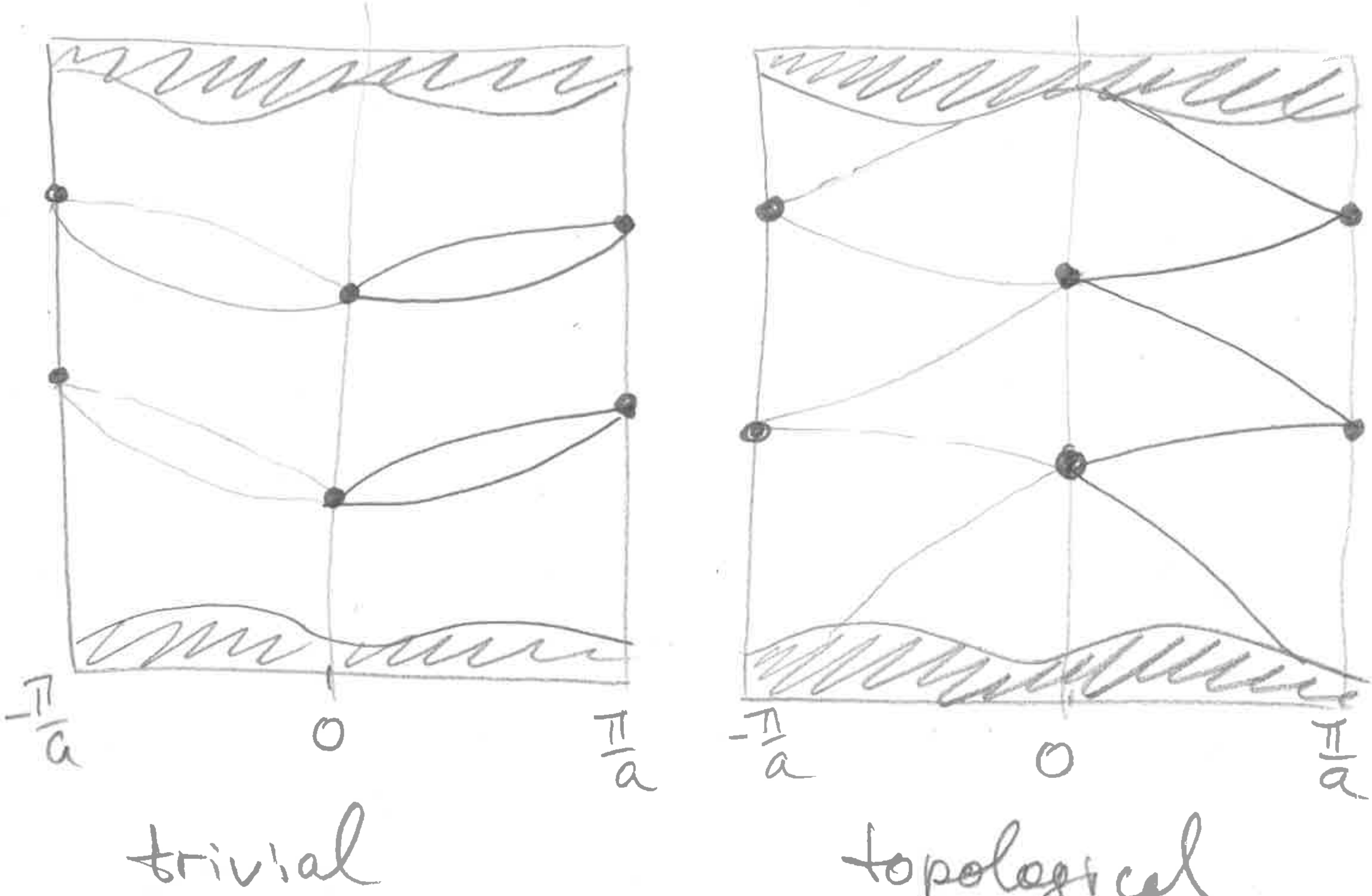
$$\mathrm{Pf}\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} = \mathrm{Pf}(A_1)\,\mathrm{Pf}(A_2)$$

$$\mathrm{Pf}\begin{bmatrix} 0 & M \\ -M^T & 0 \end{bmatrix} = (-1)^{\frac{n(n-1)}{2}} \det(M)$$

$$\boxed{\mathrm{Pf}(A) = i^{n^2} \exp\left\{\frac{1}{2} \operatorname{tr} \log\left[(\sigma_y \otimes \mathbb{1}_n)^T \cdot A\right]\right\}}$$

$$\mathrm{Pf}(\sigma_y \otimes I_n) = (-i)^{n^2}$$

$$\begin{bmatrix} & \begin{matrix} -i & & \\ & -i & \\ & & -i \end{matrix} \\ \begin{matrix} i & & \\ & i & \\ & & i \end{matrix} & \end{bmatrix}$$



TRS: $E(k) = E(-k)$

Kramers' degeneracy at $k=0$,

$k = \pm\frac{\pi}{a}$

For $k>0$:

even number of bands at given energy → trivial ≈ no edge states

odd number of bands at any energy in the bulk gap → topological

Sewing matrix:

unitary, $B_{mn}(k) = -B_{nm}(-k)$

skew-symmetric at TR-invariant points

1D case

Charge polarization:

$$P = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, A(k) = P^{I} + P^{II}$$

Chern number = 0 (does not change for a cycle)

contributions of members of Kramers' pair

$$P^{s} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, A^{s}(k)$$

$$A^{s}(k) = i\sum_{a}\langle u^{s}_{k,a}|\nabla_k|u^{s}_{k,a}\rangle$$

$$|u^{I}_{-k,a}\rangle = e^{i\chi_{k,a}}\,T\,|u^{II}_{k,a}\rangle$$

$$|u^{II}_{-k,a}\rangle = -e^{i\chi_{-k,a}}\,T\,|u^{I}_{k,a}\rangle$$

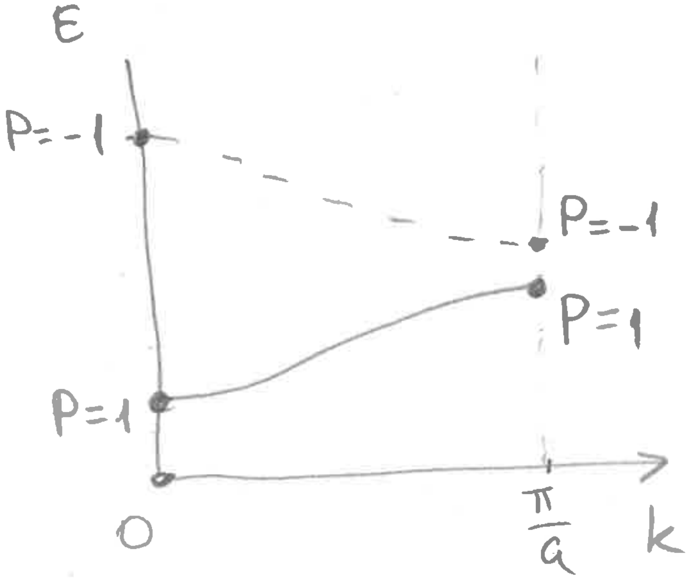
TR polarization

$$P_T \equiv P^{I} - P^{II}$$

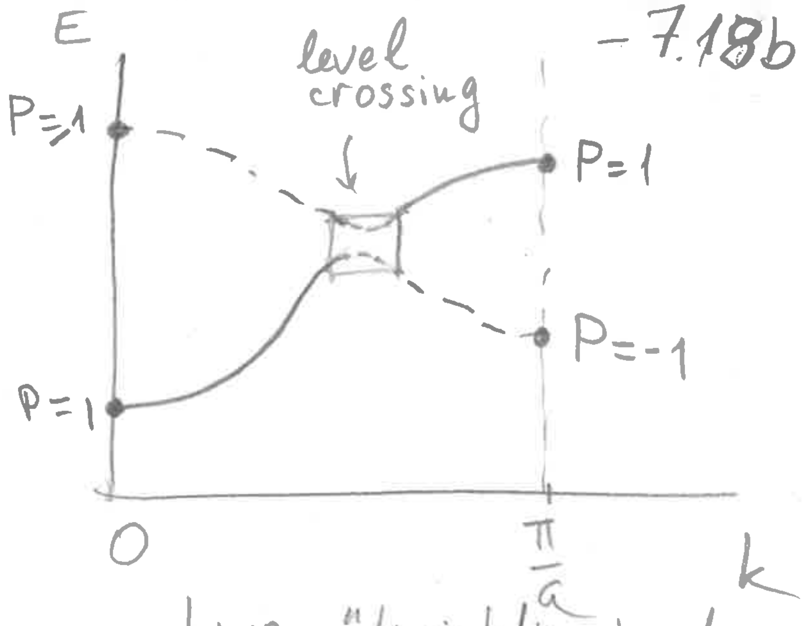
$$= \frac{1}{2\pi i}\left\{\int_0^{\pi} dk\, \underbrace{\mathrm{tr}\left(B^{+}\nabla_k B\right)}_{\nabla_k \log(\det(B(k)))} - 2\log\left(\frac{\mathrm{Pf}[B(\pi)]}{\mathrm{Pf}[B(0)]}\right)\right\}$$

$$= \frac{1}{\pi i}\log\left(\underbrace{\frac{\sqrt{\det(B(\pi))}}{\mathrm{Pf}(B(\pi))}}_{\text{sign } \mathrm{Pf}(B(\pi))}\ \underbrace{\frac{\mathrm{Pf}[B(0)]}{\sqrt{\det(B(0))}}}_{\text{sign } \mathrm{Pf}(B(0))}\right)$$

Straightforward generalization to 2D or 3D



two bands with well-defined parity



two "twisted" bands, each with opposite parities at $k=0$ and $k=\frac{\pi}{a}$

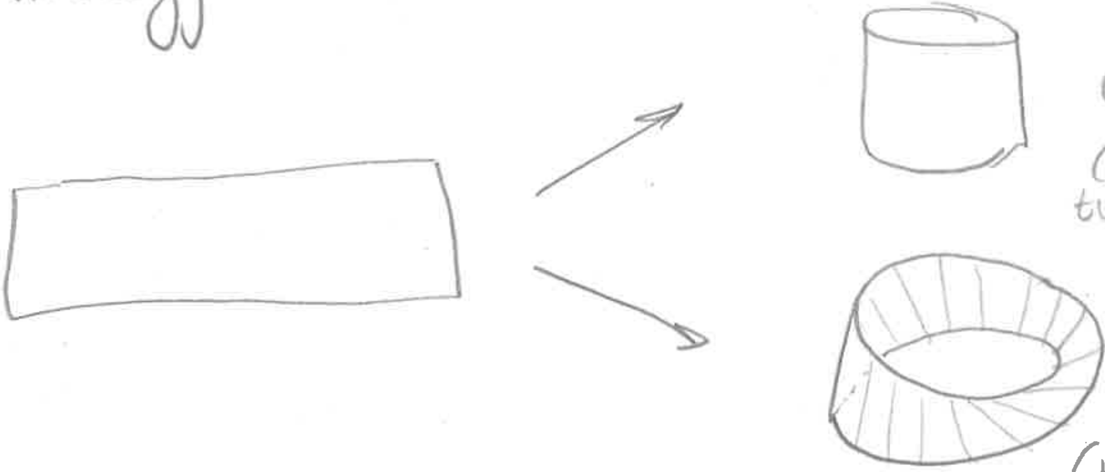
For a given band:

$$(-1)^{\rho} = \prod_{i=1}^{2^d} \delta_i \,, \qquad \underbrace{\delta_i = \pm 1}_{P=\pm 1} \text{ at } \Lambda_i$$

The product of $(-1)^{\rho}$ over all bands is always $+1$.

If inversion symmetry is not present, change parameters of the Hamiltonian along a continuous path to connect with the Hamiltonian with SIS. As long as band gaps do not close along this path (for a given band), the band has the same $\mathbb{Z}_2$ index.

Analogy: rubber band



Bloch bands constructed out of atomic orbitals, characterized by orbital ℓ and total $j = |\ell \pm \tfrac{1}{2}|$ angular momentum quantum numbers; parity quantum number $P = (-1)^{\ell}$

Crystal: no rotational symmetry, but parity (spatial inversion) may be present. Assume SIS.

P: $\vec{k} \to -\vec{k}$ $\Rightarrow$ generic Bloch state with $\vec{k}$ is not an eigenstate of P

In d spatial dimensions 2^d TR-invariant momenta $\vec{\Lambda}_i$: Bloch states at $\vec{k} = \vec{\Lambda}_i$ are eigenstates of P

Simple tight-binding limit: the bands at these points inherit parity from atomic orbitals:

$$\prod_{i=1}^{2^d} \delta_i = +1, \quad \delta_i \text{ - parity eigenvalues}$$

Another Z_2 invariant from the Pfaffian

Consider $\langle u_i(\vec{k})|T|u_j(\vec{k})\rangle \equiv M_{ik}(\vec{k})$
(different from the sewing matrix
$B_{ik}(\vec{k}) = \langle u_i(-\vec{k})|T|u_j(\vec{k})\rangle$)

M_{ik} is skew-symmetric for ALL $\vec{k}$ in BZ.

For 2×2 matrix $\langle u_i(\vec{k})|T|u_j(\vec{k})\rangle = \epsilon_{ij} P(\vec{k})$
where $P(\vec{k}) = Pf(M(\vec{k}))$

Gauge transformation $|\tilde{u}_i(\vec{k})\rangle = R_{ij}(\vec{k})|u_j(\vec{k})\rangle$
unitary

$$\tilde{P}(\vec{k}) = Pf[R^*_{im}\langle u_m(\vec{k})|T|u_n(\vec{k})\rangle(R^{*T})_{nj}]$$
$$= \det(R^*)\,P(k)$$

$P(\vec{k})$ is invariant under $SU(2)$ rotation;
$U(1)$ transformation: $U = e^{i\varphi}$
$$\Rightarrow \tilde{P}(\vec{k}) = e^{-2i\varphi} P(\vec{k})$$

Absolute value of $P(\vec{k})$ is gauge-invariant.

BZ contains special points:

(1) $T\,|u_i(k)\rangle = M_{ij}\,|u_j(k)\rangle\,, \quad |P(\vec{k})| = 1$

unitary

"even subspace"

TR-invariant points belong to this set

($T|u_i(\Lambda)\rangle$ is equivalent to $|u_i(\Lambda)\rangle$)

(2) $\langle u_1(\vec{k})\,|\,T\,|\,u_2(\vec{k})\rangle = 0\,, \quad |P(\vec{k})| = 0$

($T|u_i(\vec{k})\rangle$ is orthogonal to subspace spanned by $|u_i(k)\rangle$)

Then $P(-\vec{k}) = 0$. Indeed, $|u_j(-\vec{k})\rangle = B_{ji}(\vec{k})T|u_i(\vec{k})\rangle$

$$P(-\vec{k}) = Pf\left[\langle u_i(-\vec{k})|\,T\,|u_j(-\vec{k})\rangle\right]$$
$$= \det\left(B^*(\vec{k})\right)\left[P(\vec{k})\right]^* = 0$$

The phases of Pfaffian close to degeneracy points $\vec{k}$ and $-\vec{k}$ correspond to opposite vorticity:

$$v = \frac{1}{2\pi}\int_C d\vec{k}\; i\,\vec{\nabla}\log\left(P(\vec{k})\right)$$

where C surround the point $\vec{K}$ at which $P(\vec{K}) = 0$

Zeros of Pfaffian in half of BZ are topological invariant ($\vec{k}$ and $-\vec{k}$ belong to different halves of BZ)

Consider odd number of zeros in half of BZ
Any two of them can annihilate within this half. However, the remaining zero can only annihilate with its partner from the other half ($\vec{k} \Leftrightarrow -\vec{k}$).
This would happen at the TR-invariant point Λ. However, at Λ, the Pfaffian is nonzero: $|P(\Lambda)|=1$. Hence, one zero of $P(\vec{k})$ in half the BZ is stable globally.

Even number of zeros can annihilate within the half of the BZ without moving to the TR-invariant points, or meeting vortices from the other half not at TR-invariant points.

Z_2 Topological index:

$$I = \frac{1}{2\pi i} \int_C d\vec{k} \cdot \vec{\nabla} \log\left(P(\vec{k})\right)$$

C ← boundary of BZ/2

Total vorticity of BZ/2, even or odd

"Atomic limit": Bloch functions do not depend on momentum $\Rightarrow P(\vec{k})=1$ everywhere in BZ.
Zeros of $P(\vec{k})$ appear through closure of bulk gap.

Minimal models of 2D and 3D TR-invariant topological insulators are 4-band models with the Hamiltonian a 4x4 Hermitian matrix

$$H(\vec{k}) = \sum_{\alpha=1}^{5} d_\alpha(\vec{k})\,\Gamma_\alpha + \sum_{\alpha<\beta}^{5} d_{\alpha\beta}(\vec{k})\,\Gamma_{\alpha\beta}$$

$$[\Gamma_\alpha, \Gamma_\beta] = 2\delta_{\alpha\beta}\,, \quad \alpha,\beta = 1,2,3,4,5$$

Clifford algebra

$$\Gamma_{\alpha\beta} = \frac{1}{2i}[\Gamma_\alpha, \Gamma_\beta]$$

Take $\Gamma_\alpha = \{\sigma_x I,\ \sigma_z I,\ \sigma_y S_x,\ \sigma_y S_y,\ \sigma_y S_z\}$

(σ – sublattice, S – spin)

for the Kane-Mele model (TR-invariant)

$$T\,\Gamma_\alpha\,T^{-1} = \Gamma_\alpha \quad \text{with} \quad T = i(I \otimes S_y)K$$

TR invariance:

$$T\,\Gamma_{\alpha\beta}\,T^{-1} = -\Gamma_{\alpha\beta}$$

TR-invariant Hamiltonian

$$d_\alpha(-\vec{k}) = d_\alpha(\vec{k}), \quad d_{\alpha\beta}(-\vec{k}) = -d_{\alpha\beta}(\vec{k})$$

Example: Kane-Mele model, $\lambda_R = 0$

$$H(\vec{k}) = d_1(\vec{k})\Gamma_1 + d_2(\vec{k})\Gamma_2 + d_{12}(\vec{k})\Gamma_{12} + d_{15}(\vec{k})\Gamma_{15}$$

K-point: $d_1 = d_{12} = 0$

$$h_\uparrow(\vec{K}) = \begin{bmatrix} \lambda_v + 3\sqrt{3}\lambda_{so} & 0 \\ 0 & -(\lambda_v + 3\sqrt{3}\lambda_{so}) \end{bmatrix}$$

$$h_\downarrow(\vec{K}) = \begin{bmatrix} \lambda_v - 3\sqrt{3}\lambda_{so} & 0 \\ 0 & -(\lambda_v - 3\sqrt{3}\lambda_{so}) \end{bmatrix}$$

First consider $\lambda_v \gg \lambda_{so}$

Occupied bands:

$$E_1 = -(\lambda_v + 3\sqrt{3}\lambda_{so}), \quad |u_1(\vec{K})\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$E_2 = -\lambda_v + 3\sqrt{3}\lambda_{so}, \quad |u_2(\vec{K})\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

TR symmetry expressed via

$$T = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} K$$

$$\langle u_1(\vec{K})|T|u_2(\vec{K})\rangle = 1, \quad |P(\vec{K})| = 1$$

Now $\lambda_v < 3\sqrt{3}\lambda_{so}$ (level crossing)

$$E_1 = -(\lambda_v + 3\sqrt{3}\lambda_{so}), \quad |u_1(\vec{K})\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

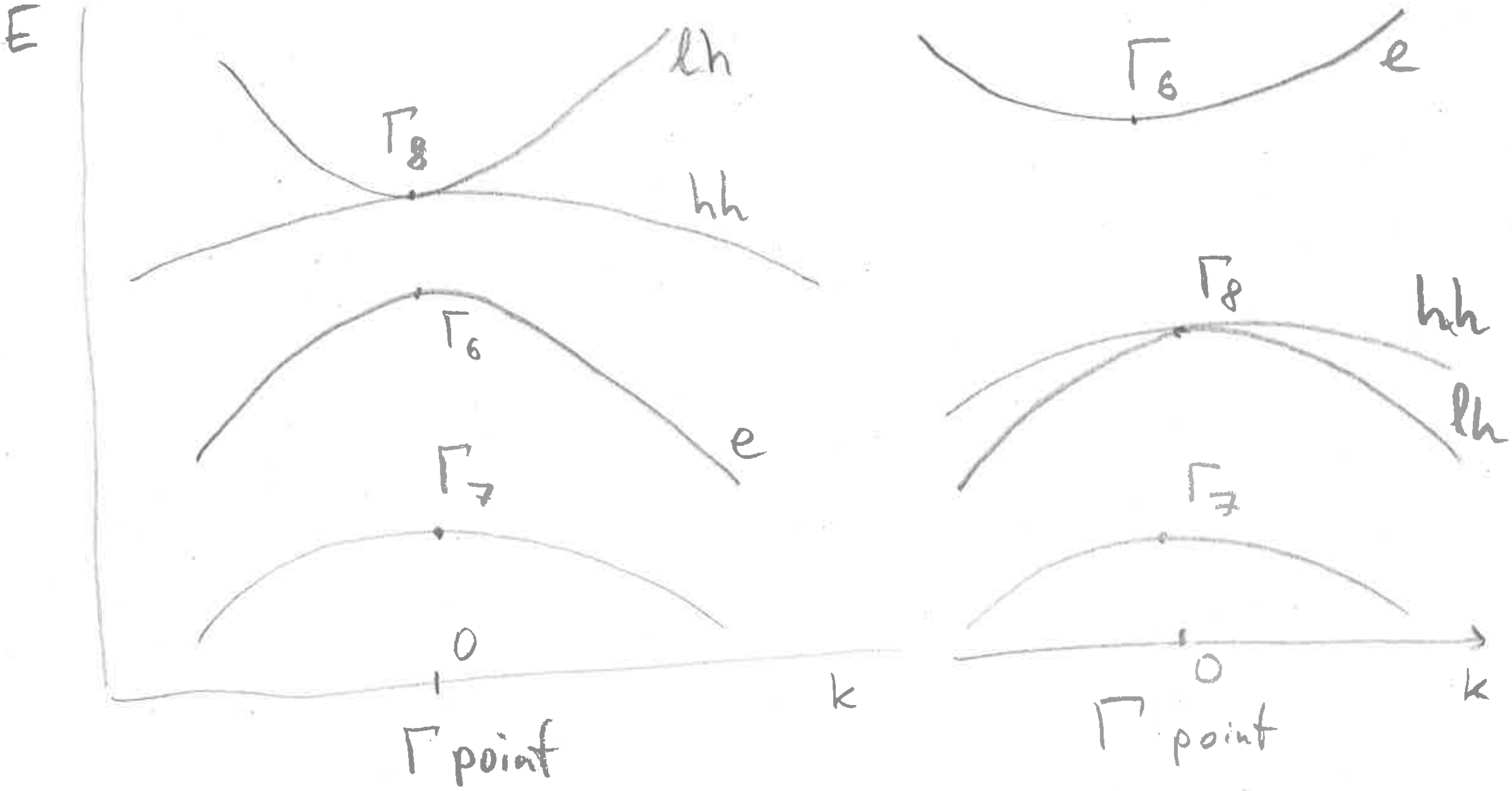
$$E_2 = \lambda_v - 3\sqrt{3}\lambda_{so}, \quad |u_2(\vec{K})\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\langle u_1(\vec{K})|T|u_2(\vec{K})\rangle = 0, \quad |P(\vec{K})| = 0$$

Zero in Pfaffian appears through level crossing

7.4 2D TR topological insulators in inverted quantum wells

3D: HgTe (inverted) CdTe (normal)



Neglect Γ_7 band

s-type Γ_6, p-type Γ_8 bands
$(s_z = \pm\frac{1}{2})$ $(s_z = \pm\frac{1}{2}, \pm\frac{3}{2})$

6-component spinor

$$\Psi = \left(|\Gamma_6, \tfrac{1}{2}\rangle, |\Gamma_6, -\tfrac{1}{2}\rangle, |\Gamma_8, \tfrac{3}{2}\rangle, |\Gamma_8, \tfrac{1}{2}\rangle, |\Gamma_8, -\tfrac{1}{2}\rangle, |\Gamma_8, -\tfrac{3}{2}\rangle \right)^T$$

combine into E1, H1, L1 bands with ↑, ↓

L1 splits off

$$H_{BHZ} = \begin{pmatrix} \epsilon(k)+m(k) & Ak_+ & 0 & 0 \\ Ak_- & \epsilon(k)-m(k) & 0 & 0 \\ 0 & 0 & \epsilon(k)+m(k) & -Ak_- \\ 0 & 0 & -Ak_+ & \epsilon(k)-m(k) \end{pmatrix}$$

$$= \epsilon(k)\sigma_0 s_0 + m(k)\sigma_z s_0 + Ak_x\sigma_x s_x - Ak_y\sigma_y s_0$$

(σ - E1-H1, s - Kramers partners)

$m(k) = M + Bk^2$, $\epsilon(k) = C + Dk^2$

$$E_k^{\pm} = \epsilon(k) \pm \sqrt{A^2k^2 + m^2(k)}$$

$$\psi_k^{(\pm)}(r) = \chi_k^{(\pm)} e^{ikr}$$

$$\chi_k^{(I,\pm)} = \frac{1}{\sqrt{1+\mu_\pm^2}}\begin{pmatrix} 1 \\ \mu_\pm e^{-i\varphi_k} \end{pmatrix}$$

Block I

$\Updownarrow$ TR

Block II

$$\chi_k^{(II,\pm)} = \frac{1}{\sqrt{1+\mu_\pm^2}}\begin{pmatrix} 1 \\ -\mu_\pm e^{i\varphi_k} \end{pmatrix}$$

$$\mu_\pm = \frac{\pm\sqrt{A^2k^2+m^2(k)} - m(k)}{A|k|}$$

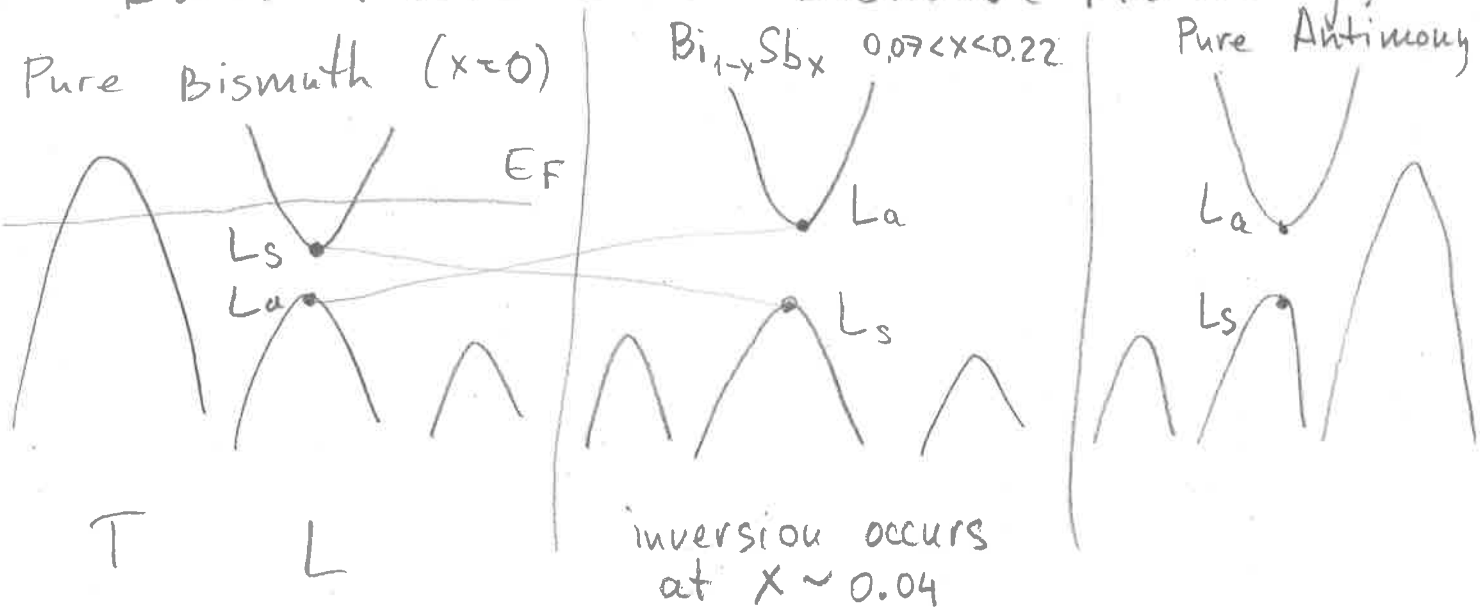
$$H_{BIA} = \begin{pmatrix} 0 & 0 & \delta_e k_+ & -\Delta_0 \\ 0 & 0 & \Delta_0 & \delta_h k_- \\ \delta_e k_- & \Delta_0 & 0 & 0 \\ -\Delta_0 & \delta_h k_+ & 0 & 0 \end{pmatrix}, \quad H_{SIA} = \begin{pmatrix} 0 & 0 & ir_e k_- & 0 \\ 0 & 0 & 0 & 0 \\ -ir_e k_+ & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Bulk inversion asymmetry

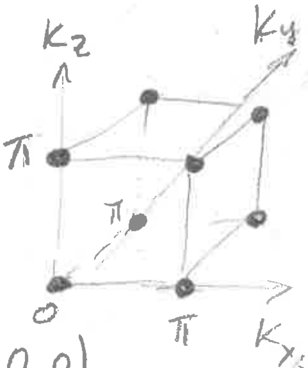
structural inversion asymmetry

7.5 3D topological insulators

Band structure of Bismuth Antimony:



8 TR invariant momenta Λ_a



$$I = \prod_{i=1}^{8} \frac{\sqrt{\det[B(\Lambda_i)]}}{\mathrm{Pf}[B(\Lambda_i)]}$$

$$\Lambda_i = \{(0,0,0), (0,0,\pi), (0,\pi,0), (0,\pi,\pi), (\pi,0,0), (\pi,0,\pi), (\pi,\pi,0), (\pi,\pi,\pi)\}$$

When $I = -1$ strong topological insulator; 2D surface state is gapless (and robust with respect to disorder – Chapter "Topology and localization")

One can introduce three more topological invariants corresponding to different facets of the cube (products over 4 TR invariant momenta, like in 2D). These define "weak topological insulators", whose surface states are not robust.