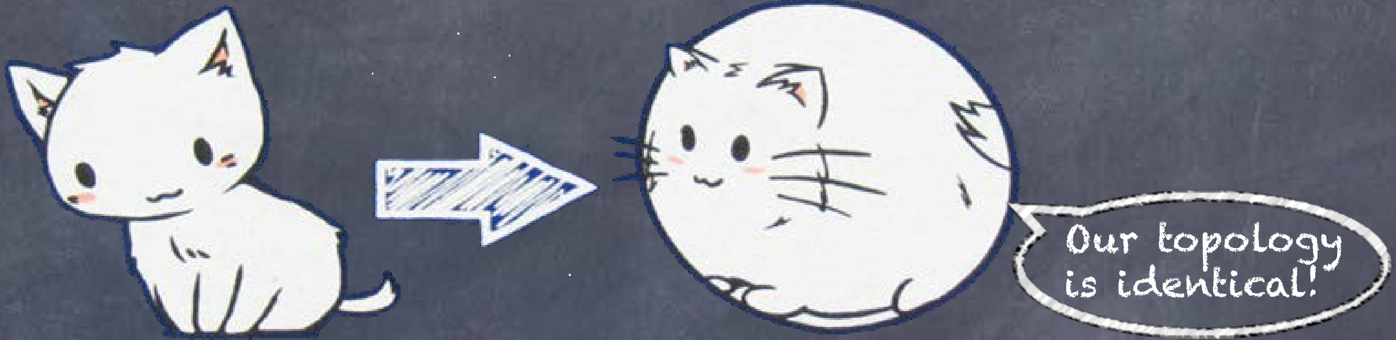
Feature-energy duality of topological boundary states in multilayer quantum spin Hall insulator



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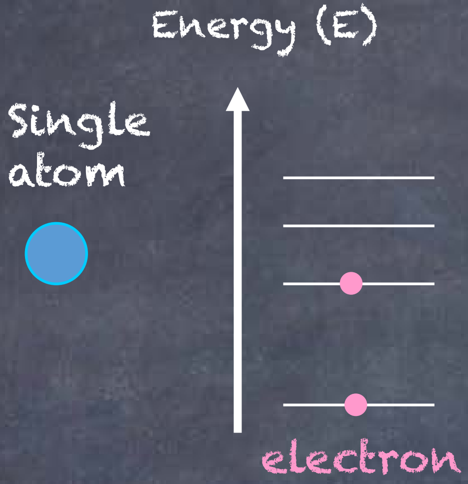
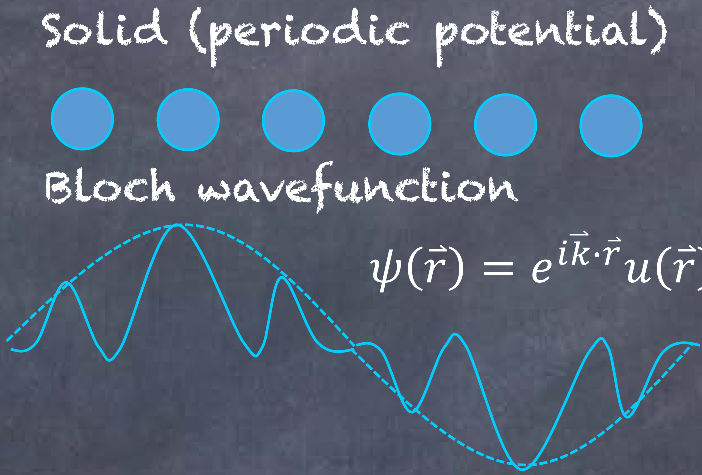
Tay-Rong Chang (張泰榕)

2024/Aug./28

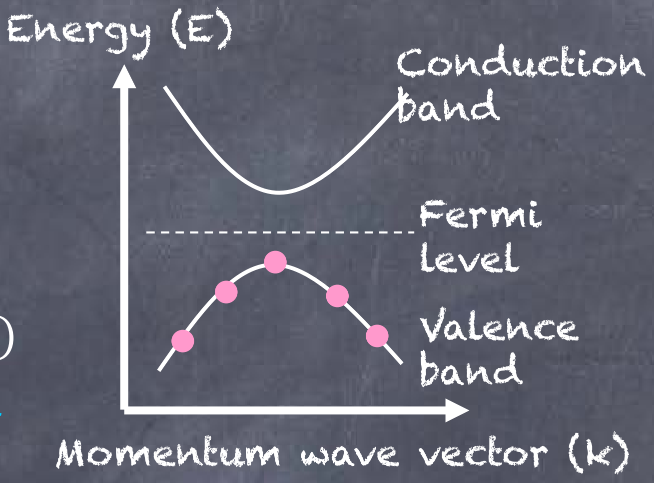
Band theory

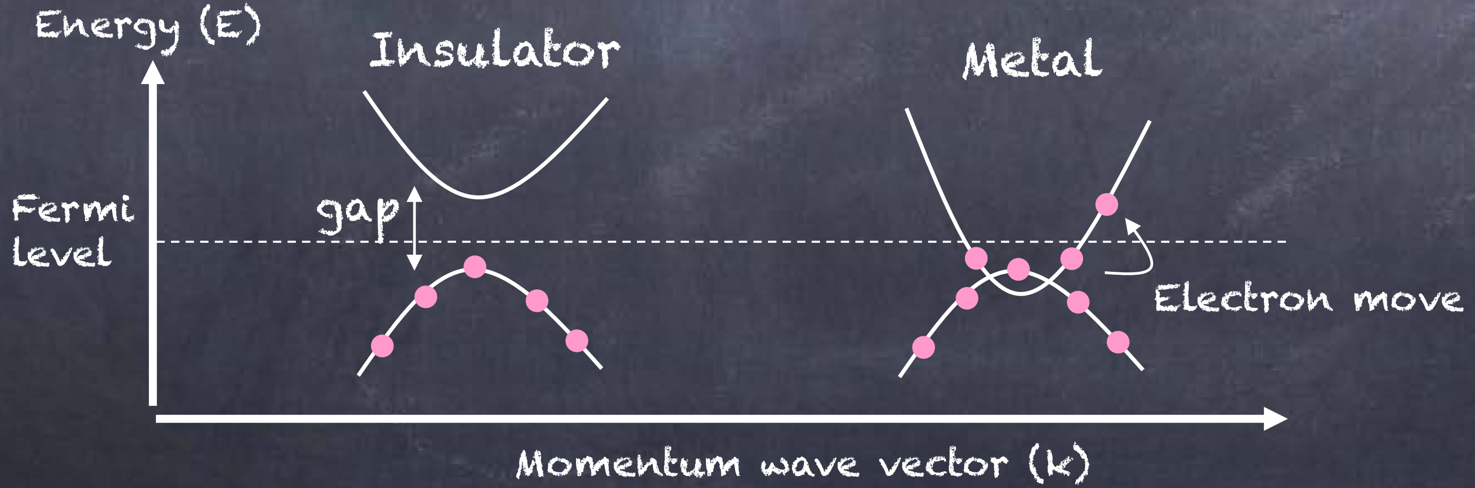




$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$$

Band structure





Band theory (topology)

Math => real space

Gauss-Bonnet Theorem:

$$\int_S K_{Gauss} ds = 4\pi(1-g)$$

Gauss curvature

genus

Phys => momentum space

TKNN theorem:

Topological invariant number

$$\frac{1}{2\pi}\sum_{m=occ}\int_{BZ} d^2k\, \underline{\vec{\nabla}\times i\left\langle u_m\middle|\vec{\nabla}\middle|u_m\right\rangle} = n$$

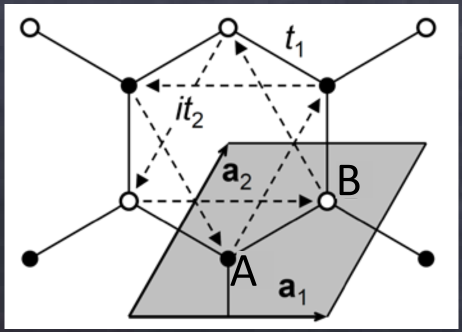
Berry curvature

Bloch wavefun

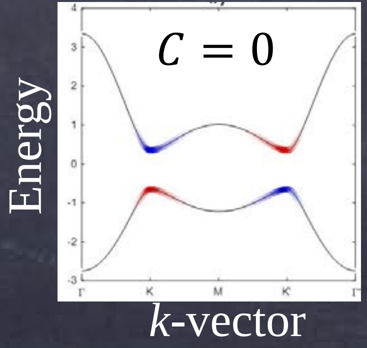
Haldane model (2D honeycomb lattice)

Ref: PRL61, 2015 (1988)

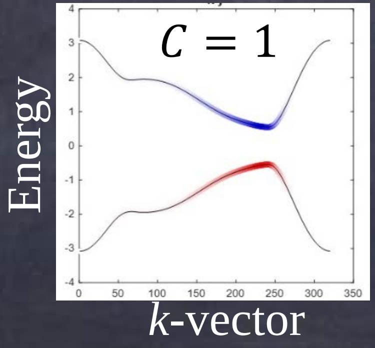
$$H=\sum_i(-1)^{\tau_i}Mc_i^\dagger c_i + t_1\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + h.c.\right) + t_2\sum_{\langle\langle ij\rangle\rangle}\left(e^{i\phi_{ij}}c_i^\dagger c_j + h.c.\right)$$



$M = 0.7, t_1 = -1, \boldsymbol{t_2 = 0}$



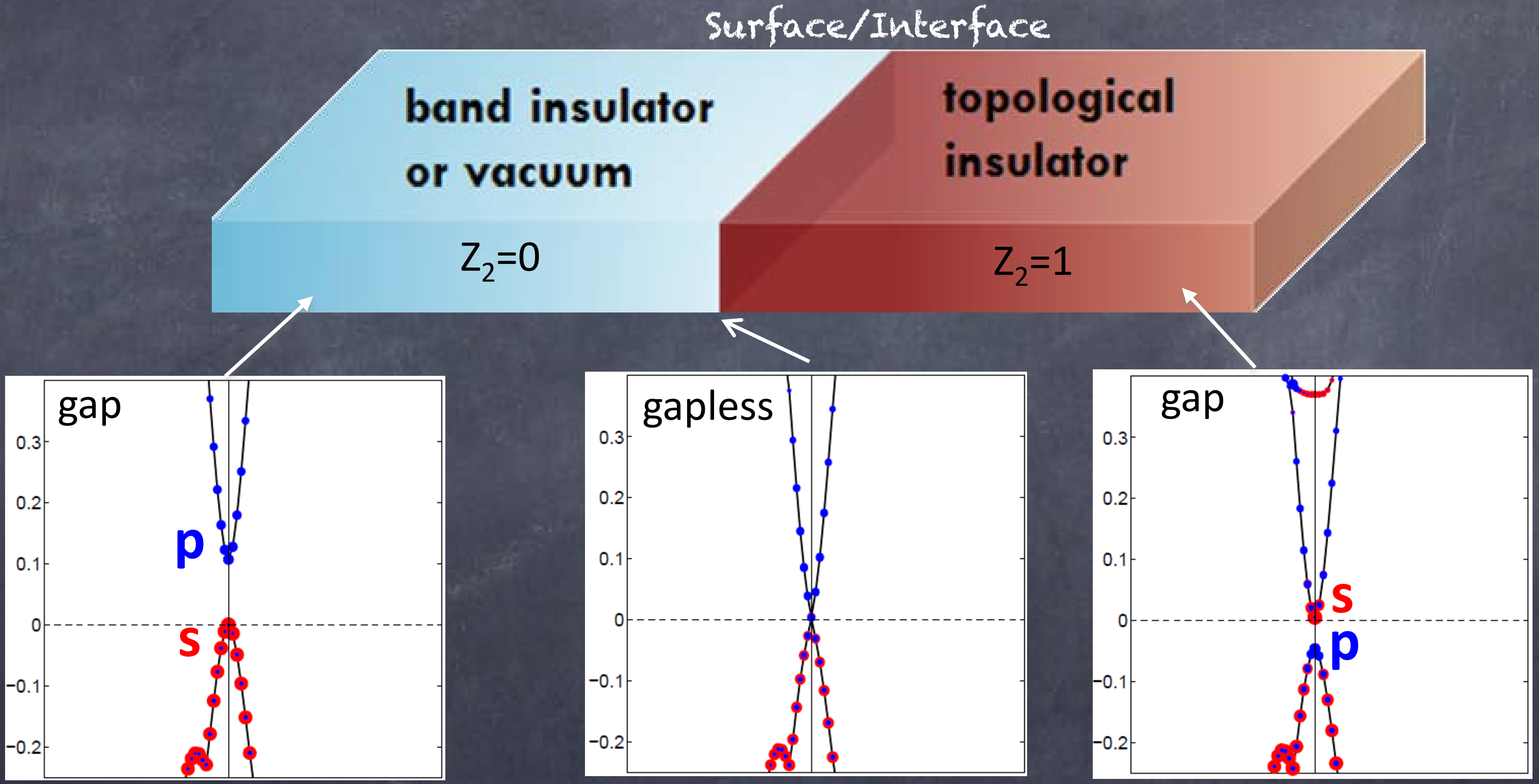
$M = 0.7, t_1 = -1, \boldsymbol{t_2 = -0.24}$



Berry curvature

Band theory (topology)

Bulk-boundary correspondence



The gapless boundary state is the hallmark of topological phase

Ref: Rev. Mod. Phys. 82, 3045 (2010)
Ref: Rev. Mod. Phys. 83, 1057 (2011)

Topological non-trivial state

Bulk property

Topological invariant number

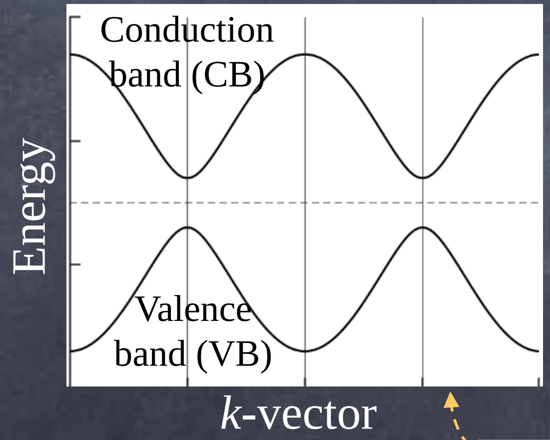
Chern number, $\mathbb{Z}_2$ index, $\mathbb{Z}_4$ index, winding number...etc

Bulk-boundary correspondence

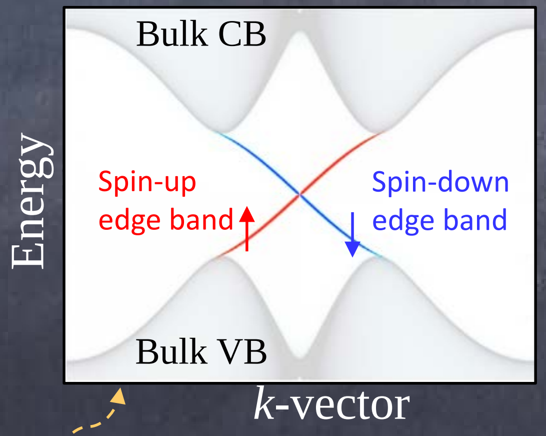
Edge property

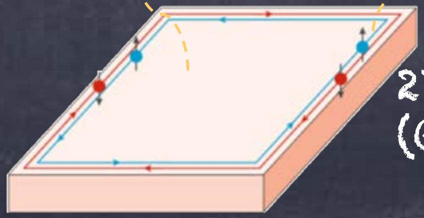
Gapless topological boundary state

Topological invariant number: $\mathbb{Z}_2$ index $(\mathbb{Z}_2 = 1)$



Gapless edge band



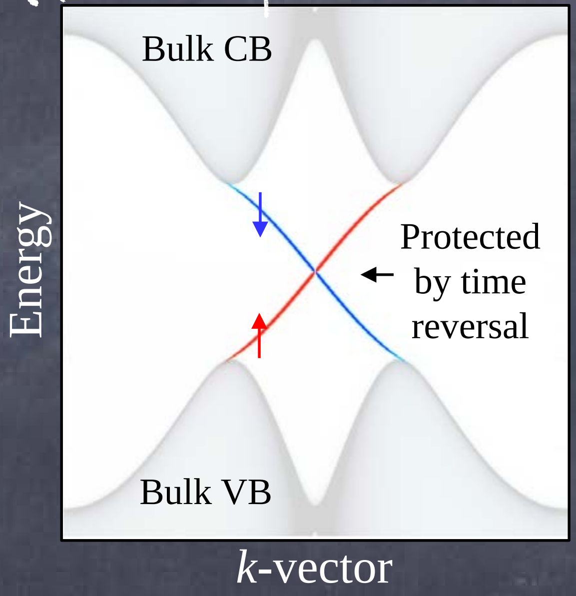


2D $\mathbb{Z}_2$ topological insulator (Quantum spin Hall insulator)

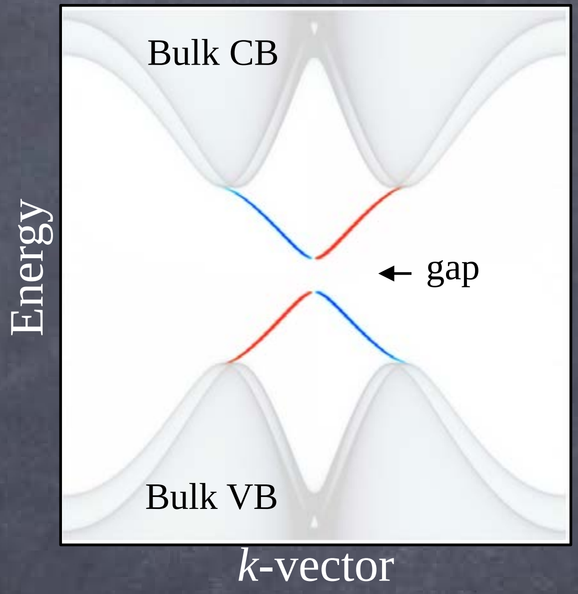
Topological non-trivial state

If we consider ....

2D $\mathbb{Z}_2$ topological insulator
(Quantum spin Hall insulator)



Symmetry breaking perturbation →



Is this system topologically trivial?

- Band structure (symmetry): trivial
- Feature Spectrum Topology: non-trivial

Outline

- Topological nontrivial state (with) symmetry protection

  2D $\mathbb{Z}_2$ topological insulator (Quantum spin Hall insulator)

The central question of this talk: If the boundary state no longer connects the valence band and the conduction band, is this system topologically trivial?

- Feature Spectrum Topology

  Kane-Mele model

  Feature-energy duality

- Material realization

  Multilayer Bi_4Br_4

Kane-Mele model w/o Rashba SOC

Ref: PRL95, 226801 (2005) · PRL95, 146802 (2005)

Kane-Mele model (2D honeycomb lattice)

$$H_0 = t\sum_{\langle i,j\rangle\alpha} c^{\dagger}_{i\alpha}c_{j\alpha} + \underbrace{\frac{i\lambda_I}{3\sqrt{3}}\sum_{\langle\langle i,j\rangle\rangle\alpha\beta} \nu_{ij}c^{\dagger}_{i\alpha}(s_z)_{\alpha\beta}c_{j\beta}}_{\text{Intrinsic SOC}}$$

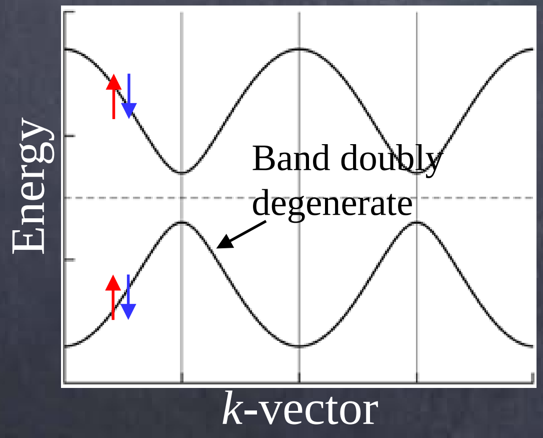
Matrix form

Basis

$$H_0 = \begin{array}{cc|c} |\uparrow\rangle & |\downarrow\rangle & \\ H^{+}_{QAH} & 0 & |\uparrow\rangle \\ 0 & H^{-}_{QAH} & |\downarrow\rangle \end{array}$$

H_{QAH} Haldane Hamiltonian (2x2 matrix)

Band structure

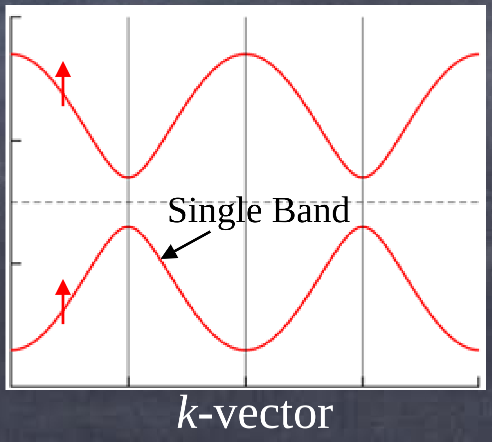


$\hat{S}_z$-conserved

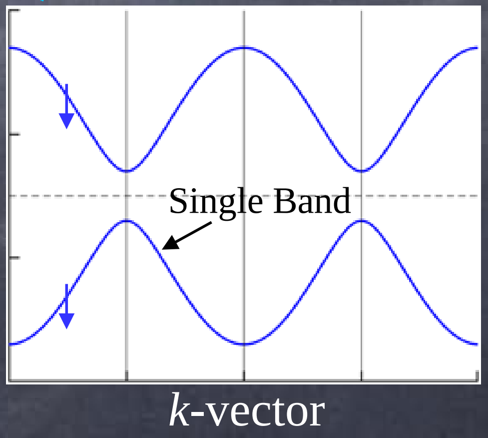
→

$|\uparrow\rangle_{VB}$ and $|\downarrow\rangle_{VB}$ separated

Spin-up (H^{+}_{QAH})



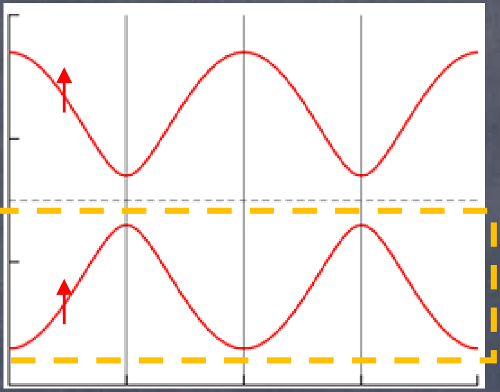
Spin-down (H^{-}_{QAH})



Kane-Mele model w/o Rashba SOC

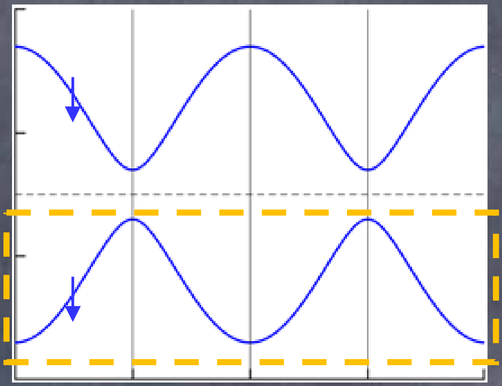
Chern number: $C = \frac{1}{2\pi} \sum_{m=occ} \int dk^2\, \vec{\nabla} \times i \left\langle u_m \middle| \vec{\nabla} \middle| u_m \right\rangle$ Bloch wavefun of VB

Spin-up (H_{QAH}^{+})



Spin-up Chern number $C_s^{\uparrow} = 1$

Spin-down (H_{QAH}^{-})



Spin-down Chern number $C_s^{\downarrow} = -1$

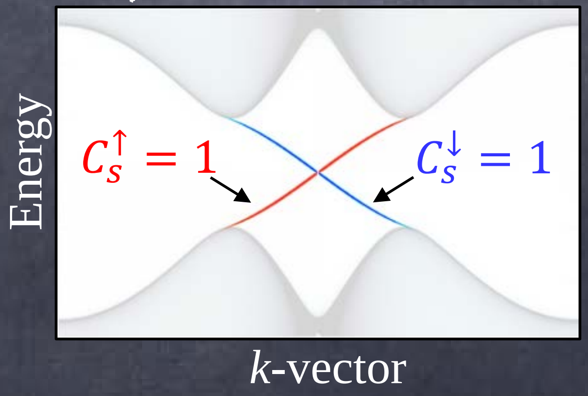
Spin Chern number (C_s)

$$C_s = \frac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1$$

$$\mathbb{Z}_2 = mod(C_s, 2) = 1$$

Bulk-boundary correspondence

Gapless edge bands



Kane-Mele model is a quantum spin Hall insulator

Kane-Mele model ($\mathcal{T}$-broken)

Kane-Mele model (2D honeycomb lattice)

$$H_M = H_0 \underbrace{- i\frac{2}{3}\lambda_{so}\sum_{\langle\langle i,j\rangle\rangle\alpha\beta}\mu_i c^{\dagger}_{i\alpha}\left(\boldsymbol{s}\times\hat{\boldsymbol{d}}_{ij}\right)^{z}_{\alpha\beta}c_{j\beta}}_{\text{Rashba SOC: off-diagonal terms (break } \hat{S}_z \text{ symmetry)}} + \underbrace{M\sum\nolimits_{i\alpha} c^{\dagger}_{i\alpha}s_z c_{i\alpha}}_{\text{Zeeman exchange field (break } \mathcal{T}\text{)}} - l\sum\nolimits_{i\alpha}\mu_i c^{\dagger}_{i\alpha}c_{i\alpha}$$

Kane-Mele
($\hat{S}_z$ conserved)

Matrix form

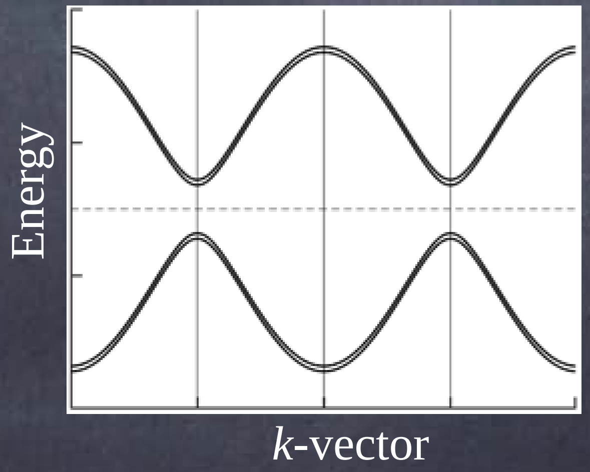
$$H_M = \begin{array}{cc} \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \quad \text{Basis} \end{array} & \\ \begin{pmatrix} H^{+}_{QAH} + M & -H_R \\ H_R & H^{-}_{QAH} - M \end{pmatrix} & \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Rashba SOC

Zeeman

H_{QAH} Haldane Hamiltonian

Band structure



$|\uparrow\rangle_{VB}$ and $|\downarrow\rangle_{VB}$ mixed

Kane-Mele model ($\mathcal{T}$-broken)

Matrix form

Basis

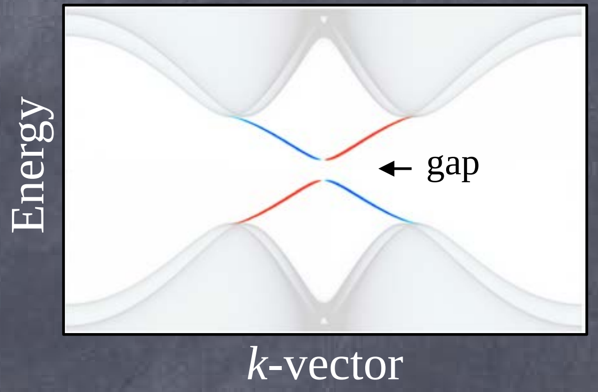
$$\begin{array}{cc} & \begin{array}{cc} |\uparrow\rangle & \qquad\qquad |\downarrow\rangle \end{array} \\ H_M = & \begin{pmatrix} H^{+}_{QAH} + M & -H_R \\ H_R & H^{-}_{QAH} - M \end{pmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Rashba SOC

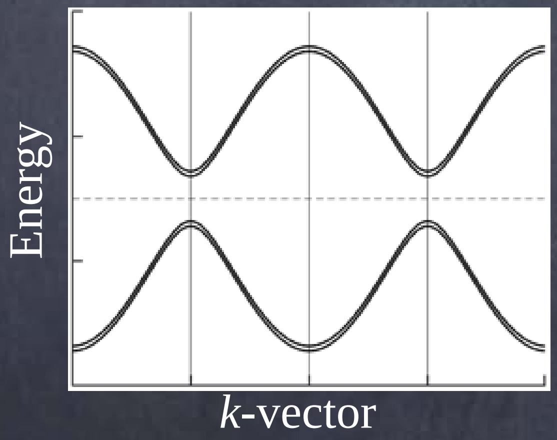
Zeeman

H_{QAH} Haldane Hamiltonian

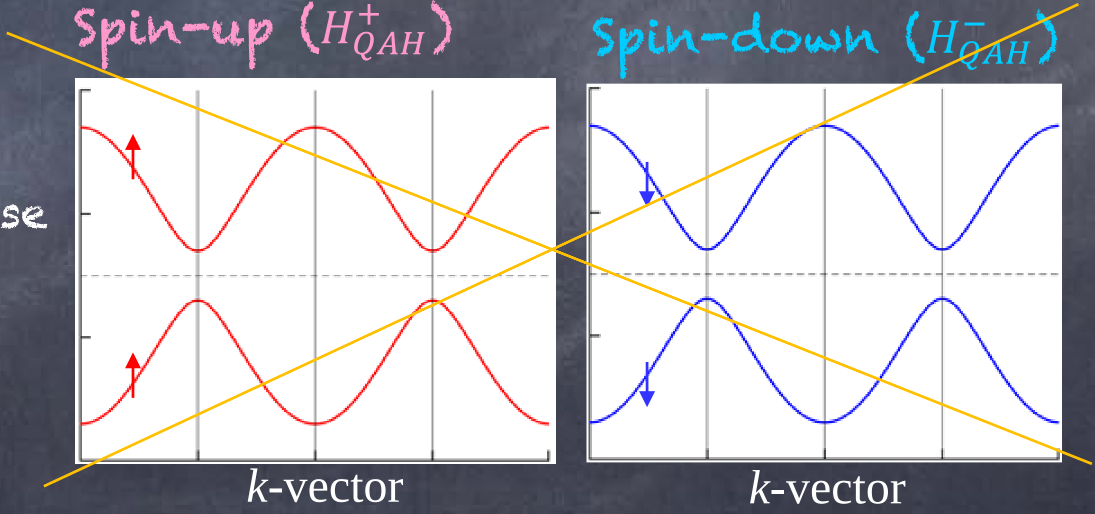
Edge bands



Band structure



decompose



Spin-up (H^{+}_{QAH})

Spin-down (H^{-}_{QAH})

How to deal with topological phase in this model?

Feature Spectrum Topology

Ref: E. Prodan PRB 80, 125327 (2009), H. Lin arXiv:2310.14832v1 (2023)

Band structure:

eigenvalue

$$\hat{H}|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

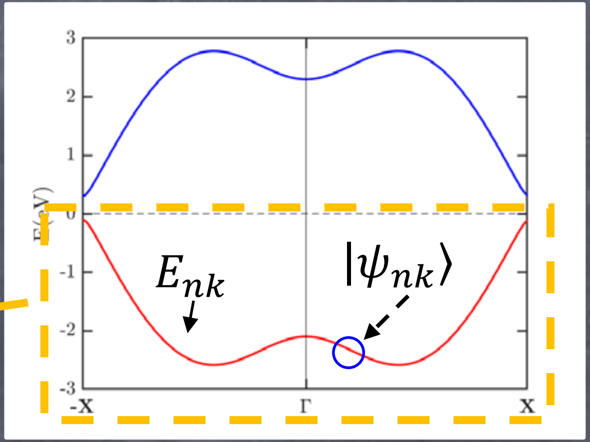
Hamiltonian

eigenstate

$$C = \frac{1}{2\pi}\sum_{m=occ}\int dk^2\Omega_m$$

The nature of band topology mainly comes from valence electron

Band structure



Feature Spectrum Topology:

Feature eigenvalue

$$\widehat{\mathbb{F}}_O|\tilde{\psi}_{mk}\rangle = O_{mk}|\tilde{\psi}_{mk}\rangle$$

Feature operator

$$\widehat{\mathbb{F}}_O = P\hat{O}P$$

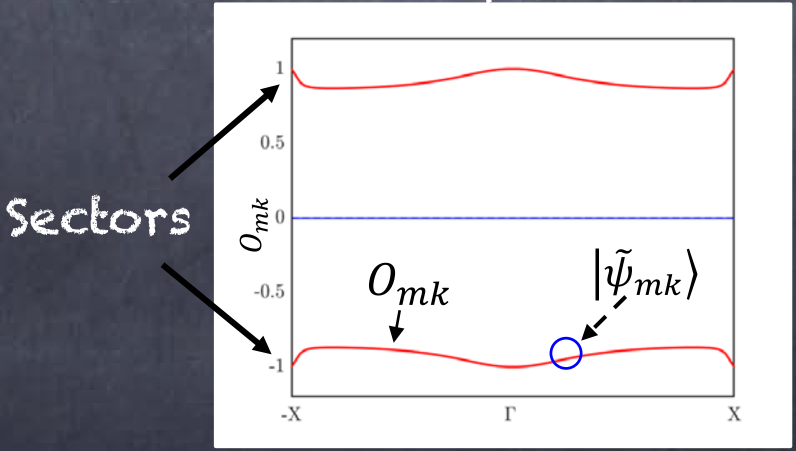
Quantum operator

Projector (project to the occupied state)

Feature eigenstate

$$|\tilde{\psi}_{mk}\rangle = \sum_{i=occ} a_i|\psi_i\rangle_{VB}$$

Feature spectrum



Topological invariant number: Feature Chern number

Feature Spectrum Topology

Kane-Mele model

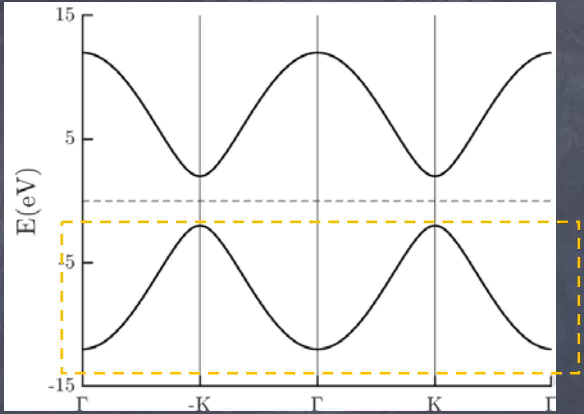
$\hat{H}$ (4x4 matrix)

Projected $\hat{S}_z$ onto the VB of the KM model →

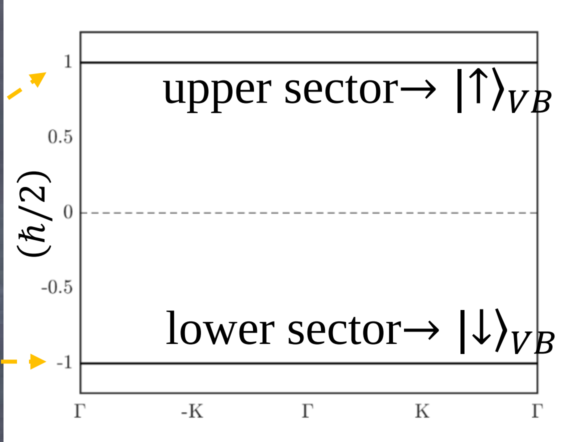
Feature operator

$\hat{\mathbb{F}}_{S_z} = P\hat{S}_zP$ (2x2 matrix)

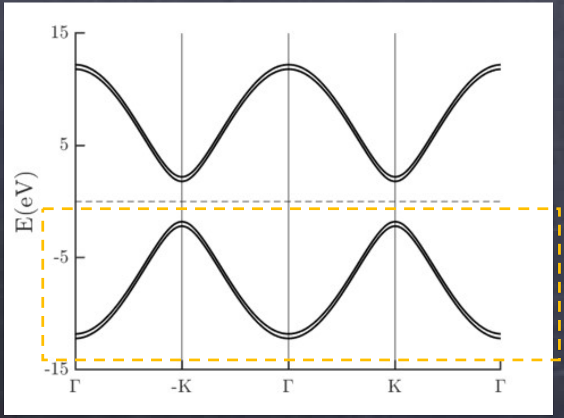
Band structure (w/o Rasba SOC)



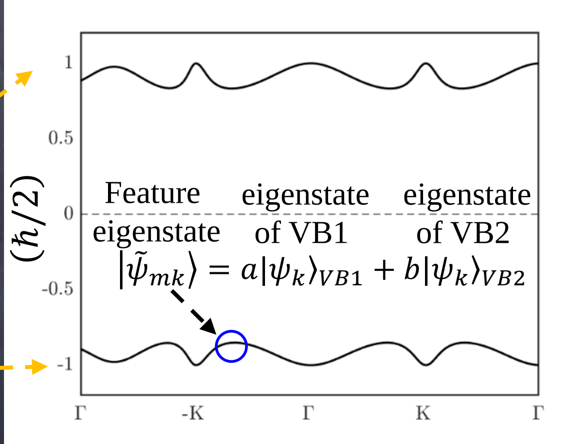
Feature spectrum



Band structure (w/ Rasba SOC, w/o $\mathcal{T}$)



Feature spectrum



Feature Spectrum Topology

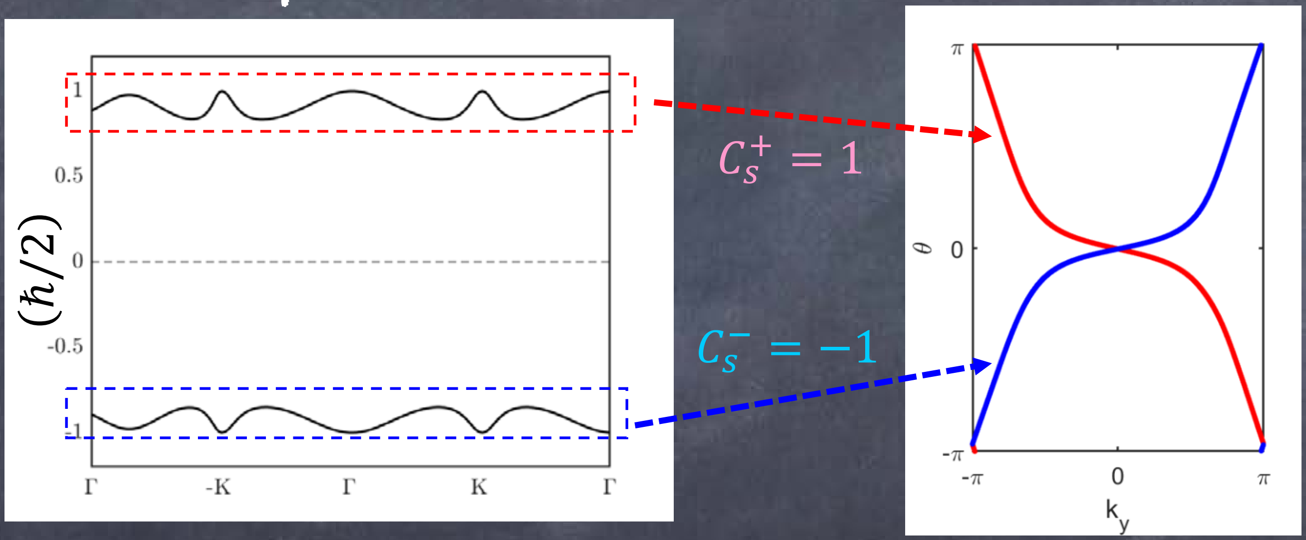
PRB109, 155143 (2024)

Feature operator

$$\hat{\mathbb{F}}_{s_z} = P\hat{S}_z P$$

Feature spectrum

Wilson loop



$C_s^+ = 1$

$C_s^- = -1$

Spin Chern number (C_s)
from feature eigenstates
(feature Chern number) $= C_s = \dfrac{(C_s^+ - C_s^-)}{2} = 1$

Kane-Mele model (with Rasba SOC and break $\mathcal{T}$) is still a QSHI

Feature Spectrum Topology

Bulk property

Topological invariant number

Bulk-boundary correspondence

↔

Edge property

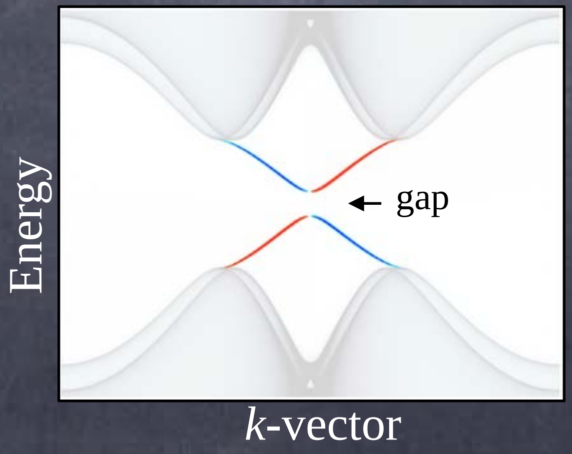
Gapless topological boundary state

Spin Chern number
(feature Chern number)

$$C_s = \frac{(C_s^+ - C_s^-)}{2} = 1$$

?

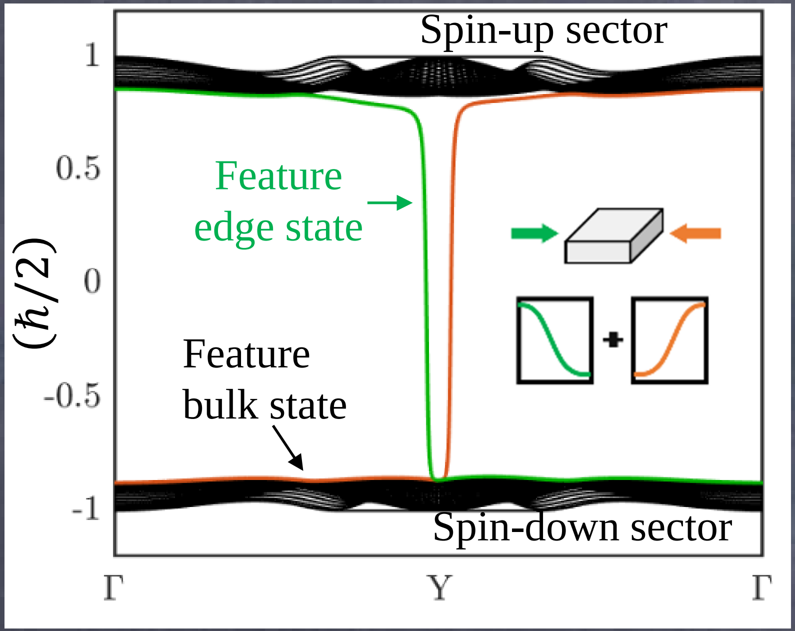
↔



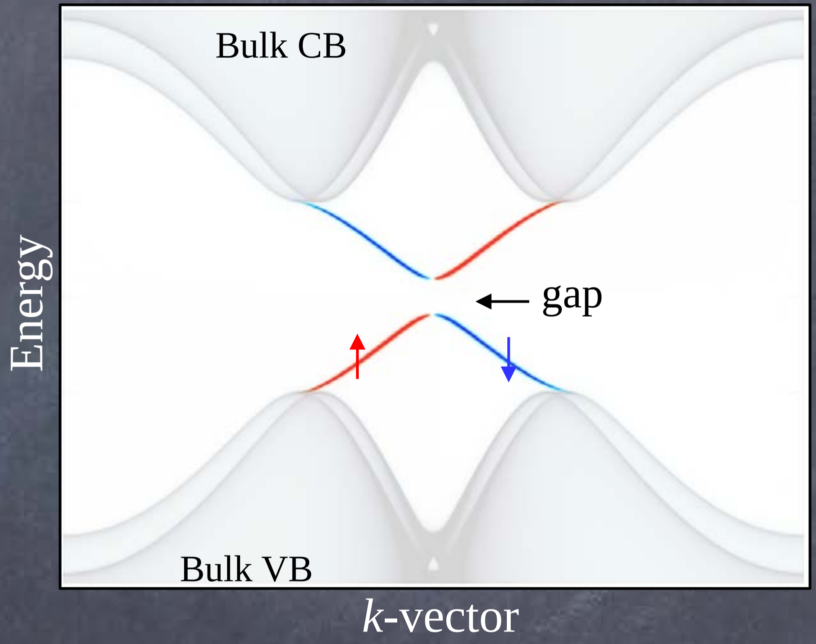
Edge Feature Spectrum

PRB109, 155143 (2024)

Edge feature bands



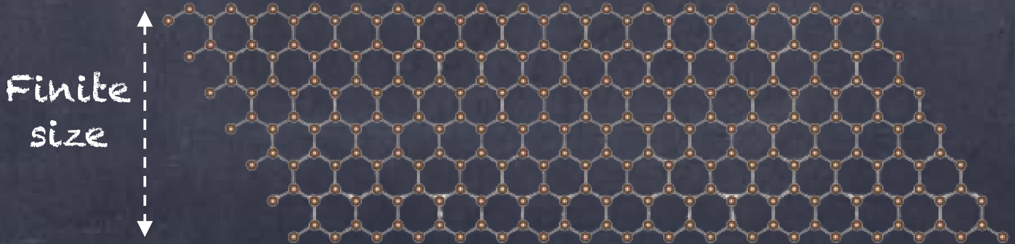
Edge bands (w/o $\mathcal{T}$)



Spin Chern number
(feature Chern number)

$$C_s = \frac{(C_s^{+} - C_s^{-})}{2} = 1$$

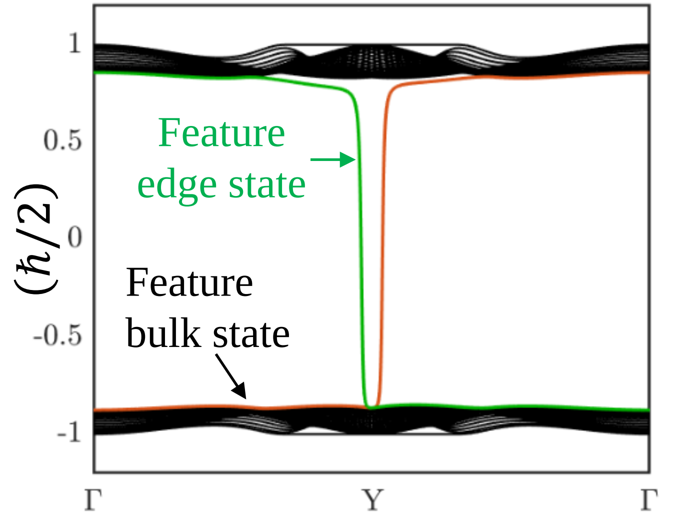
1D ribbon structure



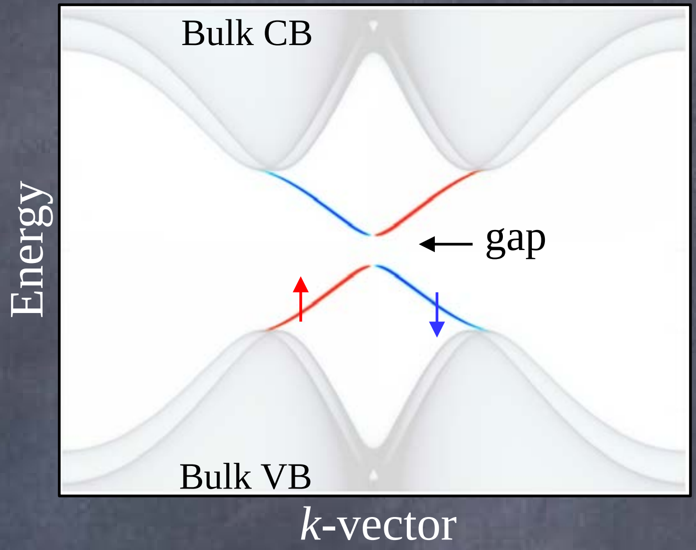
Edge Feature Spectrum

PRB109, 155143 (2024)

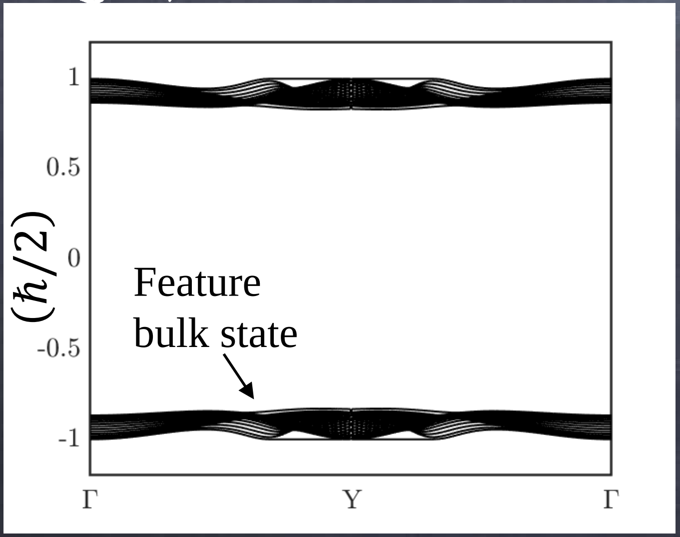
Edge feature bands (w/o $\mathcal{T}$)



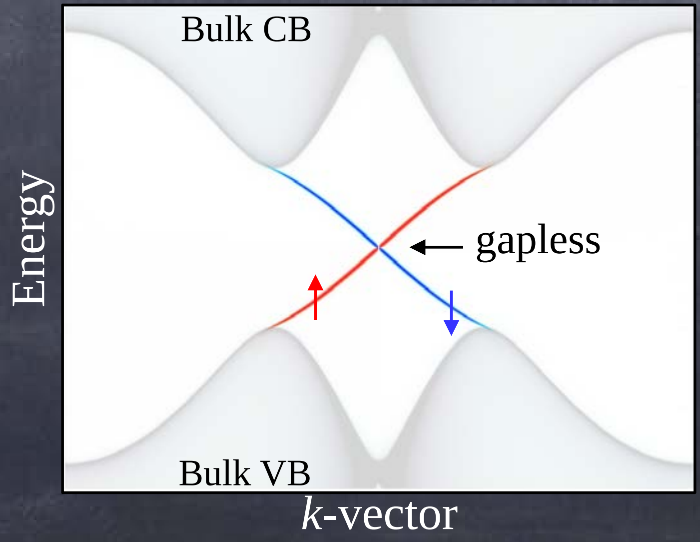
Edge bands (w/o $\mathcal{T}$)



Edge feature bands (w/ $\mathcal{T}$)



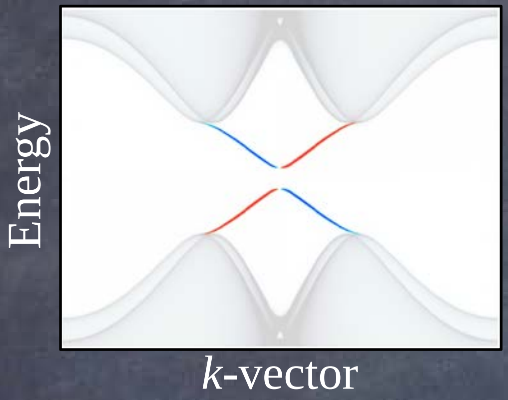
Edge bands (w/ $\mathcal{T}$)



Feature-energy duality

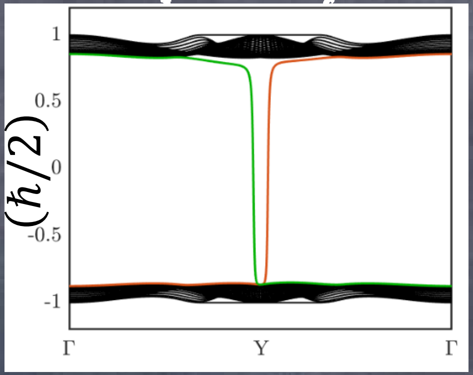
PRB109, 155143 (2024)

Band (w/o $\mathcal{T}$) | # of gapless edge states | **Feature** (w/o $\mathcal{T}$) | # of gapless edge states | Spin Chern number



0

+

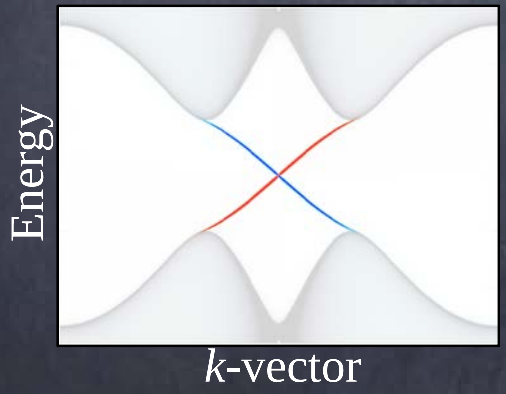


1

=

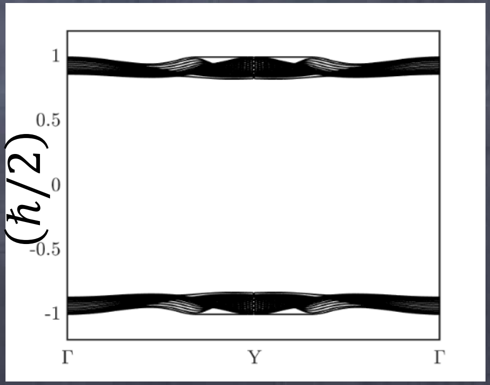
$C_s = 1$

or (w/ $\mathcal{T}$)



1

(w/ $\mathcal{T}$)



0

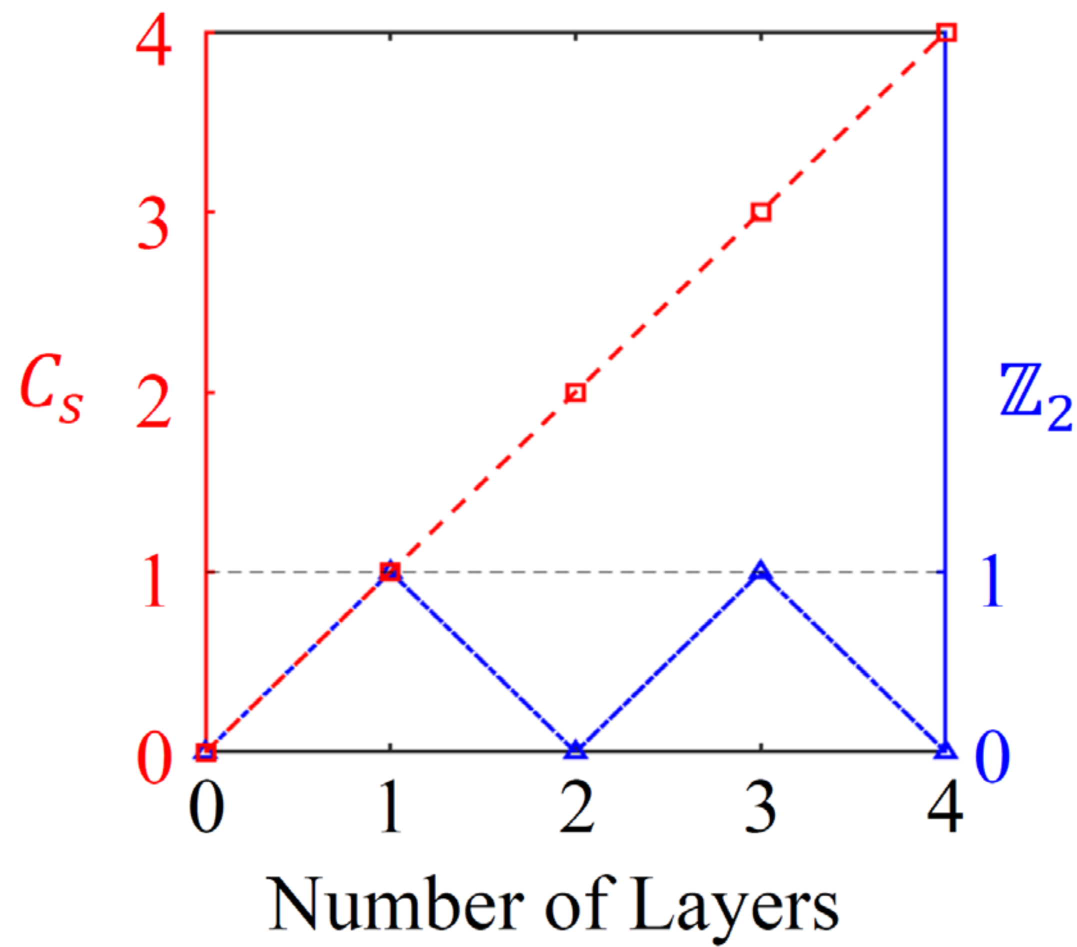
$C_s = 1$

Feature-energy duality: Total number of gapless edge states on the band structure, combined with the non-trivial edge states in the feature spectrum, equals the spin Chern number of QSHI.

Multilayer Kane-Mele model

PRB109, 155143 (2024)

Multilayer Kane-Mele model



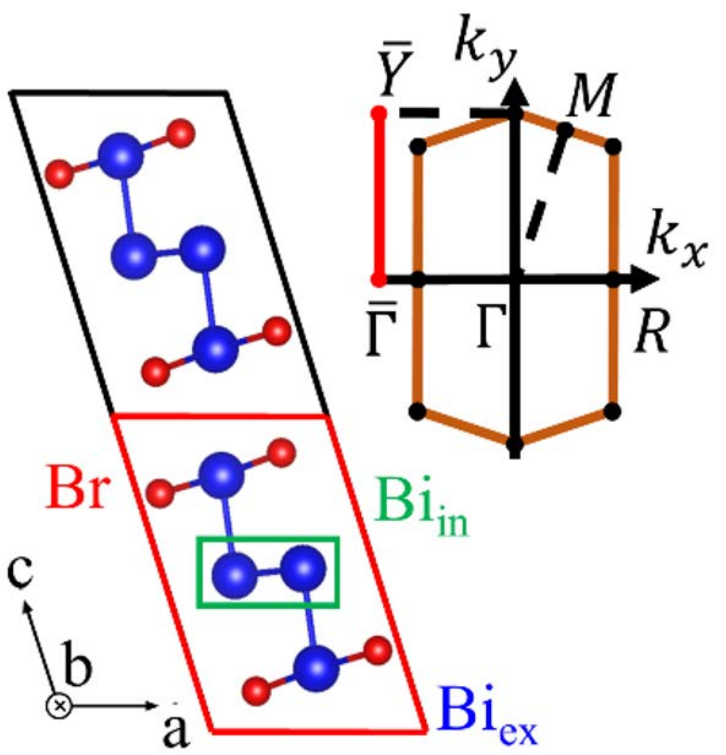
Feature eigenstates:
Spin Chern number C_s exhibits linear increases with the number of layers.

Bloch eigenstates:
$\mathbb{Z}_2$ index oscillates between 1 and 0 for odd and even number of layers, respectively.

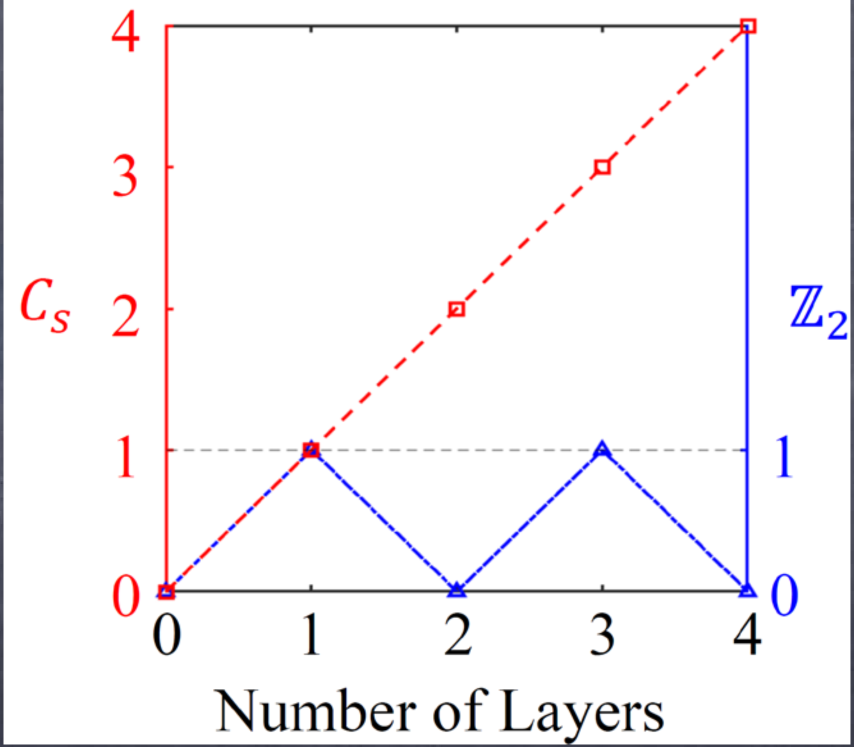
Material realization Bi_4Br_4

PRB109, 155143 (2024)

Quasi-1D structure



Same as multilayer Kane-Mele model



Material realization Bi_4Br_4

PRB109, 155143 (2024)

Monolayer Bi_4Br_4

$C_s = 1, \mathbb{Z}_2 = 1$

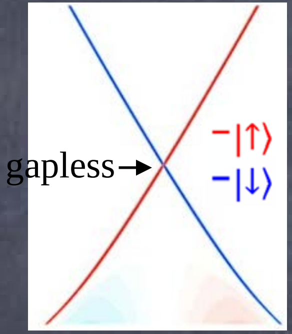
Bilayer Bi_4Br_4

$C_s = 2, \mathbb{Z}_2 = 0$

Trilayer Bi_4Br_4

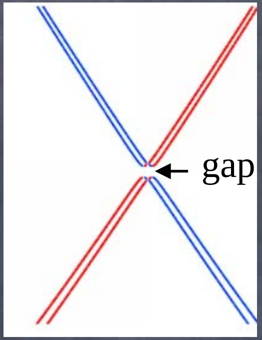
$C_s = 3, \mathbb{Z}_2 = 1$

Bands



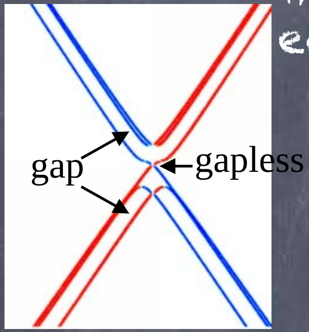
\# of gapless edge states

1



\# of gapless edge states

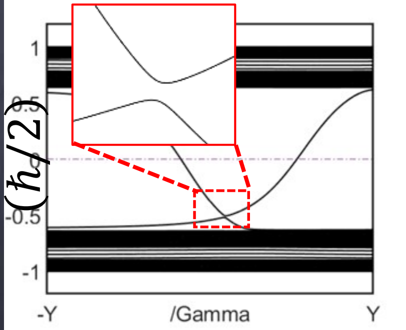
0



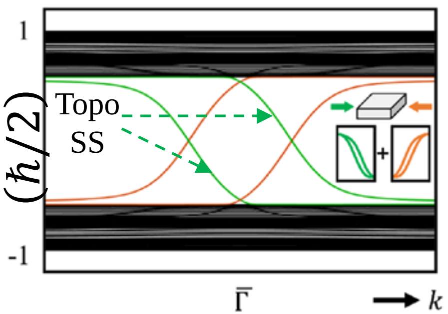
\# of gapless edge states

1

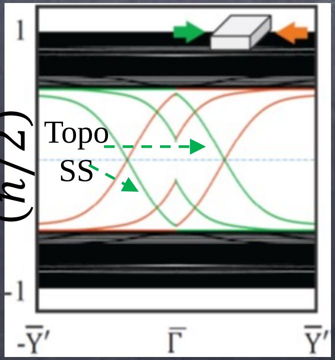
Feature



0



2



2

Conclusion

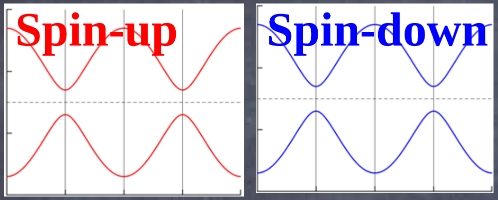
Kane-Mele model ($\hat{S}_z$ conserved)

Rashba SOC w/o $\mathcal{T}$

Kane-Mele model (w/ Rashba SOC) (w/o $\mathcal{T}$)

$\widehat{\mathbb{F}}_{s_z} = P\hat{S}_z P$

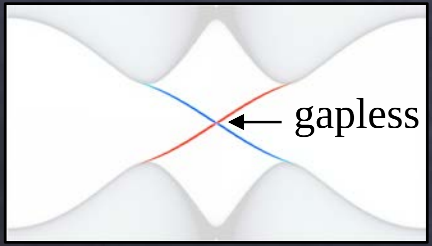
Feature operator



Spin Chern number (Bloch eigenstate)

$$C_s = \frac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1$$

Gapless boundary states in the band structure

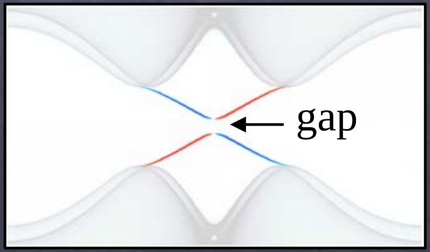


Sz is no longer a good quantum number

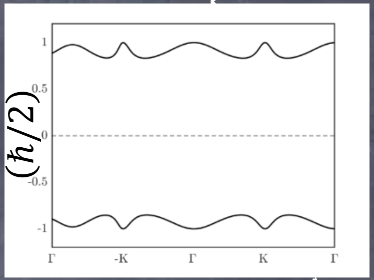
~~Spin Chern number (Bloch eigenstate)~~

$$\cancel{C_s = \frac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1}$$

Gap boundary states in the band structure



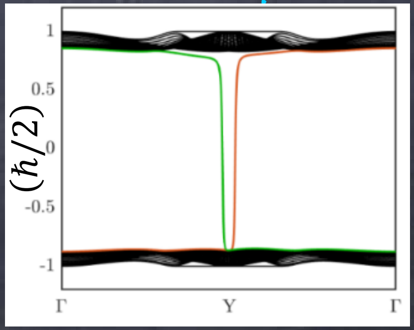
Feature spectrum



Spin Chern number (feature eigenstate)

$$C_s = \frac{(C_s^{\uparrow} - C_s^{\downarrow})}{2} = 1$$

Gapless boundary states in the feature spectrum



Feature-energy duality

Acknowledgements

Feature-energy duality of topological boundary states in a multilayer quantum spin Hall insulator

Phys. Rev. B 109, 155143 (2024)
arXiv:2312.11794 (2023)

My master student

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Hsin Lin (Sinica)

Yi-Chun Hung
(Northeastern U.)

Feature Spectrum Topology
arXiv:2310.14832 (2023)

Thank you !

NSTC 國家科學及技術委員會
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1931

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Center for Quantum Frontiers of Research & Technology

NCTS
Physics Division

To see a world in a grain of sand … —William Blake