Spin-Resolved Topology, Partial Axion Angles, and Half Quantum Spin Hall Surface States in Higher-Order Topological Crystalline Insulators

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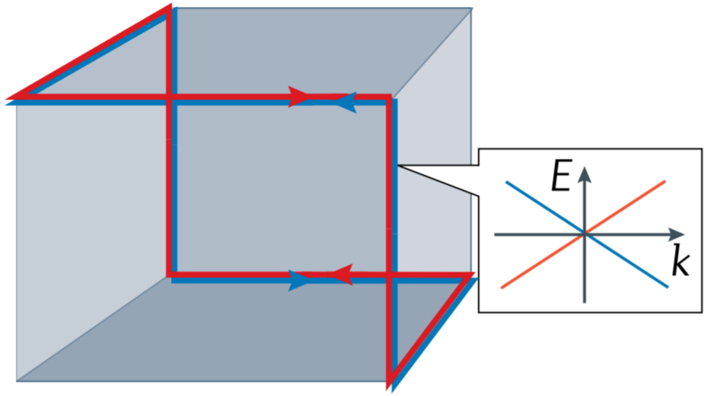
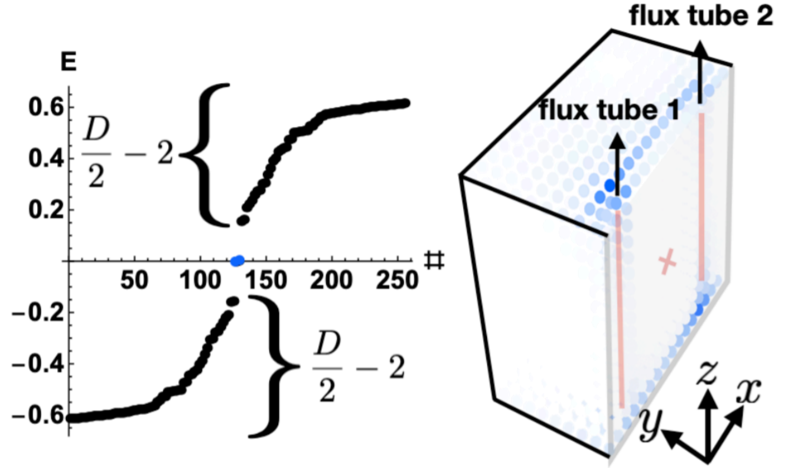
Hiring postdoc Fall 2022/Winter 2023, reach out if interested!

Outline

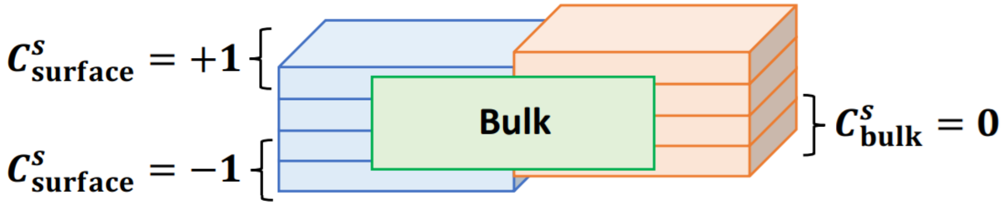


- **Introduction:**
  - Band topology vs. robustness
  - (Higher-order) topological crystalline insulators (HOTIs)



- **What is "robust" about 3D HOTIs?**
  - <u>Signatures without invoking 1D hinges</u>
  - New magnetic flux response
  - Spin-resolved topological invariants and constructions

- **Findings:**
  - ½ quantum spin Hall surface states
  - "Partial" axion angles and parity anomaly
  - Bulk spin-magnetoelectric effect



Schindler, Tsirkin, Neupert, Bernevig, **BJW**, *arXiv:2207.10112*, *To Appear in Nat. Comm.* (2022)
K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Research Teams

Flux insertion numerics:

Schindler, Tsirkin, Neupert, Bernevig, **BJW**, *arXiv:2207.10112, To Appear in Nat. Comm.* (2022)

Frank Schindler
(Princeton)

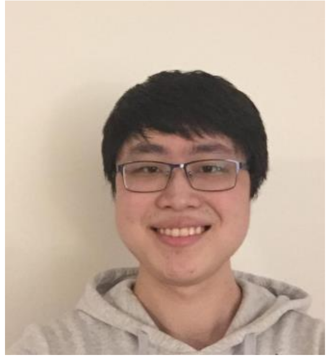
Stepan Tsirkin
(UZH)

Titus Neupert
(UZH)

Andrei Bernevig
(Princeton)

Spin Wilson numerics and theory:

K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)



Kuan-Sen Lin
(UIUC)

Giandomenico Palumbo
(Dublin IAS)

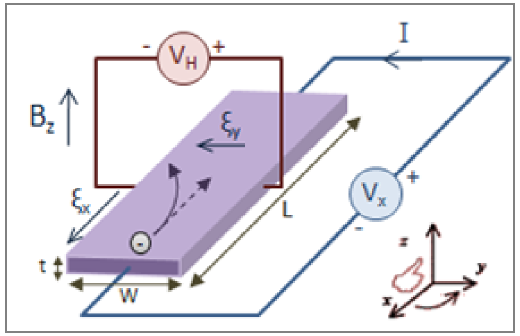
Barry Bradlyn
(UIUC)

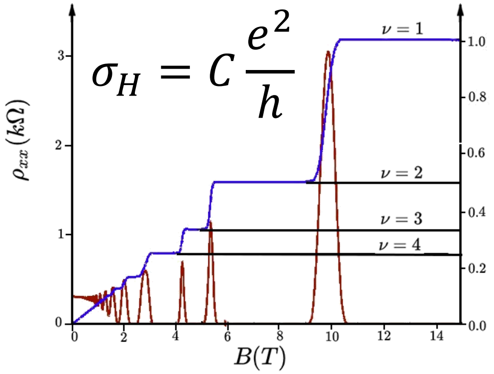
Greg Fiete
(Northeastern/MIT)

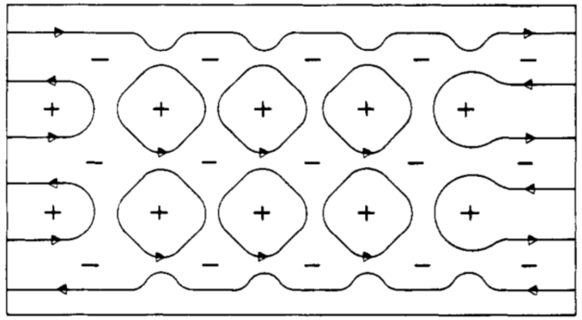
DFT:
Zhaopeng Guo (IOP)
Zhijun Wang (IOP)

Why Do We Care About Topological States?

- **Unambiguous Experimental Robustness – Quantum Hall States**
  - σ_H extremely quantized, robust to disorder, does not *require* band theory



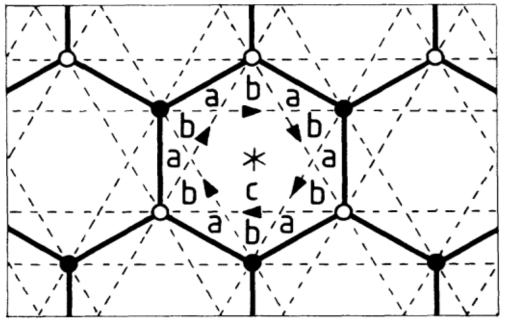




Von Klitzing *et al.*, *PRL* (1980)
Chalker, Coddington, *J. Phys. C.* (1988)

- **Elegance and Accessibility of Band Topology, Connection to Real Materials**
  - Compute invariants, boundary states in tight-binding, DFT
  - Add symmetry (time-reversal, crystal, etc.)

Haldane, *PRL* (1988)
Kane, Mele, *PRL* (2005)
Bernevig, Hughes, Zhang, *Science* (2006)

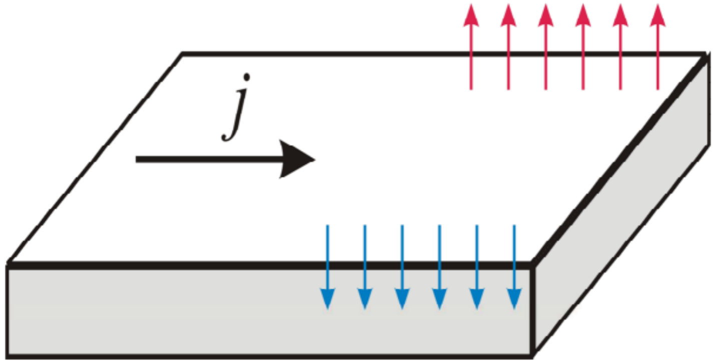


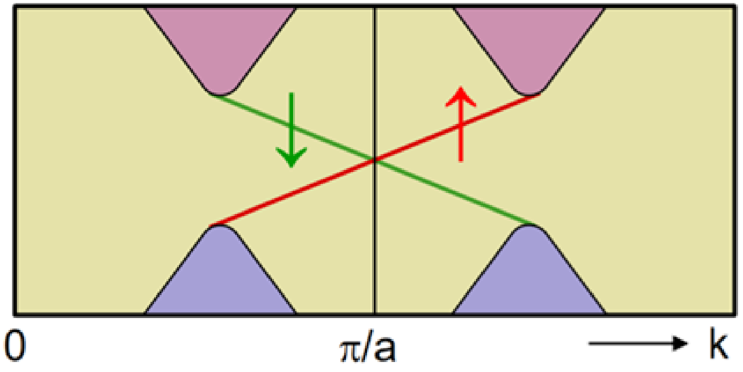
Many Topological States Have Unclear Robust Bulk Properties

- **Ex: 2D $\mathbb{Z}_2$ topological insulators (TIs) have boundary helical modes**
  - But no quantized spin Hall conductivity w/o S^z symmetry

Kane and Mele, *PRL* (2005)

Dyakonov and Perel, *JETP Lett.* (1971)
Murakami, *et al.*, *Science* (2003)

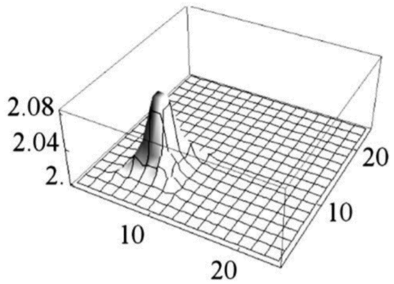


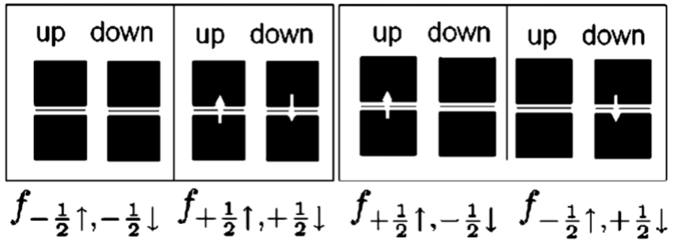


- **Robust bulk signature of 2D TI *does* exist – but very theoretical**

SPT order	Symmetry	Classification	Chain end/SPT probe
2F quantum spin Hall states	$U^f(1) \times U^f(1)$	Z	Spin-charge Hall conductance
2F topological insulator	$[U^f(1) \rtimes Z_4^T]/Z_2$	Z_2	π flux carries charge-0 Kramers doublet

Y. Ran *et al.*, *PRL* (2008)
X.-L. Qi and S.-C. Zhang, *PRL* (2008)
X. G. Wen, *RMP* (2017)

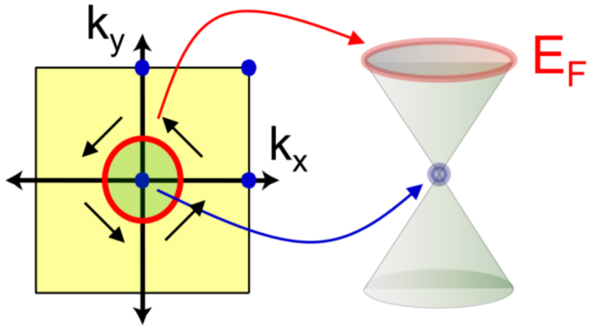




Everything is Clear in 3D TIs

- **Unpaired twofold Dirac cone surface state from time-reversal *(T)* symmetry**
  - Condensed-matter realization of "parity anomaly"

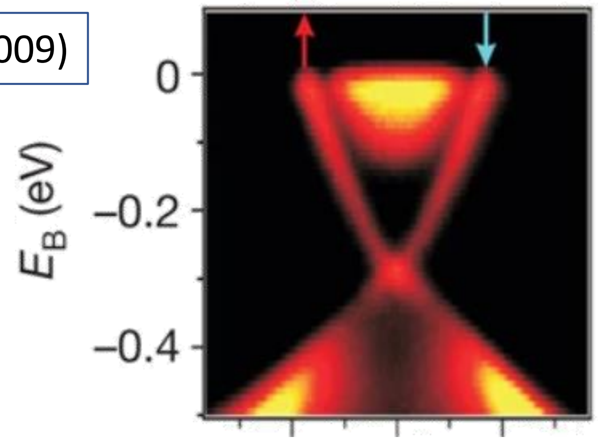
L. Fu, Kane, and Mele, *PRL* (2007)
Qi, Hughes, and Zhang, *PRB* (2008)



- **Fu-Kane parity criteria simplifies diagnosis through coreps**
  - Determine if $\nu_0 = 1$ from inversion symmetry eigenvalues

$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \qquad (-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i$$

Hsieh, … , Cava, Hasan, *Nature* (2009)



- **Detect surface Dirac cones in ARPES**
  - 1^{st} generation: $Bi_{1-x}Sb_x$
  - 2^{nd} generation: Bi_2Se_3

Fu and Kane, *PRB* (2007)
Hasan and Kane, *Rev. Mod. Phys* (2010)

- **Robust *bulk* signatures of 3D TIs also known, "simple"…**

The Response Theory of 3D TIs is Axion Electrodynamics

- **Axion Electrodynamics**
  - Modified E&M with magnetic monopoles
  - Magnetoelectric (ME) term ($\boldsymbol{E} \cdot \boldsymbol{B}$)
  - Originated in high-energy theory

$$\Delta \mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h} \mathbf{E} \cdot \mathbf{B}$$

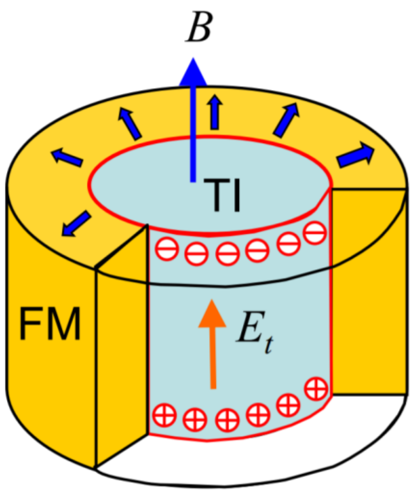
$$\theta = -\frac{1}{4\pi} \int_{\mathrm{BZ}} d^3k \epsilon_{ijk} \mathrm{Tr}\left[\mathcal{A}_i \partial_j \mathcal{A}_k - i\frac{2}{3} \mathcal{A}_i \mathcal{A}_j \mathcal{A}_k \right]$$

Wilczek, *PRL* (1978, 1987)
X.-L. Qi, Hughes, S.-C. Zhang, *PRB* (2008)
Essin, Moore, Vanderbilt, *PRL* (2009)

- **$\boldsymbol{\theta}$ is axion angle (defined mod $\boldsymbol{2\pi}$)**
  - $\theta = 0, \pi$ quantized by $\boldsymbol{E} \cdot \boldsymbol{B}$-odd symmetries
  - $\Delta\theta = \pi$ boundaries bind ½ Chern states

- **<u>3D TIs are "Axion Insulators" with $\boldsymbol{\theta = \pi}$</u>**
  - Topological ME effect confirmed in optical exp.

L. Wu, …, Armitage, *Science* (2016)
Mogi *et al., Nat. Phys.* (2022)



$$\mathbf{P}_t = \left(n + \frac{1}{2}\right) \frac{e^2}{hc} \mathbf{B}$$

3D TIs are Device Ready

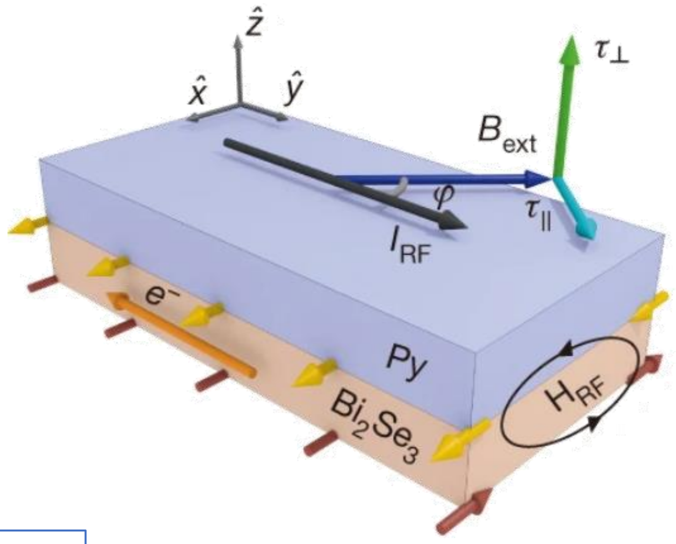
- **Experiments driven by well-understood theory, accessible materials**
  - Can outperform conventional materials in:
  - **Spintronics:**

Published: 23 July 2014

Spin-transfer torque generated by a topological insulator

A. R. Mellnik, J. S. Lee, A. Richardella, J. L. Grab, P. J. Mintun, M. H. Fischer, A. Vaezi, A. Manchon, E.-A. Kim, N. Samarth & D. C. Ralph

Nature **511**, 449–451 (2014) | Cite this article



  - **Current rectification:**

Letter | Open Access | Published: 12 May 2022

Giant magnetochiral anisotropy from quantum-confined surface states of topological insulator nanowires

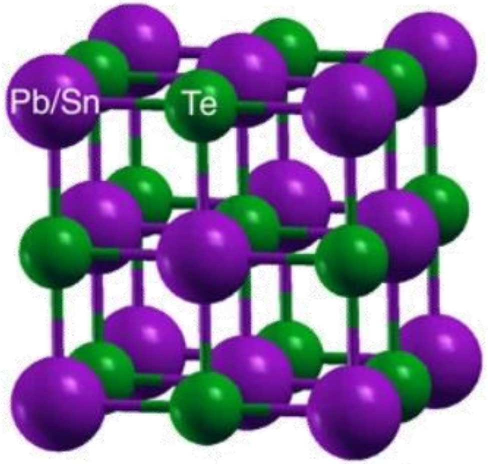
Henry F. Legg, Matthias Rößler, Felix Münning, Dingxun Fan, Oliver Breunig, Andrea Bliesener, Gertjan Lippertz, Anjana Uday, A. A. Taskin, Daniel Loss, Jelena Klinovaja & Yoichi Ando

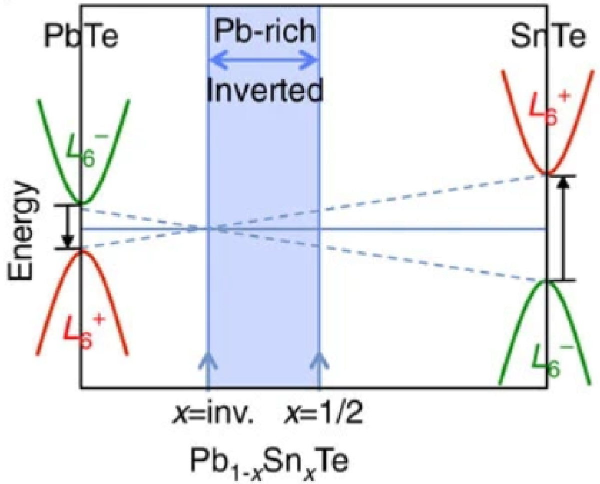
Nature Nanotechnology **17**, 696–700 (2022) | Cite this article

What about other topological states?

Topological Crystalline Insulators (TCIs) Also Exist

- **Protected by <u>bulk</u> spatial symmetry**
- **1st Proposal** L. Fu, *PRL*(2011)



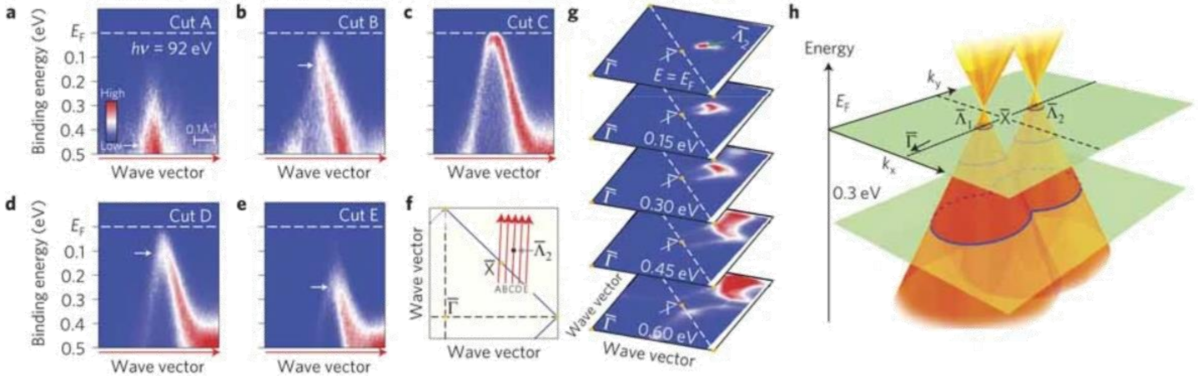


- **Ex: Mirror TCI: SnTe**
  - 2 surface Dirac cones on mirror lines

T. Hsieh, *et al.*, *Nat. Comm.* (2012)
Y. Tanaka, *et al.*, *Nat. Phys.* (2012)
S.-Y. Xu, *et al.*, *Nat. Comm.* (2012)

- **Now many, many variants**
  - <u>Exhaustively enumerated</u>

Z. Song, *et al.*, *Nat. Comm.* (2018)
Khalaf, *et al.*, *PRX* (2018)
Elcoro*, **BJW***, *et al.*, *Nat. Comm.* (2021)
B. Peng, *et al.*, *PRB* (2022)



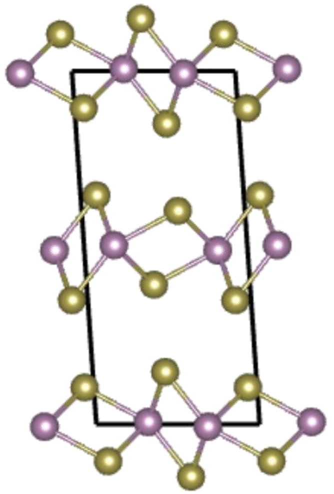
Efficient Numerical Searches Reveal Many TIs, TCIs

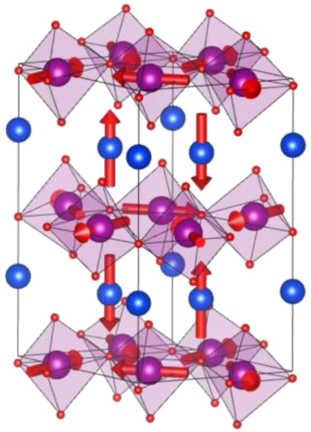
- **Material screening from symmetry-based indicators**
  - Generalized Fu-Kane formulas from symmetry eigenvalues/corep combinatorics
  - Diagnose topology from WF at high-symmetry ***k*** points

Po, *et al.*, *Nat. Comm.* (2017)
Z. Song, *et al.*, *Nat. Comm.* (2018)
Elcoro*, **BJW***, *et al., Nat. Comm.* (2021)

- **High-throughput DFT reveals abundant band topology**
  - Over 6,000 nonmagnetic TIs and TCIs
  - Over 100 new topological magnets
  - Publicly available repositories:

T. Zhang *et al., Nature* (2019)
F. Tang *et al., Nature* (2019)
Vergniory,* **BJW.***, …., Regnault, *Science* (2022)





Y. Xu, Elcoro, Z. Song, **BJW** *et al., Nature* (2020)

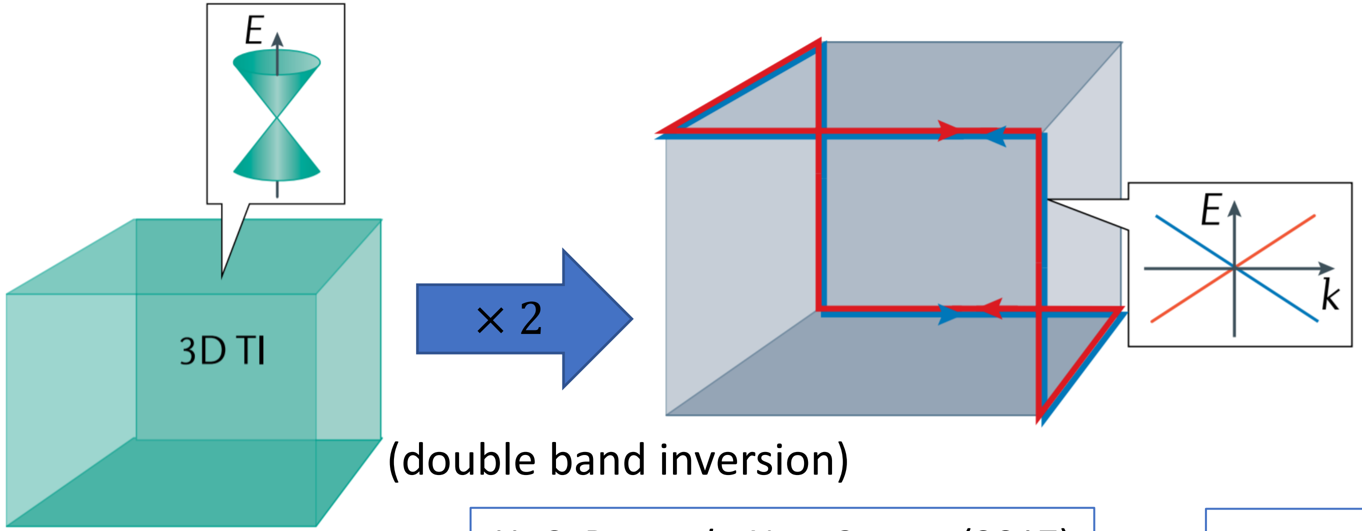
Topological Materials Database

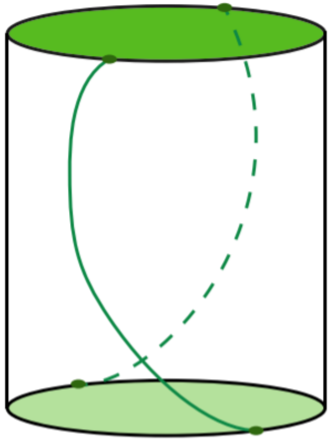
www.topologicalquantumchemistry.com

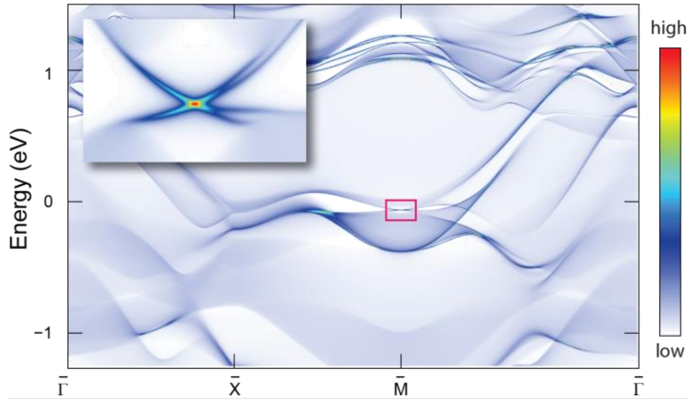
www.topologicalquantumchemistry.fr/magnetic/

Robust Properties of TCIs Remain Puzzling

- **More Dirac cones, what else?**
- **“Doubled” TIs have (some or all) gapped surfaces, are axion-trivial $\theta = 0$**
  - “Higher-order TIs” (HOTIs) – fourfold Dirac surface states and 1D helical “hinge” modes







H. C. Po *et al., Nat. Comm.* (2017)
F. Schindler *et al., Sci. Adv.* (2018)

C. Fang and L. Fu, *Sci. Adv.* (2019)

BJW *et al., Science* (2018)

- **Experimentally accessible material candidates**
  - Bismuth, $MoTe_2$, WTe_2, BiBr

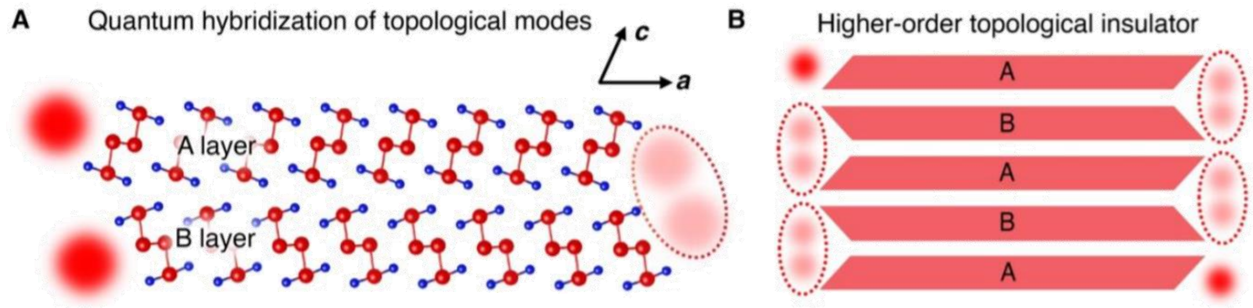
F. Schindler *et al., Nat. Phys.* (2018)
Z. Wang*, **BJW*** *et al., PRL* (2019)
F. Tang *et al., Nat. Phys.* (2019)

- **Little progress on response theory**

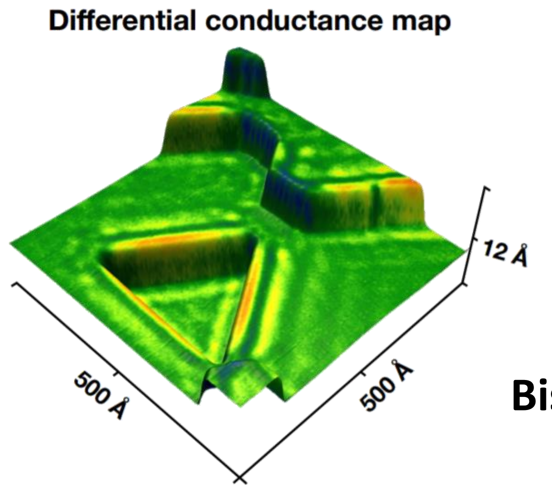
P. Lopes *et al., PRB* (2016)
S. Ramamurthy *et al., PRL* (2017)

Hinge-States are Well-Documented in Candidate HOTIs

- **STM experiments reveal 1D channels**

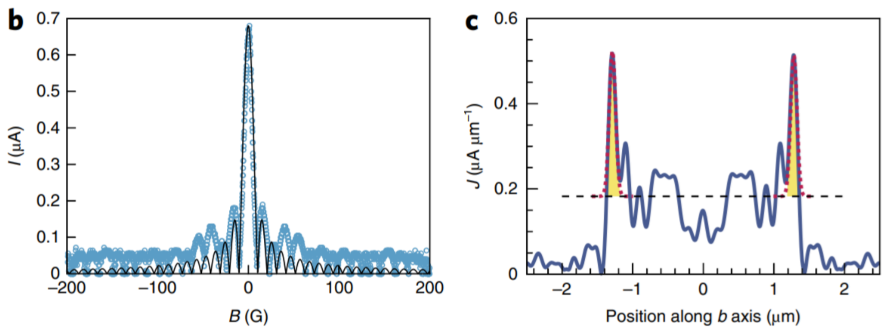


BiBr



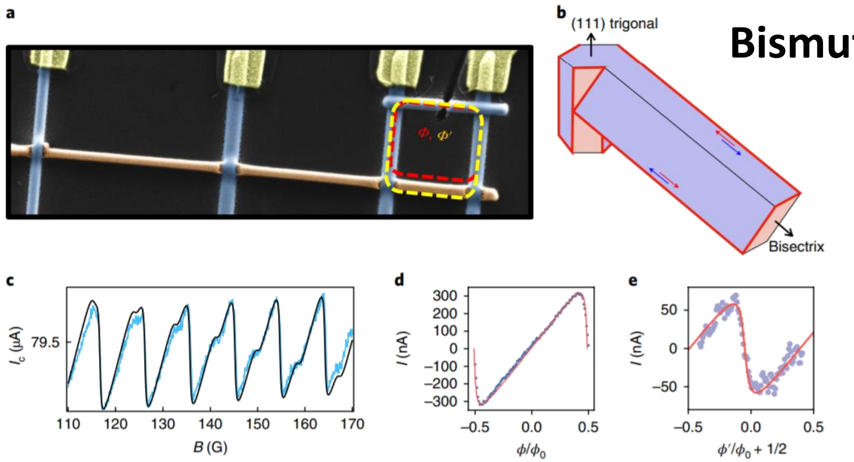
Bismuth

- **Supercurrent oscillations suggest hinge states**
  - Ballistic edge transport in Bi measured at Orsay



WTe_2

Schindler *et al., Nat. Phys.* (2018)
Y.-B. Choi *et al., Nat. Mater.* (2020)
N. Shumiya *et al., Nat. Mater.* (2022)

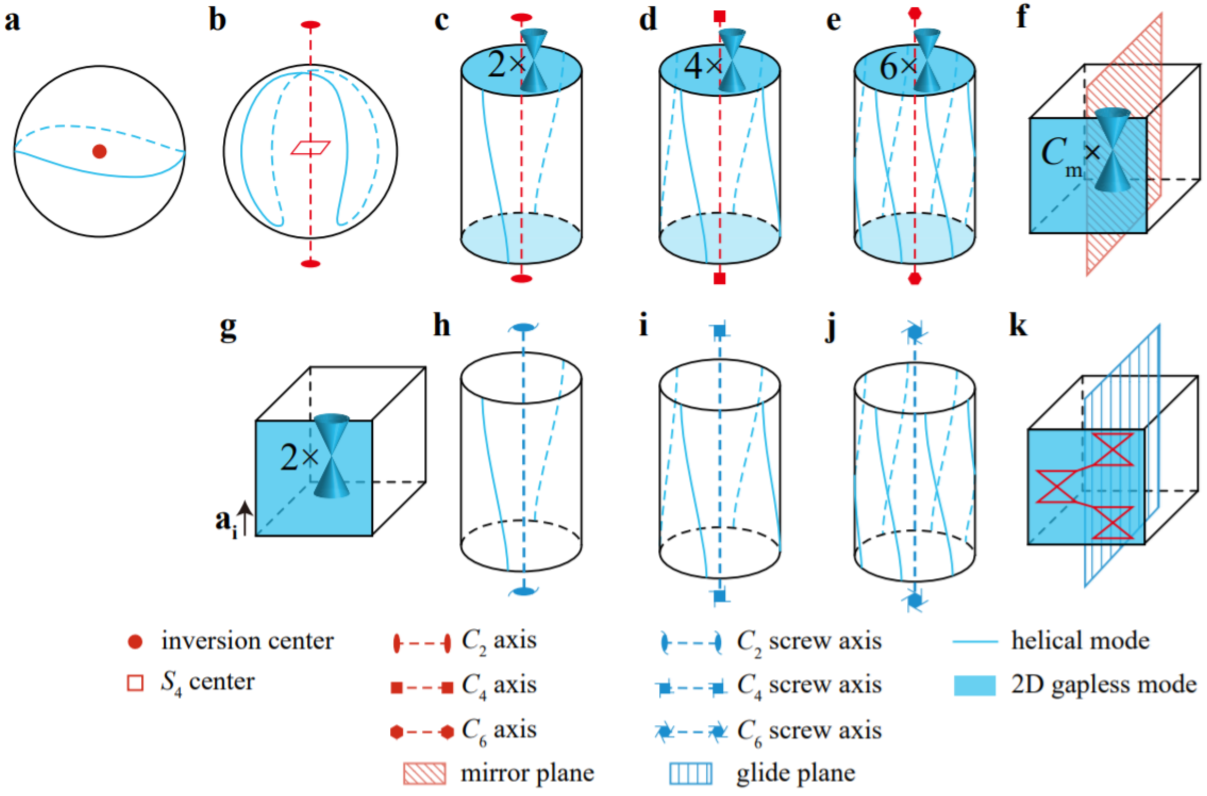


Bismuth

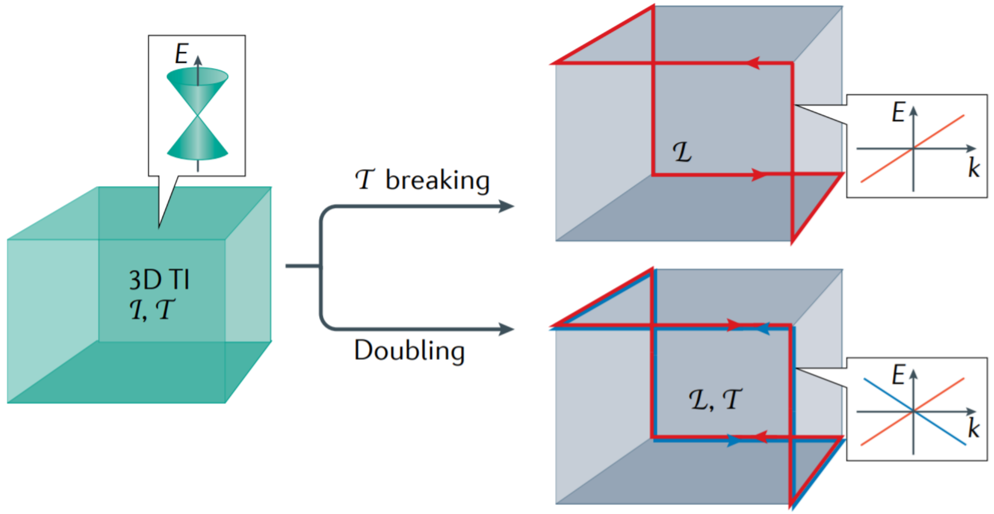
- **Several issues:**
  - Questions about classification of bismuth, WTe_2
  - Theoretical limitations of higher-order topology….

Higher-Order Topology is a Useful Theory Framework

- **Provides complete TCI classification through exact global symmetry in models**



- **Count 2D Dirac & 1D hinge modes**
  - Indicates topological distinction
- **Theory reveals chiral HOTIs also exist**



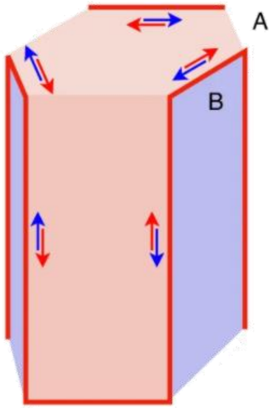
B.J.W. *et al., Nat. Rev. Mater.* (2022)

Benalcazar *et al., PRB* (2017)
F. Schindler *et al., Sci. Adv.* (2018)
E. Khalaf *et al., PRX* (2018)
Z. Song *et al., Nat. Comm.* (2018)

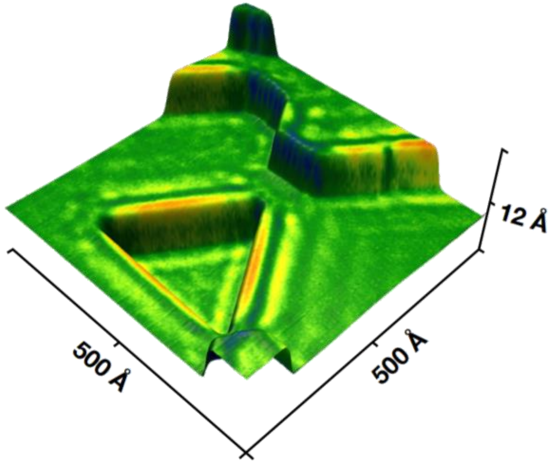
Higher-Order Topology is Experimentally Ambiguous

- **Real material samples do not have perfect global symmetries:**
  - No insight provided in absence of global sample symmetry

Bismuth does not look like this:



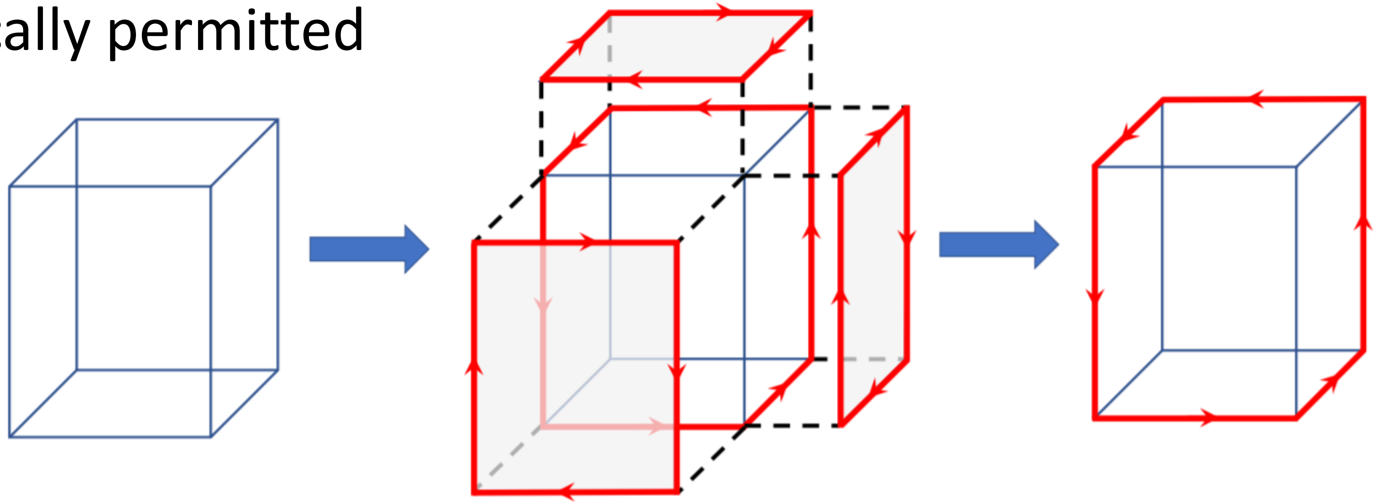
Bismuth looks like this:



F. Schindler *et al., Nat. Phys.* (2018)
A. Nayak *et al., Sci. Adv.* (2019)

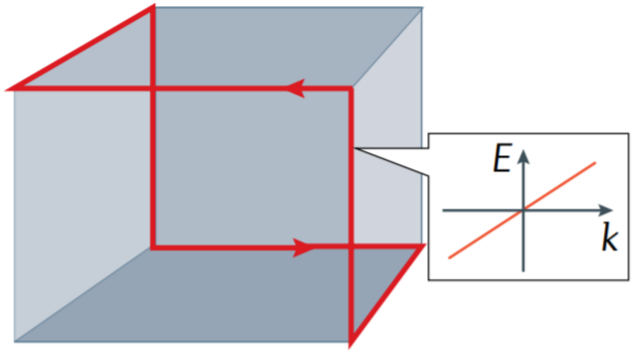
- **Trivial materials can exhibit "extrinsic" hinge states**
  - "Gluing" 2D surface phases is realistically permitted
  - Equivalent to surface band inversions

B.J.W. and Bernevig, *arXiv:1810.02373* (2018)



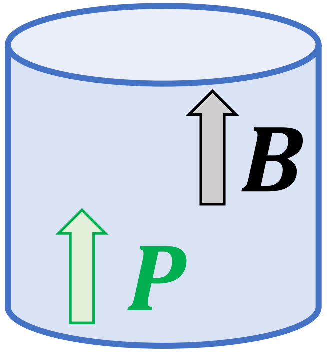
Signature of 3D Chiral HOTIs: Axion Electrodynamics

- **All spinful chiral HOTIs have $\boldsymbol{\theta = \pi}$**
  - Replace higher-order topology with <u>axion electrodynamics</u>



Elcoro*, **B.J.W.*** *et al., Nat. Comm.* (2021)

- **Break global symmetry (on boundary), remove hinge modes**
  - $\theta = \pi$ still quantized in bulk
  - Detect chiral HOTI through magnetoelectric effect



$$\mathbf{P}_t = \left(n + \frac{1}{2}\right)\frac{e^2}{hc}\mathbf{B}$$

Qi, Hughes, Zhang, *PRB* (2008)
Essin, Moore, Vanderbilt, *PRL* (2009)

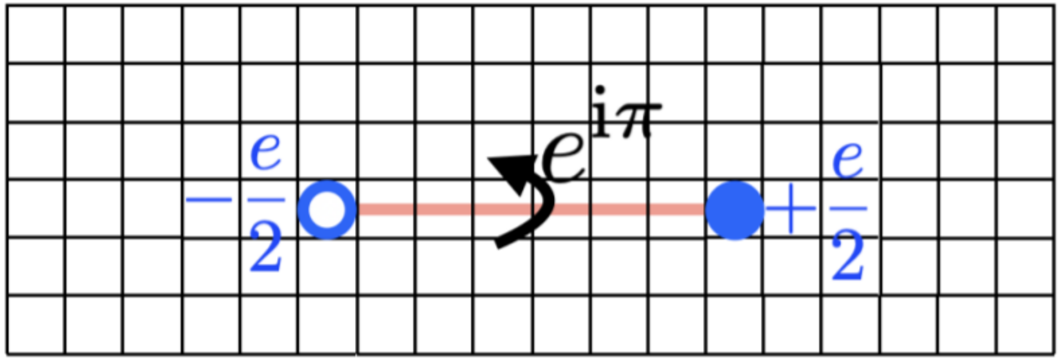
- **But helical HOTIs, $\boldsymbol{\theta = 0}$…**
  - Surfaces have $C = 0$ ($\sigma_H = 0$ from T symmetry)

Does there exist something "like" θ to replace global symmetry arguments in theory of <u>inversion-symmetric</u> helical HOTIs?

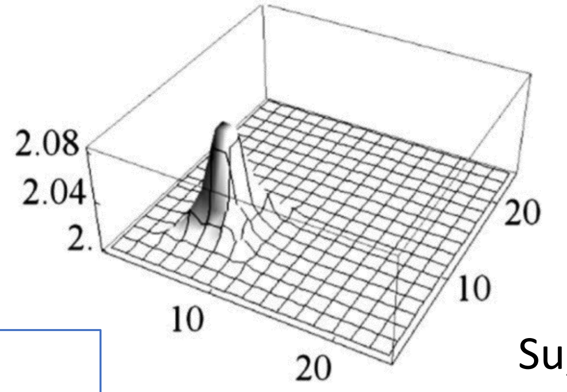
Test: Dislocations and Magnetic Flux Insertion

- **Dislocations and flux insertion can (sometimes) detect bulk topology**
  - For HOTIs, flux provides clearest theoretical topological signature
- **2D C=1 Chern insulator: singly degenerate π-flux states, $q \bmod e = e/2$**

D.-H. Lee *et al.*, *PRL* (2007)
Schindler, … , **BJW**, *arXiv:2207.10112, To Appear in Nat. Comm.* (2022)

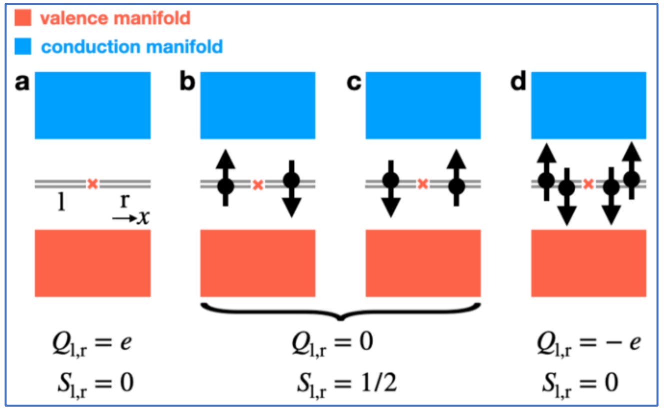


- **2D $\mathbb{Z}_2$ TI (quantum spin Hall):**
  Doubly degenerate π-flux states w/ fractionalization (spin-charge separation)



Y. Ran *et al.*, *PRL* (2008)
X.-L. Qi and S.-C. Zhang, *PRL* (2008)

"Reversed" spin-charge relations
Su, Schrieffer, Heeger (SSH), *PRL* (1979)
Flood and Heeger, *PRB* (1983)



Test Case: Chiral HOTI (Axion Insulator)

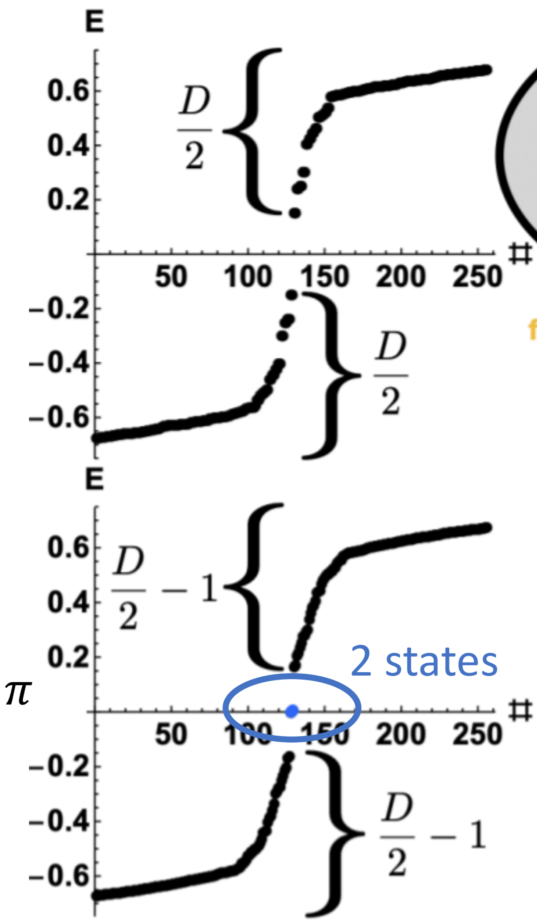
- **Surfaces carry ½ the π-flux response of C=1 Chern insulators**

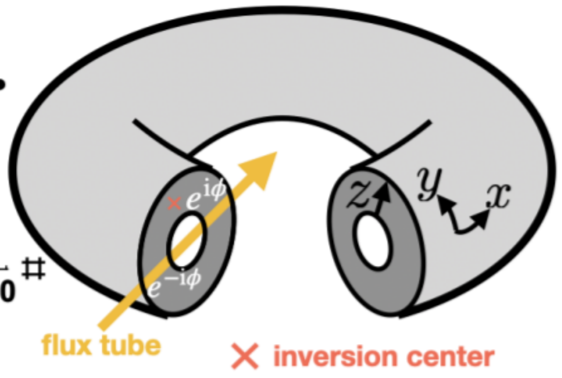
- **Bulk looks like a "thick" (magnetic) chain with nontrivial polarization e/2**

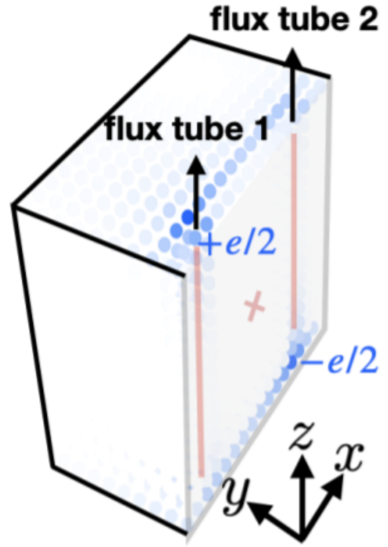
- **Consistent with $\theta = \pi$**

$$\mathbf{P}_t = \left(n + \frac{1}{2}\right)\frac{e^2}{hc}\mathbf{B}$$

Filling anomaly at $\phi = \pi$







G. Rosenberg, H.-M. Guo, and Franz, *PRB* (2010)
B.J.W. and Bernevig, *arXiv:1810.02373* (2018)
Benalcazar, T. Li, and Hughes, *PRB* (2019)

Beyond θ in Helical HOTIs

- **Surfaces carry ½ the π-flux response of $\mathbb{Z}_2$ TIs!**
  - *Cannot remove* by gluing surface 2D TIs

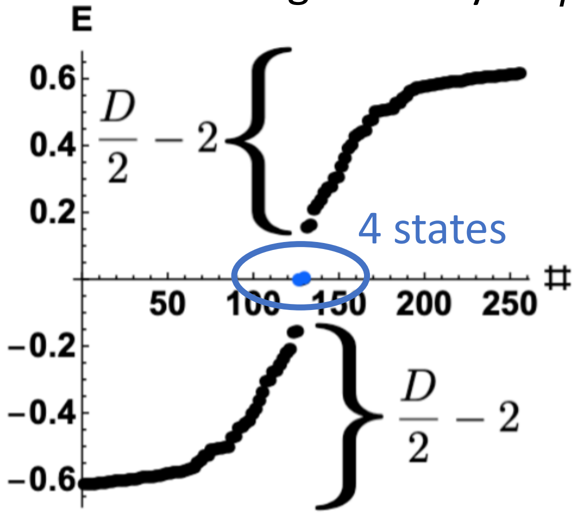
- **Bulk looks like a "thick" *T*-doubled chain with nontrivial *partial* polarization e/2**
  - Polarization per "half" of states

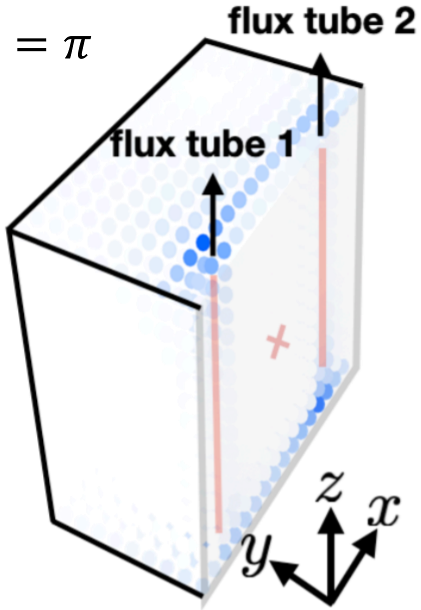
L. Fu and Kane, *PRB* (2006)

- **B flux induces *partial polarization* $P^{\uparrow\downarrow}$!**
  - Reduces to spin accumulation with S^z symmetry
  - ***1st signature without invoking hinges!***

Schindler, … , **BJW**, *arXiv:2207.10112, To Appear in Nat. Comm.* (2022)

Filling anomaly at $\phi = \pi$

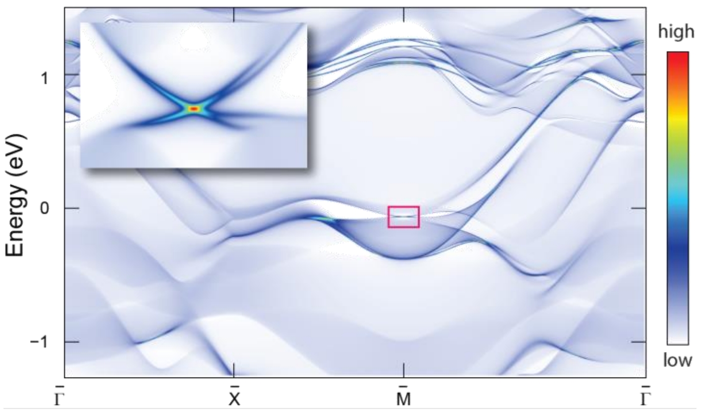




How do we make sense of this?

Theory Interpretation of Flux Insertion

- **Surface derives from anomalous fourfold Dirac fermion**
  - Two copies of TI surface parity anomaly



BJW *et al., Science* (2018)
Z. Wang*, **BJW.*** *et al., PRL* (2019)

- **Helical HOTIs with *I* and *T* admit an S^z-preserving limit with $\boldsymbol{\theta}^{\uparrow\downarrow} = \boldsymbol{\pi}$**
  - Derive from 8-fold Dirac $k \cdot p$ theory

BJW *et al., PRL* (2016)

$$H_{HOTI} = \tau^y k_x + \mu^y \tau^x k_y + \tau^x \mu^x S^z k_z + m\tau^z, \qquad T = iS^y K, I = \tau^z$$

- **Theta "per spin" $\boldsymbol{\theta}^{\uparrow}$ is nontrivial (3D generalization of 1D $\boldsymbol{P}^{\uparrow}$)**

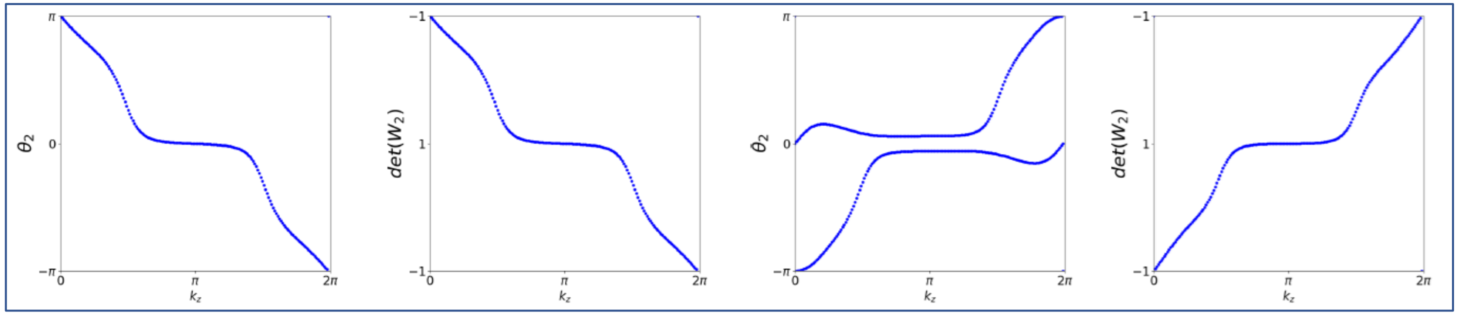
How much of this picture survives ***quantitatively*** *without S^z symmetry?*

Employ numerical tools: Wilson loops and Chern markers (layer-resolved)

Verifying New Axion $\boldsymbol{\theta}$ Angles in HOTIs

- **Gauge-invariant analytic formula for partial axion angle $\boldsymbol{\theta}^{\uparrow\downarrow}$ is coming soon**

- **For now, build on numerical methods for computing $\boldsymbol{\theta}$**
  - Use non-Abelian Berry phase, hybrid Wannier
  - Could diagnose $\theta^{\uparrow\downarrow}$ if applied to “half” of states



BJW and Bernevig, *arXiv:1810.02373* (2018)
Varnava, Souza, and Vanderbilt, *PRB* (2020)

$$\frac{\theta}{\pi} = C_{\gamma_2} \bmod 2$$

- **Does there exist a gauge-invariant *numerical* way of dividing systems in “half”?**
  - *YES, the “spin” spectrum!* E. Prodan, *PRB* (2009)

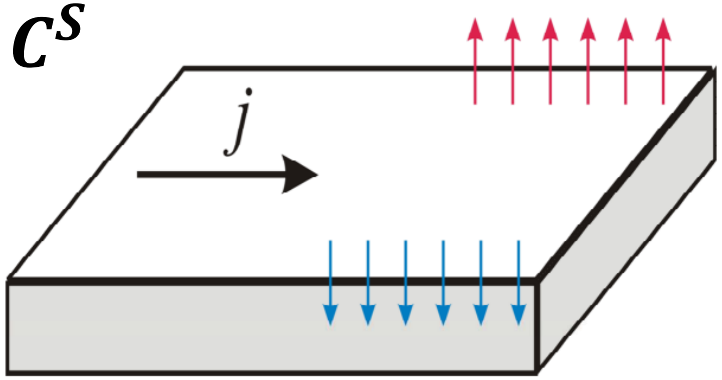
K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Revisiting 2D TIs: Quantum Spin Hall or $\mathbb{Z}_2$ TI?

- **With S^z symmetry, define spin Hall conductivity $\sigma_H^S = \frac{e}{4\pi} C^S$**

Murakami, *et al.*, *Science* (2003)
Bernevig and S.-C. Zhang, *PRL* (2006)

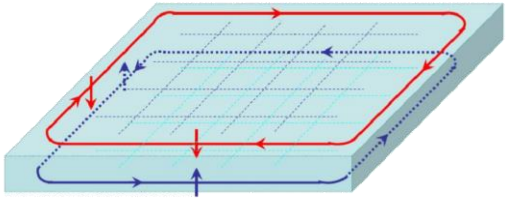
$$C^S = C^{\uparrow} - C^{\downarrow}$$



Spin Hall Effect

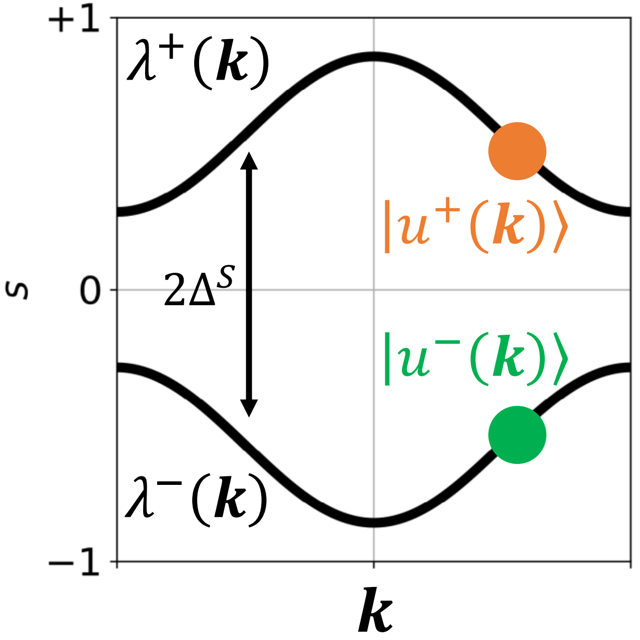
- **Spin-orbit coupling (SOC) destroys ↑↓ S^n sector labels**

Kane and Mele, *PRL* (2005)



- **But, can *restore* labels if gap in $P_k^{occ} S^n P_k^{occ}$, *even with SOC***
  - Gauge-invariant S^n spin spectrum
  - "Emergent" U(1) spin if spin gap Δ^S

$$\sigma_H^S \sim \Delta^S \frac{e}{4\pi}(C^+ - C^-)$$

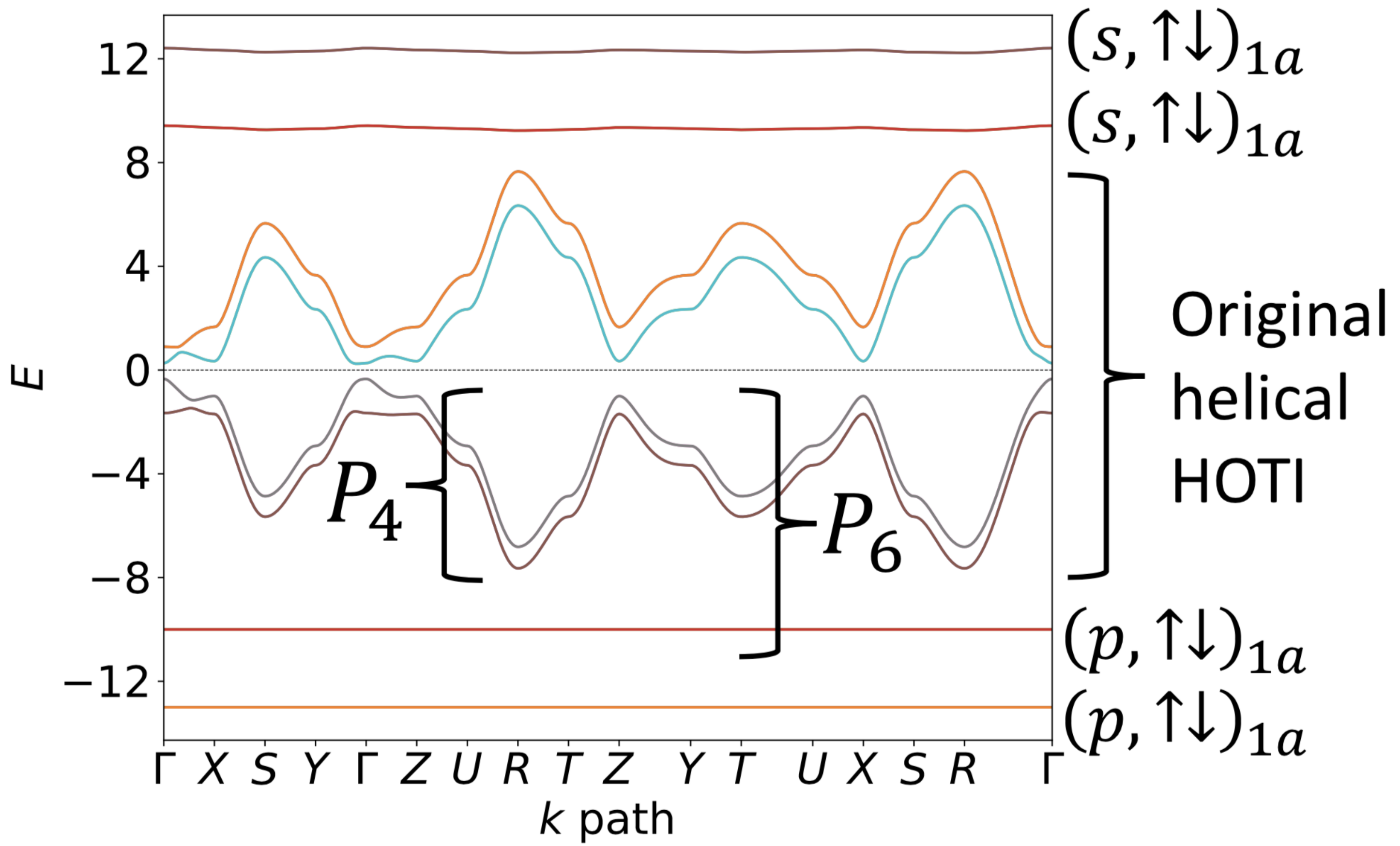


- **Predicts bulk contribution to σ_H^S**
  - Response beyond $\mathbb{Z}_2$ topological class

E. Prodan, *PRB* (2009)
Monaco, Ulčakar, *PRB* (2020)

Spin Band Topology of a Helical HOTI?

- **Extract partial $\boldsymbol{\theta^{\pm}}$ angles of a 3D helical HOTI *with a spin gap***



- **Compute partial $\boldsymbol{\theta^{\pm}}$ angles for $\boldsymbol{P_6}$ bands**
- **Wilson loop spectrum easier to see in non-minimal model**
  - P_4 alone has "fragile" winding

Model adapted from:
BJW and Bernevig, *arXiv:1810.02373* (2018)
Z. Wang*, **BJW*** *et al., PRL* (2019)

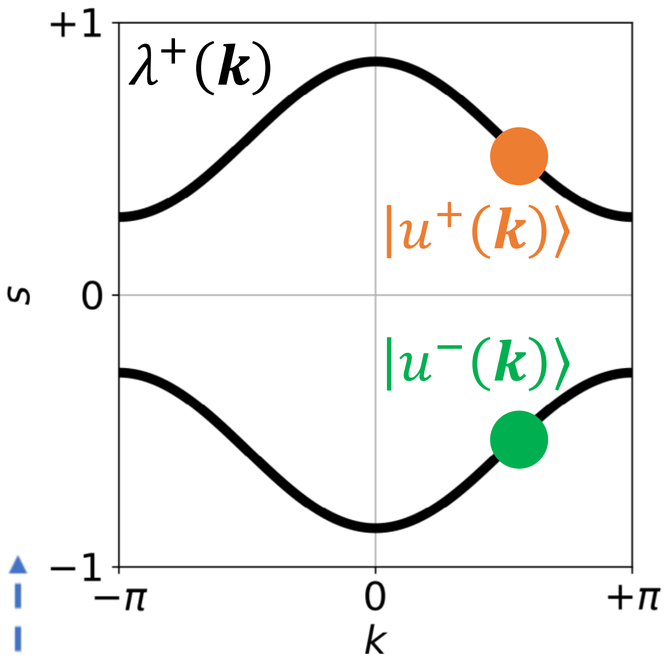
P_4 = 4 valence bands of helical HOTI

$P_6 = P_4 \oplus$ 2 trivial bands from *p* orbitals at $\boldsymbol{r} = \boldsymbol{0}$ (1a Wyckoff position)

Introduce Spin Wilson Loops for Partial Axion Angles

- Compute 1st spin Wilson loop (non-Abelian Berry phase)

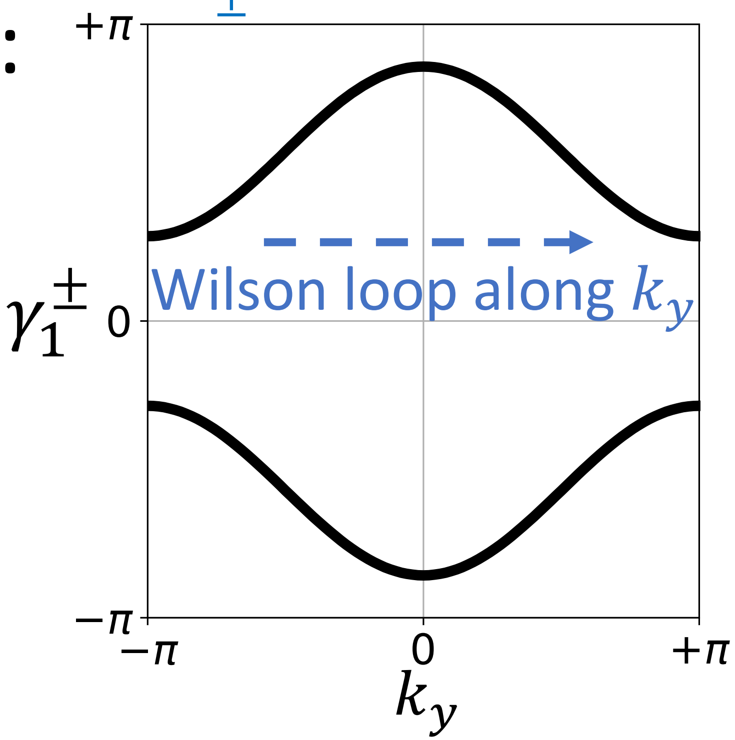
$$[W_1^{\pm}]_{mn} = \langle u_m^{\pm}(\boldsymbol{k}+\boldsymbol{G})| \prod_{\boldsymbol{q}}^{\boldsymbol{k}+\boldsymbol{G}\leftarrow\boldsymbol{k}} P_{\pm}(\boldsymbol{q})\,|u_m^{\pm}(\boldsymbol{k})\rangle$$



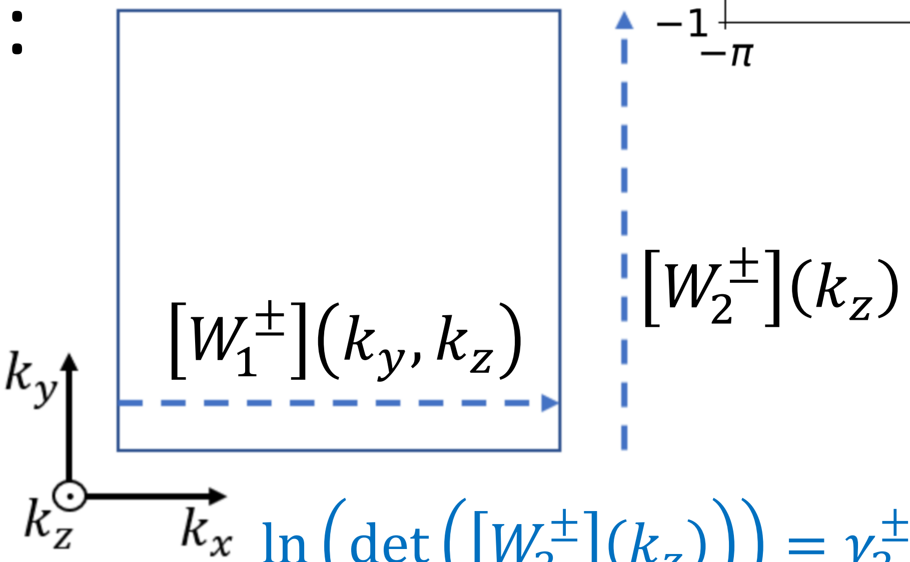
- Compute 2nd spin Wilson loop – nested Spin Wilson loop

$P_{\pm}$-Wannier bands

W_1:



W_2:

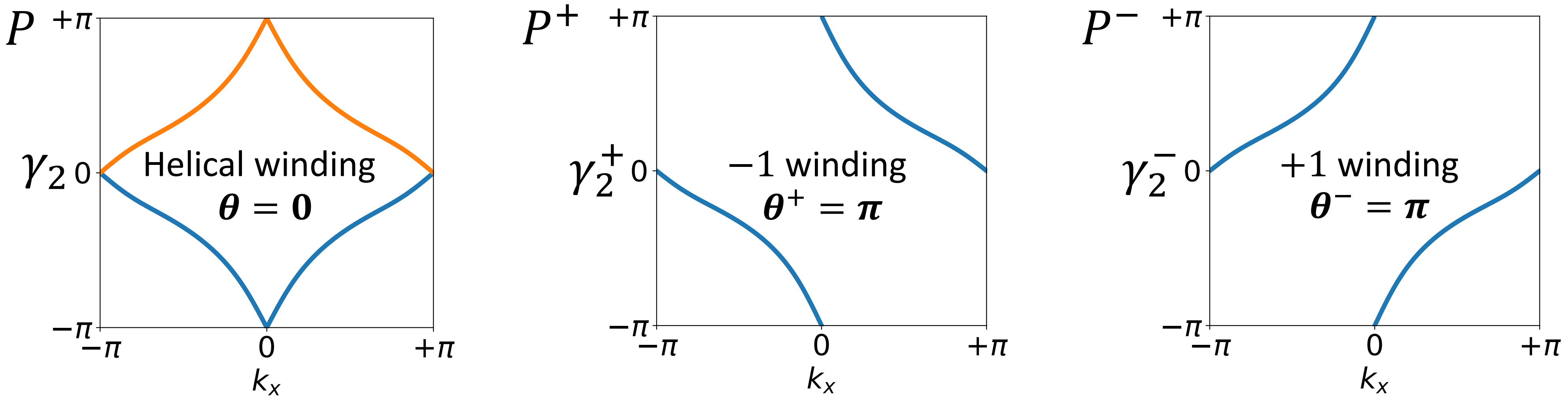


$\ln\left(\det\left([W_2^{\pm}](k_z)\right)\right) = \gamma_2^{\pm}(k_z)$

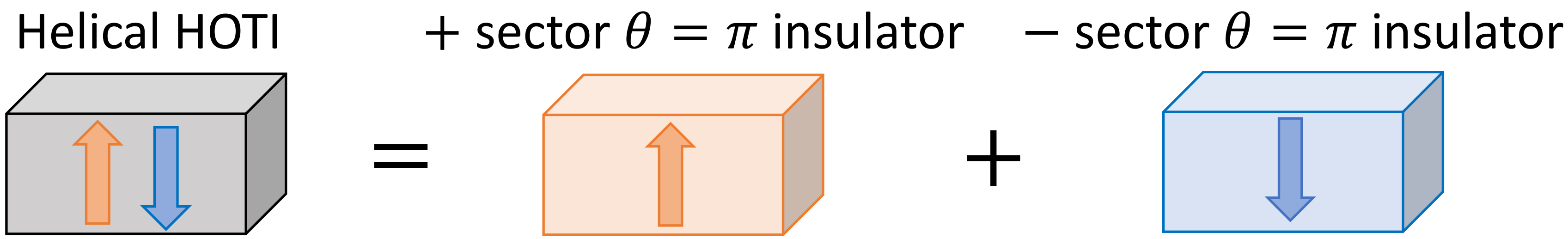
B.J.W. and Bernevig, *arXiv:1810.02373* (2018)

Helical HOTI Spin-Wilson Matches $\boldsymbol{\theta = \pi}$ Axion Insulator

- **Nested Wilson loop indicates $\boldsymbol{\theta^{\pm} = \pi}$ quantized by inversion symmetry**



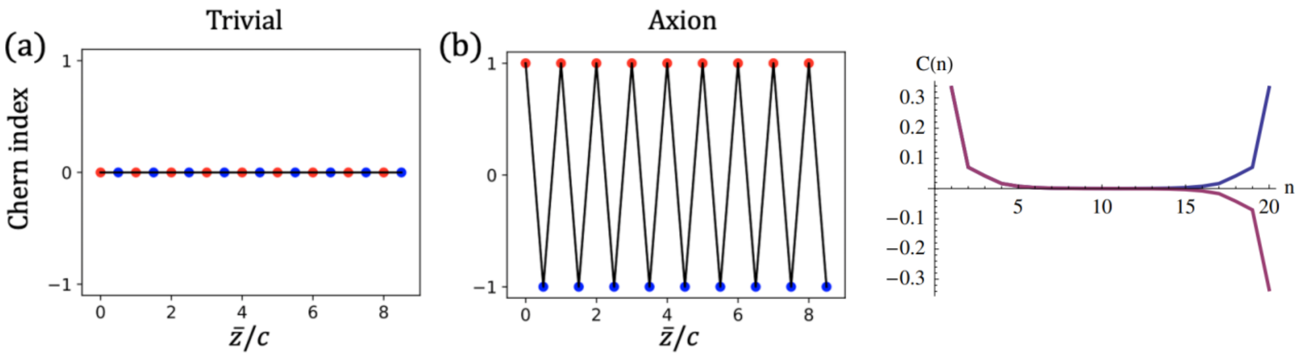
- **Confirms physical interpretation of flux response *without* invoking unrealistic $\boldsymbol{S^z}$ symmetry**
  - 3D generalization of "partial polarization" L. Fu and Kane, *PRB* (2006)



K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Position-Space Chern Number Also Measures $\boldsymbol{\theta}$

- **Known result: compute layer-resolved Chern number for 3D TCI**
  - For magnetic $\theta = \pi$ insulators, C oscillates in the bulk (zero on average)
  - Saturates at ½ integer value on surfaces



Essin, Moore, Vanderbilt, *PRL* (2009)
Varnava, Souza, Vanderbilt, *PRB* (2020)

$$C(\mathbf{R}) = -\frac{2\pi i}{A_{\text{cell}}} \sum_{\alpha=1}^{N_{\text{sta}}} \langle \mathbf{R}, \alpha | \left[\widehat{x}_P, \widehat{y}_P \right] | \mathbf{R}, \alpha \rangle$$

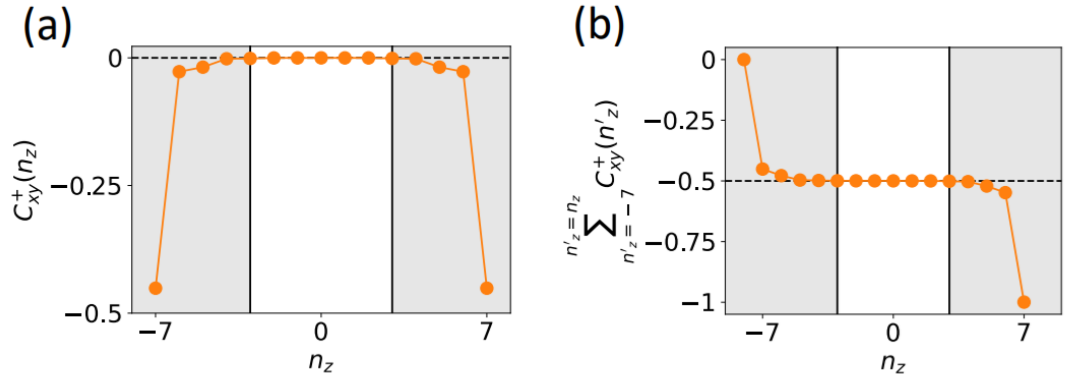
- **Consequence of parity anomaly**
  - Odd numbers of twofold Dirac cones cannot be symmetry-stabilized in pure 2D
  - If gapped, each Dirac cone would give ½ quantum Hall state
  - Surfaces of 3D TIs evade parity anomaly -> gapped surfaces of AXIs have C mod 1 = ½

L. Fu, Kane, and Mele, *PRL* (2007)
Qi, Hughes, and Zhang, *PRB* (2008)

Position-Space Calculations Reveal a New Anomaly

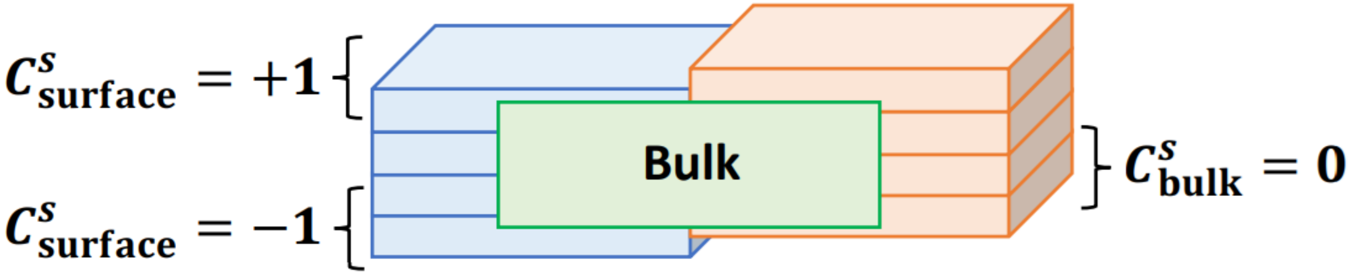
- **Compute layer-resolved, spin-resolved (partial) Chern number**
  - Chern number per $\pm$ sector saturates in ½ integer value (**robust to SOC!**) Levin, Stern, *PRL* (2009)
  - $C^S = C^+ - C^-$ saturates in odd-integer value (disallowed under *T* in 2D)
  - **"Partial" parity anomaly –** clarifies TCI fermion doubling in: **BJW** *et al., Science* (2018), C. Fang and L. Fu, *Sci. Adv.* (2019)

$$C^{\pm}(\mathbf{R}) = -\frac{2\pi i}{A_{\text{cell}}} \sum_{\alpha=1}^{N_{\text{sta}}} \langle \mathbf{R}, \alpha | \left[\widehat{x}_{P_{\pm}}, \widehat{y}_{P_{\pm}} \right] | \mathbf{R}, \alpha \rangle$$



- **More generally, C^s vanishes in the bulk, surface-only response**
  - **"Spin-magnetoelectric effect"**
  - Different from 3D QSH
  - Previous field theory

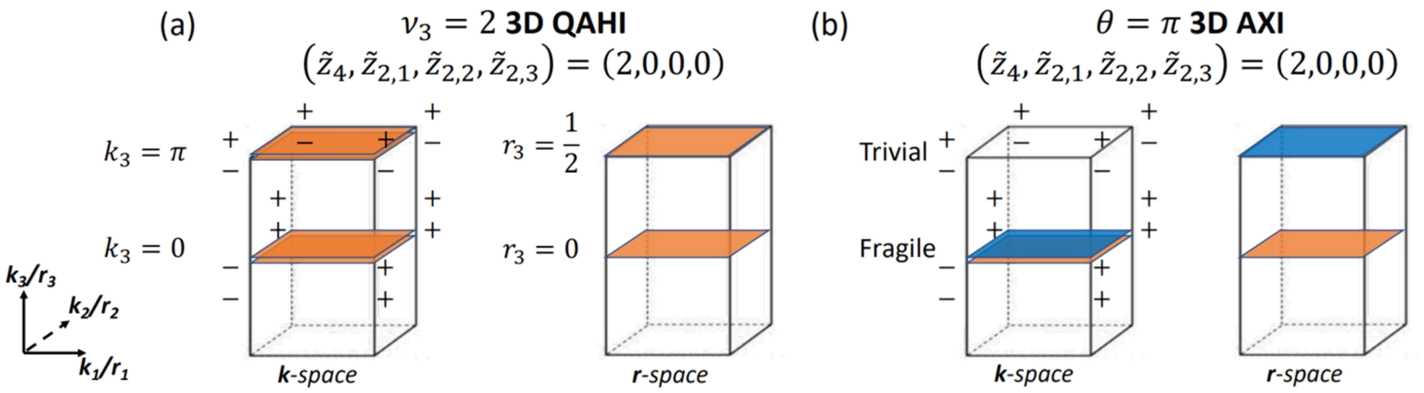
P. Ye, J. Wang, *PRB* (2013)



K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Understandable From Layer Construction Perspective

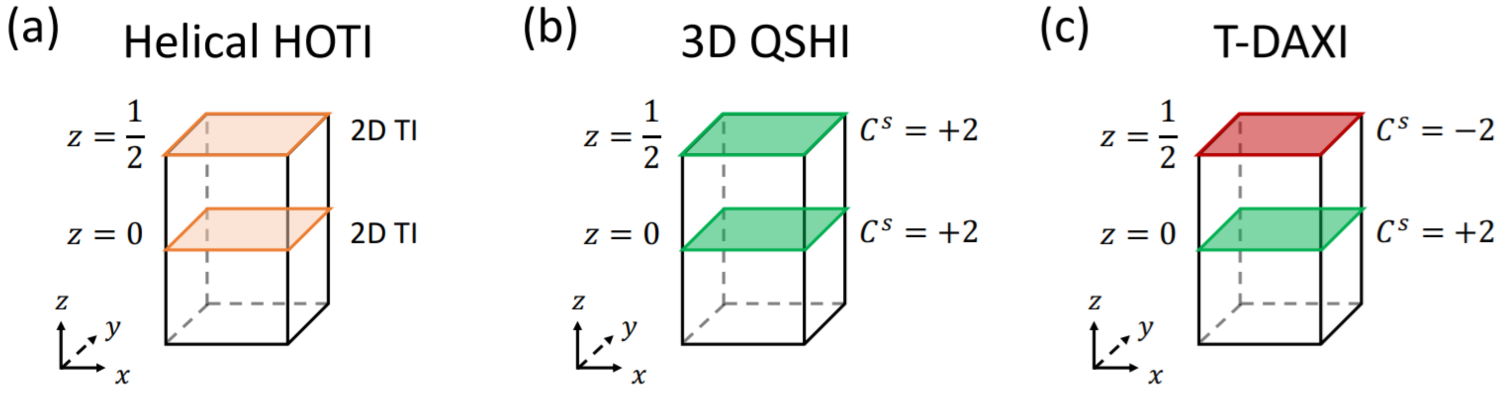
- **Some 3D states constructable from 2D layers + symmetry (here inversion)**



S.J. Huang *et. al., PRB* (2017)
Z .Song *et al., Nat. Comm.* (2018)
Elcoro*, **BJW*** *et al., Nat. Comm.* (2021)

- **New concept for resolved responses: <u>spin-resolved layer constructions</u>**
  - Start with "spin-space group" with U(1) spin
  - Add SOC w/o closing spin gap

Brinkman *et al., Proc. Royal Soc. London.* (1966)



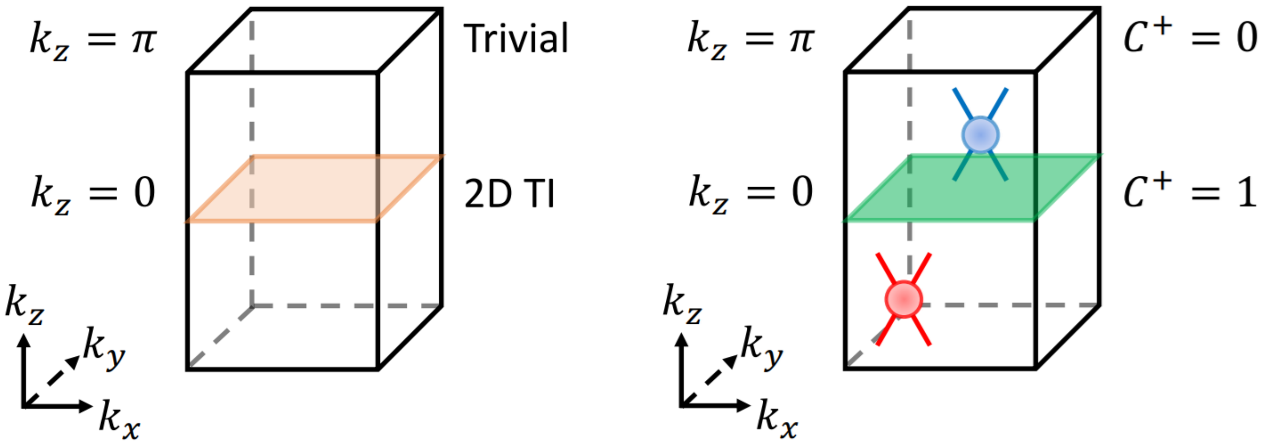
Case with $\theta^{\pm} = \pi$

K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Finer Classification of Insulators: Spin-Resolved Topology

- ***PsP* spectrum provides gauge-invariant information beyond band topology**
  - Indicates topological contribution to spin-electromagnetic responses
  - Response transitions from both **energy & spin gap closures**

- **In 3D, *PsP* gap closures are stable w/o symmetry: "spin-Weyl fermions"**
  - 3D TI *must* have spin Weyl points



- **Helical HOTI can be 3D QSH, T-DAXI ($\theta^{\pm} = \pi$), or spin-Weyl**
  - "Doubled-strong TI" limit is spin-Weyl

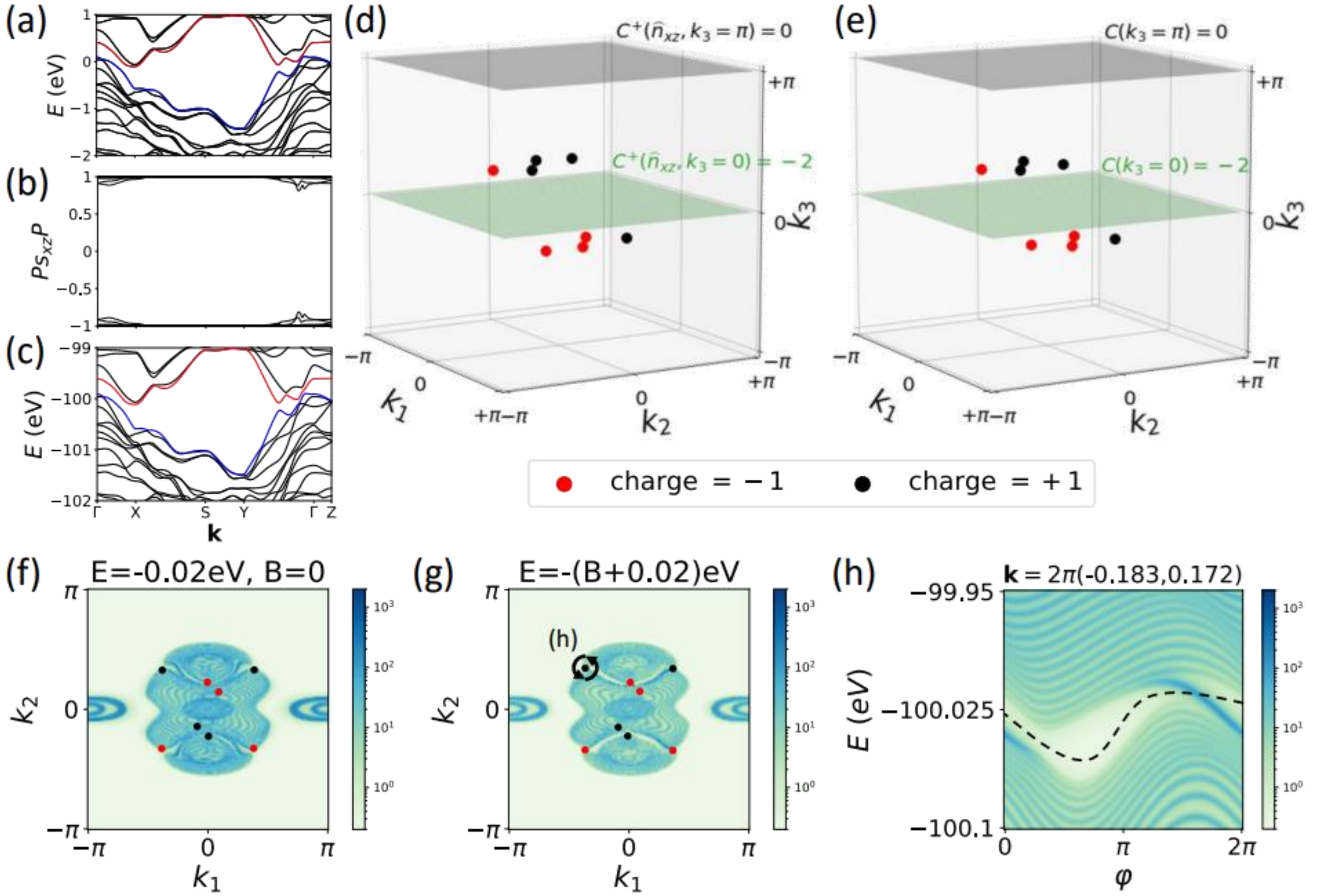
H. C. Po *et al., Nat. Comm.* (2017)

K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Finer Classification of Insulators: Spin-Resolved Topology

- **Spin spectrum and Wilson loops computable in real materials**
- **Ex: Helical HOTI β-MoTe$_2$ ($P2_1/m1'$, SSG #11.51)**
  - Spin-Weyl semimetal: surface Fermi arcs under strong Zeeman field

Z. Wang*, **BJW*** *et al., PRL* (2019)
F. Tang *et al., Nat. Phys.* (2019)



K.-S. Lin, Palumbo, Z. Guo, …, Z. Wang, Fiete, **BJW**, Bradlyn, *arXiv:2207.10099* (2022)

Conclusions

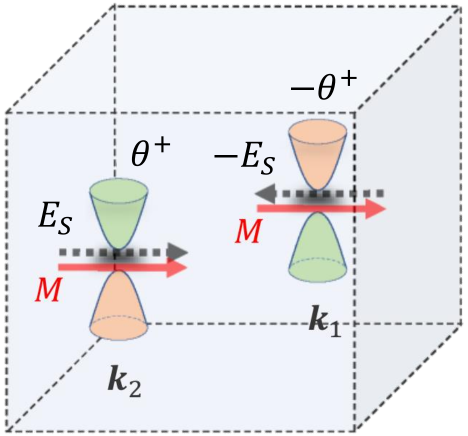
- **3D TCIs can have $\theta^{\pm} = \pi$, <u>topological bulk spin-magnetoelectric effect</u>**
  - Like spin Hall effects, should be a magnetic counterpart
  - Proved in adiabatic pumping, field theory & linear response with SOC needed next
  - <u>Need materials for *T*-DAXI ($\theta^{\pm} = \pi$) regime</u>

- **Flux and sector-resolved Wilson loops can detect 3D bulk response, indicate topological field theory**
  - Gaps in a gauge-invariant PsP-like spectrum facilitate additional responses
  - **Ex: charge-density wave in a Weyl semimetal with <u>emergent valley-axion</u> response**

E_S and B_S from strain, torsion

$$\Delta L \propto \theta^{+}(E_e \cdot B_S + B_e \cdot E_S)$$

J. Yu, **BJW**, C.-X. Liu, *PRB* (2021)



Thank You!

Questions?

Extra Slide for Zoom Whiteboard