Axion insulators

NSF DMR-1408838

David Vanderbilt
Rutgers University

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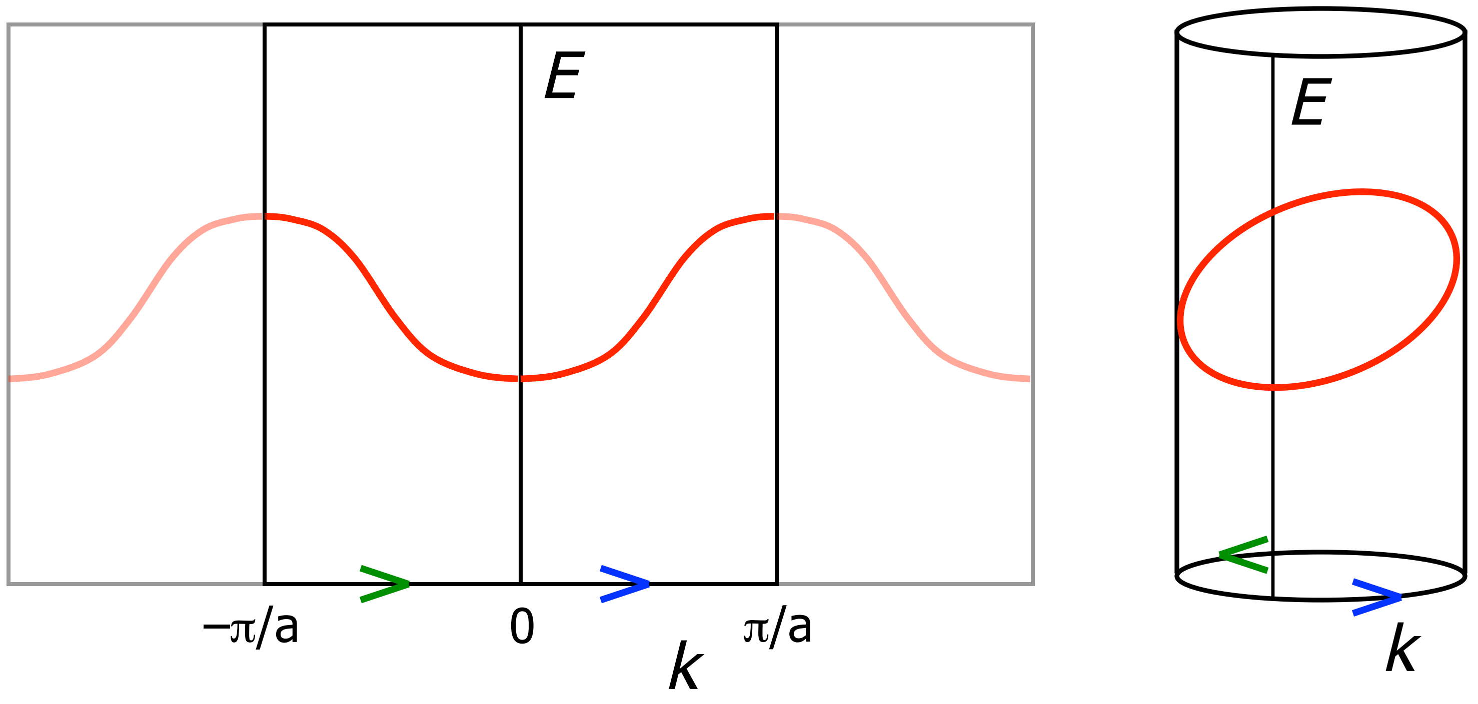
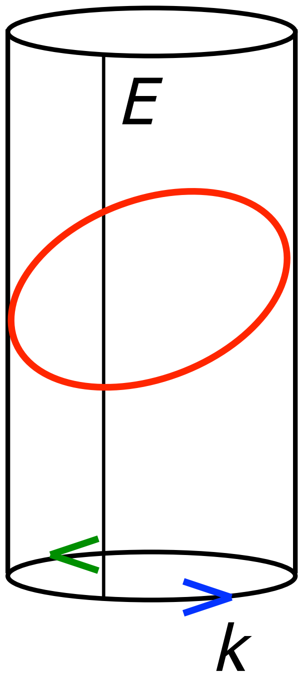
1D Brillouin zone as a loop

- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop



Berry phase in 1D Brillouin zone



Berry phase ϕ

$$u_k(x) = e^{-ikx}\psi_k(x)$$

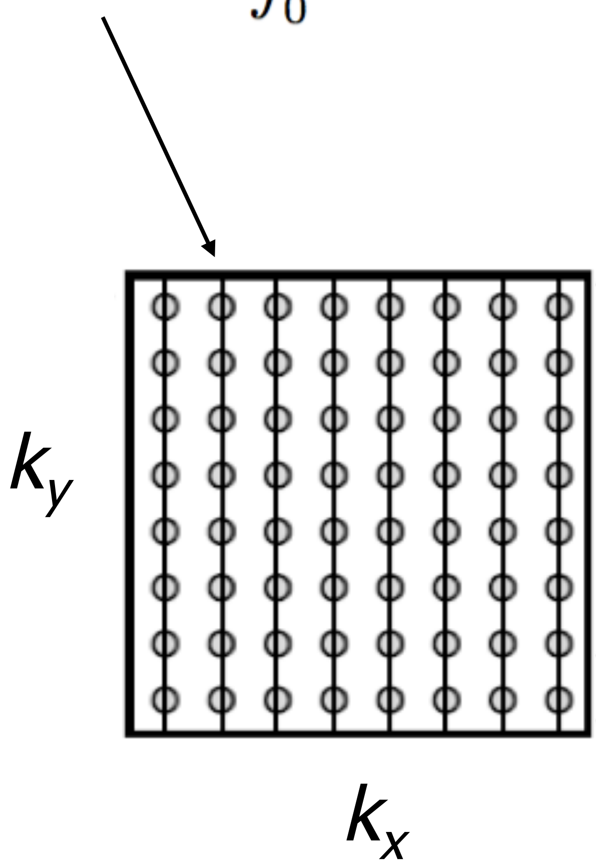
$$\phi_n = \int_0^{2\pi/a} \langle u_{nk} | \, i\frac{d}{dk} \, | u_{nk} \rangle \, dk$$

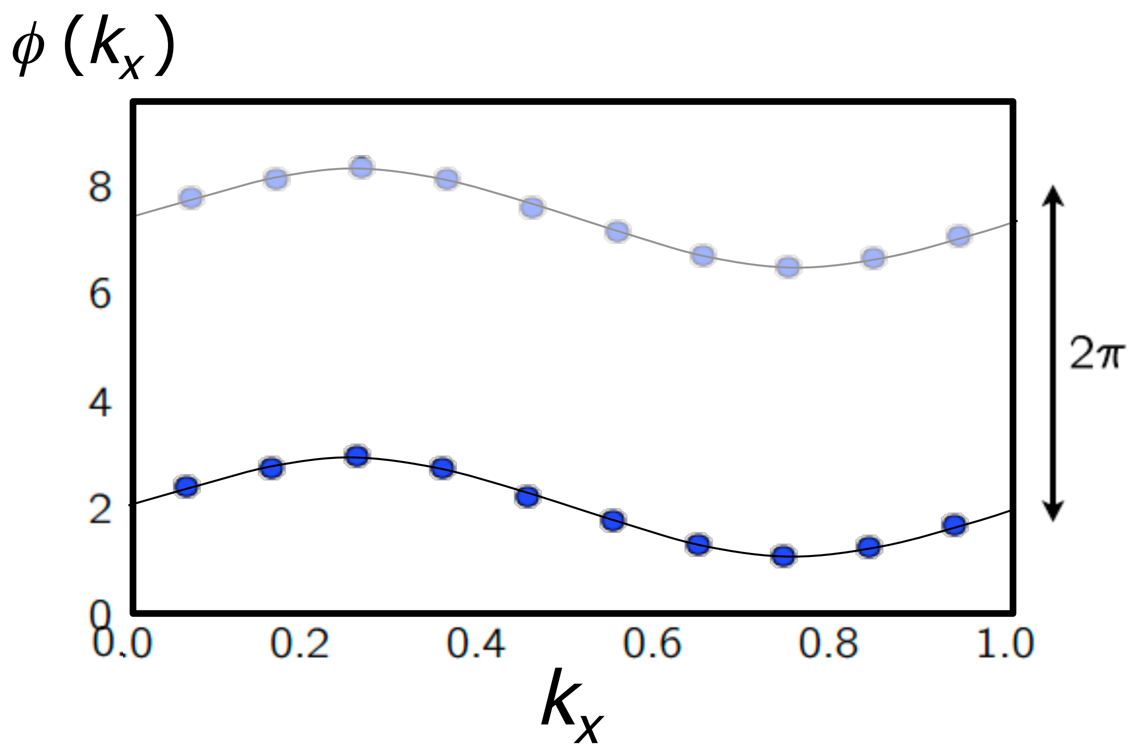
Berry curvature

$$A_{nk} = \langle \, u_{nk} \, | \, i\frac{d}{dk} \, | \, u_{nk} \, \rangle$$

String Berry phases of 2D insulator

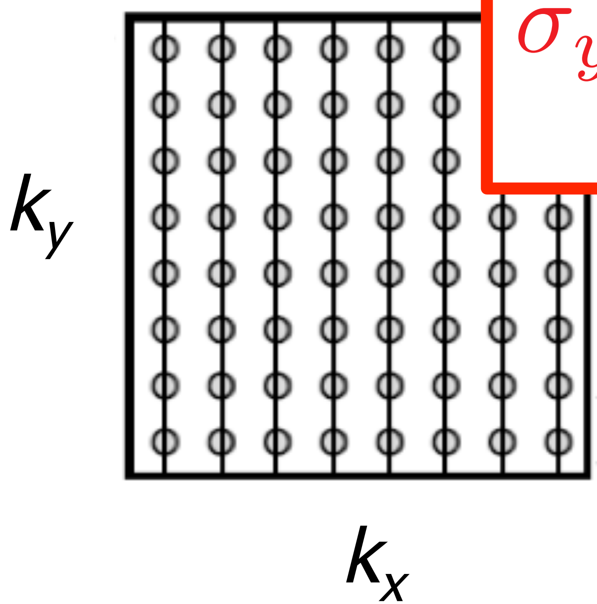
$$\phi\left(k_x\right) = \int_0^{2\pi/a} \langle u_{nk}|\, i\frac{d}{dk_y} |u_{nk}\rangle \, dk$$



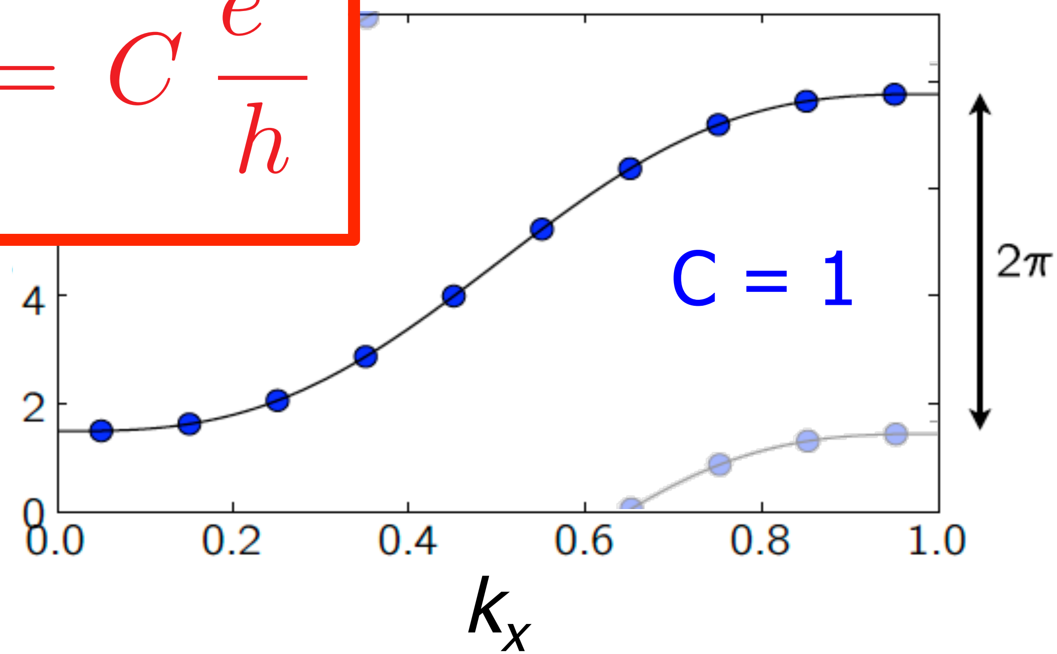


String Berry phases of 2D Chern insulator

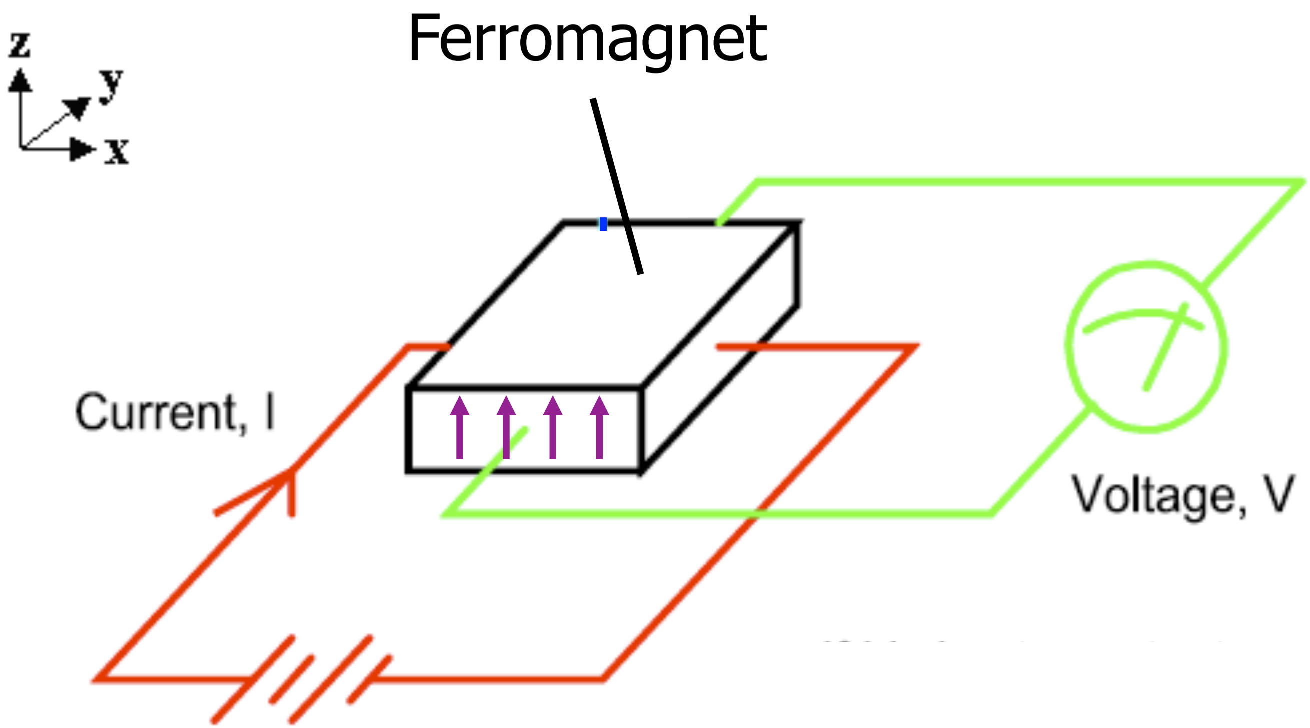
$$\phi\,(k_x) = \int_0^{2\pi/a} \langle u_{nk}|\, i\frac{d}{dk_y}\, |u_{nk}\rangle\, dk$$



$$\sigma_{yx} = C\,\frac{e^2}{h}$$



Anomalous Hall conductivity (AHC)



Measure σ_{yx} in ***absence*** of *B*-field

Chern insulator = QAH insulator

"Quantum anomalous Hall"

Berry curvature

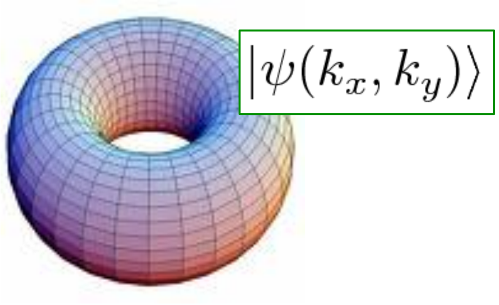
$$\Omega(\mathbf{k}) = \partial_{k_x} A_y - \partial_{k_y} A_x$$

Chern number

$$C = \frac{1}{2\pi} \int d^2k \, \Omega(\mathbf{k})$$

Anomalous Hall conductivity (AHC)

$$\sigma_{\mathrm{AHC}} = C \, \frac{e^2}{h}$$

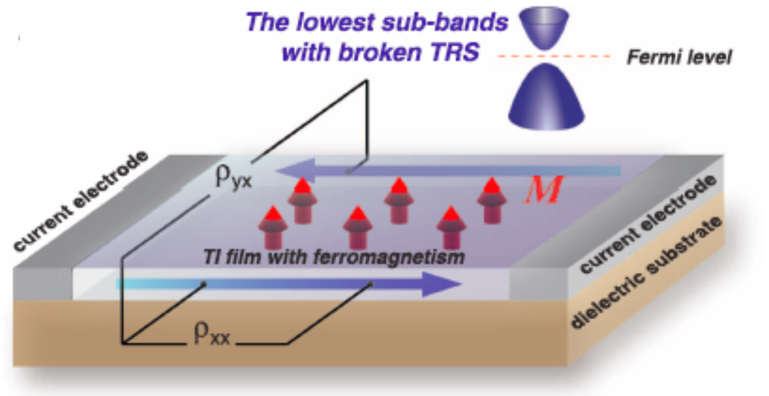


Chern theorem:
C = integer

Conclusion so far: 2D insulators

Any isolated 2D insulator either has:

- $\sigma_{AHC} = 0$
  - All non-magnetic
  - Most magnetic
- σ_{AHC} = integer x (e^2/h)
  - QAH or Chern insulator
  - First discovery 2013



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C.-Z. Chang … Q.-K. Xue, Tsinghua U.

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AHC of surface of insulator

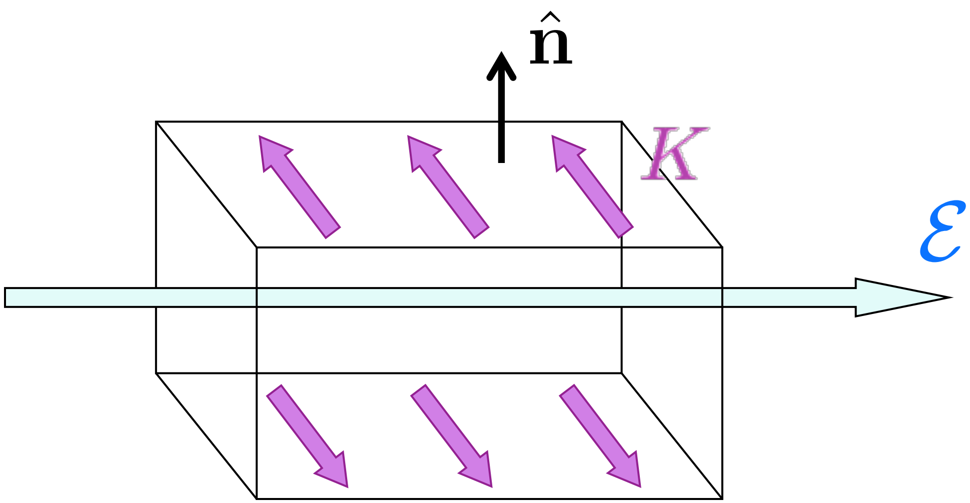
Trick question:

- What is the AHC at the insulating surface of an insulating crystal?

Tempting answer:

"Anomaly"

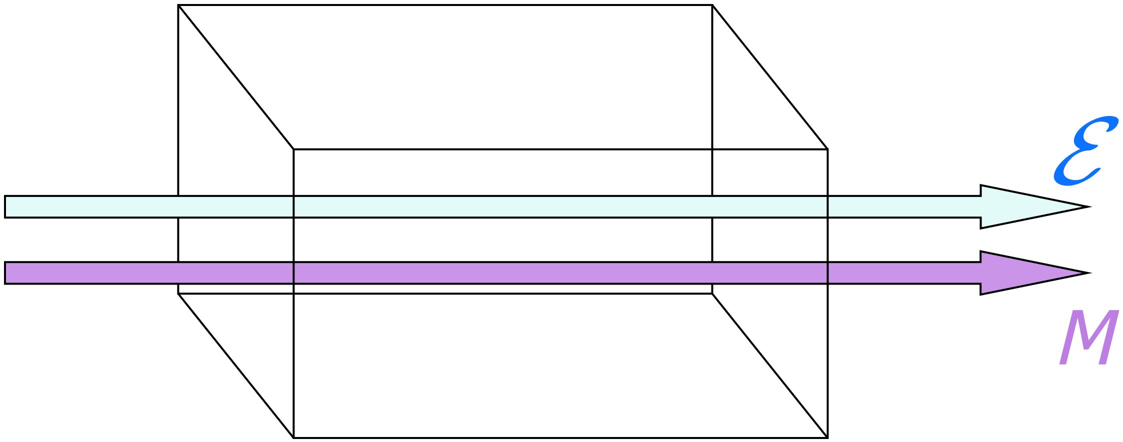
- ~~0 or integer multiple of e^2/h~~



$$\mathbf{K} = \sigma_{\rm AHC}^{\rm surf}\,\hat{\mathbf{n}} \times \mathcal{E}$$

defines $\sigma_{\rm AHC}^{\rm surf}$

Magnetoelectric coupling (MEC)



$$\mathbf{M} = \alpha\,\boldsymbol{\mathcal{E}}$$

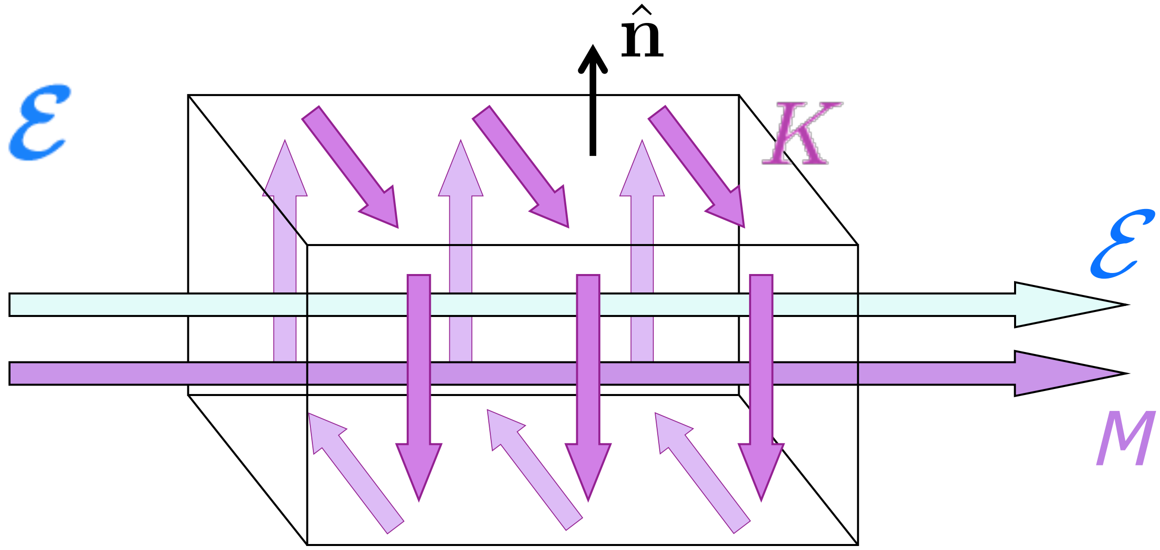
α = "magnetoelectric coefficient"

Comments: "axion"

- Assume α is isotropic (in general, it is a 3x3 tensor)
- Consider electronic (not lattice-mediated) part
- Consider orbital (not spin) part

Surface σ_{AHC} = MEC

$$\mathbf{M} = \alpha\,\mathcal{E}$$

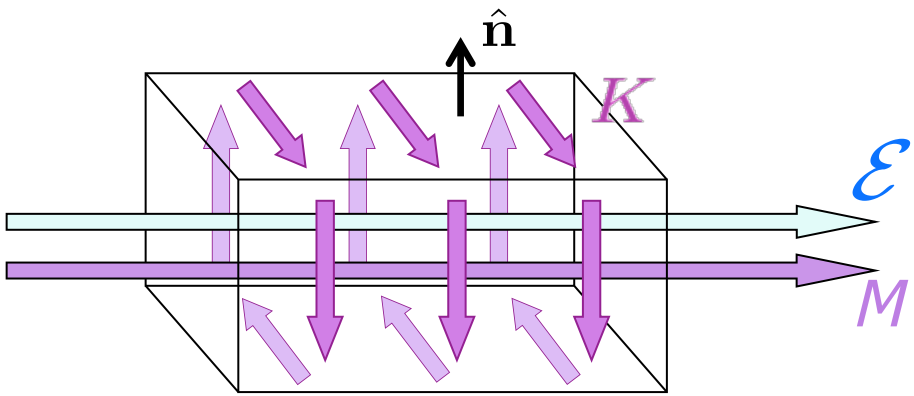


$$\mathbf{K} = \mathbf{M} \times \hat{\mathbf{n}}$$

$$\mathbf{K} = \sigma^{\mathrm{surf}}_{\mathrm{AHC}}\,\hat{\mathbf{n}} \times \mathcal{E}$$

$$\sigma^{\mathrm{surf}}_{\mathrm{AHC}} = -\alpha$$

MEC = "axion coupling"



Let

$$\alpha = \frac{\theta}{2\pi}\frac{e^2}{h}$$

- θ has Berry-phase like formula
- θ is only well-defined modulo 2π
- θ = "axion coupling"

Axion coupling

- Lagrangian has a term proportional to $\mathcal{E} \cdot B$
- Suggested for the fundamental Lagrangian of our universe:
  - Static field θ: Some bizarre consequences
    - Electric charges acquire magnetic monopole
  - Dynamic field $\theta(\mathbf{r},t)$: Quantum is "axion"
    - Possible dark matter candidate
- Here, $\theta(\mathbf{r}) \neq 0$ inside a magnetoelectric insulator
  - Emergent property of insulating ground state

Berry-phase like formula

*Qi, Hughes and Zhang, PRB **78**, 195424 (2008)*
*Essin, Moore and Vanderbilt, PRL **120**,146805 (2009)*

$$\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\,\epsilon_{abc}\,\mathrm{tr}\left[\mathrm{A_a}\partial_{\mathrm{b}}\mathrm{A_c} - \frac{2\mathrm{i}}{3}\mathrm{A_a}\mathrm{A_b}\mathrm{A_c}\right]$$

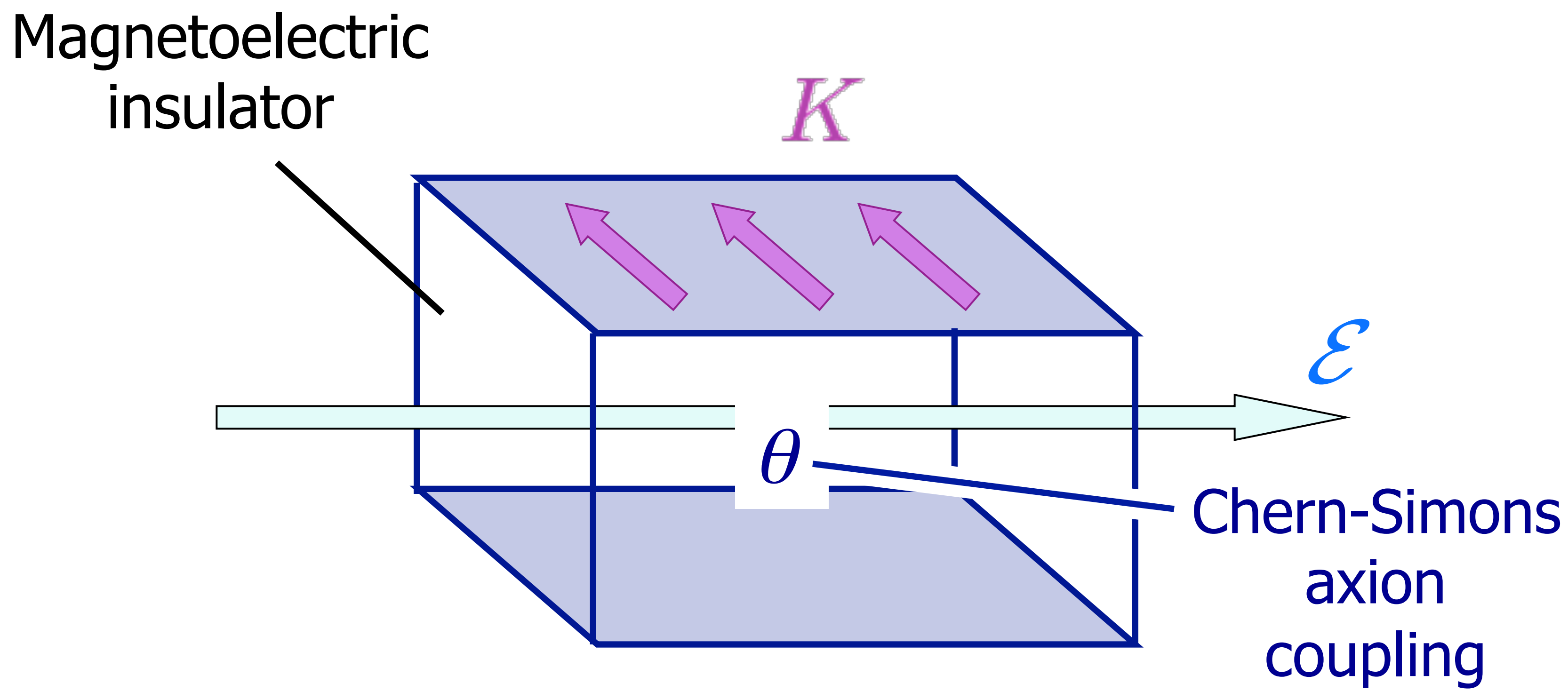
$$\text{Berry connection:}\quad A_{a,nm} = i\,\langle u_{n\mathbf{k}}|\,\frac{\partial}{\partial k_a}\,|u_{m\mathbf{k}}\rangle$$

Compare Berry phase:

$$\phi = \int_{\mathrm{BZ}} dk\ \mathrm{tr}[\mathrm{A}]$$

θ and ϕ are gauge-invariant only modulo 2π

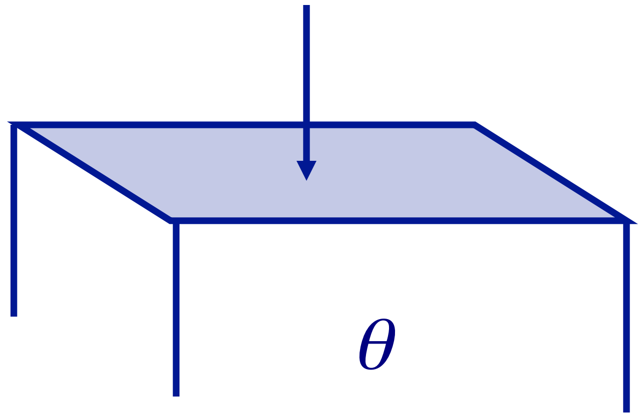
Surface AHC


Magnetoelectric
insulator
K
ℰ
θ
Chern-Simons
axion
coupling

Insulating surface of bulk insulator

Surface AHC

$$\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[\frac{-\theta}{2\pi} + \text{integer}\right]$$



θ is ill-defined modulo 2π

When can θ be equal to π ?

- θ is gauge-invariant, modulo 2π
- T or I symmetry operator maps θ into $-\theta$
- Two values of θ are allowed (Z_2 classification):
  - Case of $\theta = 0$ $\Leftrightarrow$ trivial insulator
  - Case of $\theta = \pi$ $\Leftrightarrow$ strong topological insulator (T)
    axion insulator (I)
- $\theta = \pi$ implies half-integer surface quantum AHC !

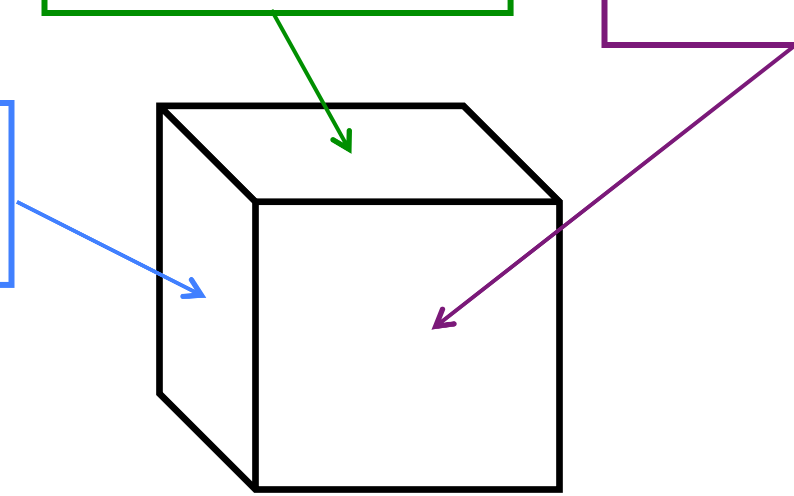
Half-integer surface QAH?

- $\theta = \pi$ implies half-integer surface quantum AHC !

$$\sigma^{\rm surf}_{\rm AHC} = +\frac{1}{2}\frac{e^2}{h}$$

$$\sigma^{\rm surf}_{\rm AHC} = +\frac{3}{2}\frac{e^2}{h}$$

$$\sigma^{\rm surf}_{\rm AHC} = -\frac{1}{2}\frac{e^2}{h}$$



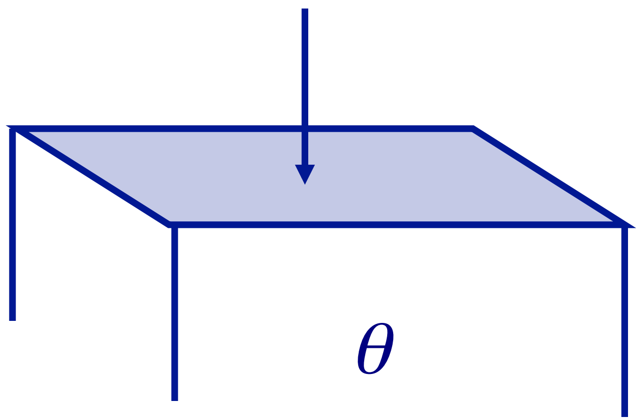
But T symmetry ⇒ surface AHC = 0.

Is this a contradiction?

Metallic surface of bulk insulator

Anom. Hall conductivity

$$\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[-\frac{\theta}{2\pi} + \text{int} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k})\right]$$

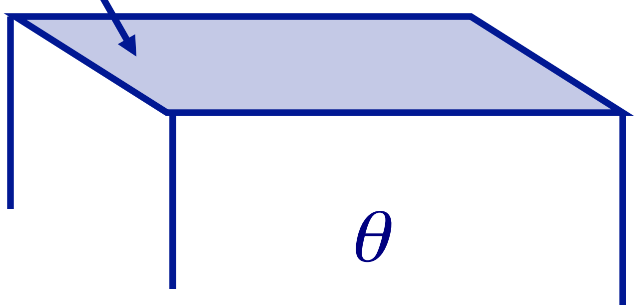


θ is ill-defined
modulo 2π

Surface AHC of strong topological insulator

if surface is metallic

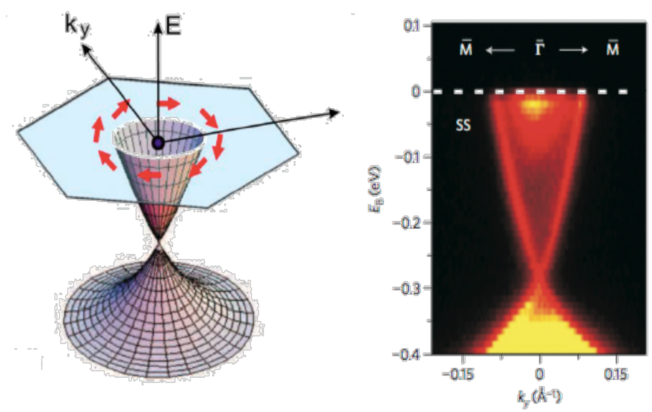
$$\sigma^{\rm surf}_{\rm AHC} = -\frac{e^2}{h}\left[-\frac{\theta}{2\pi} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k}) \right]$$



Bulk θ is defined modulo 2π

Strong topo. insulator:

- Bulk θ contrib. = π
- Metallic contrib. = π
- Total surface AHC = 0



Figures from Hasan and Kane, RMP, 2010 (Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009).

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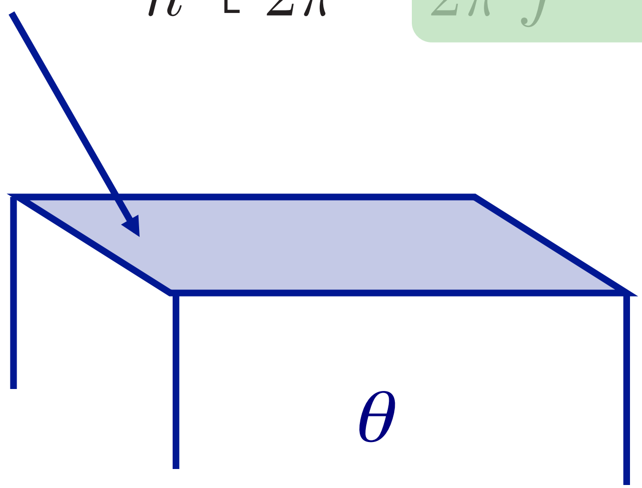
Surface AHC of axion insulator

if surface is metallic

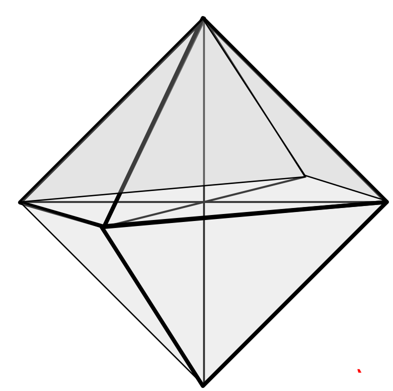
$$\sigma_{\mathrm{AHC}}^{\mathrm{surf}} = -\frac{e^2}{h}\left[-\frac{\theta}{2\pi} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k})\right]$$



Bulk θ is defined modulo 2π

<u>Axion insulator</u>:

- $\theta = \pi$
- Surface contrib. = 0
- Surface AHC = ± $e^2/2h$



What is an axion insulator?

- Axion $\theta = \pi$ protected by I symmetry
- But I is never a good symmetry at a surface
- Surfaces are naturally gapped!
- Surfaces carry half-integer QAH response!
- Problem:
  - We don't know any materials realizations!*
  - Future plan: look for new materials

* Except magnetically doped thin films of Bi_2Se_3-class topological insulators

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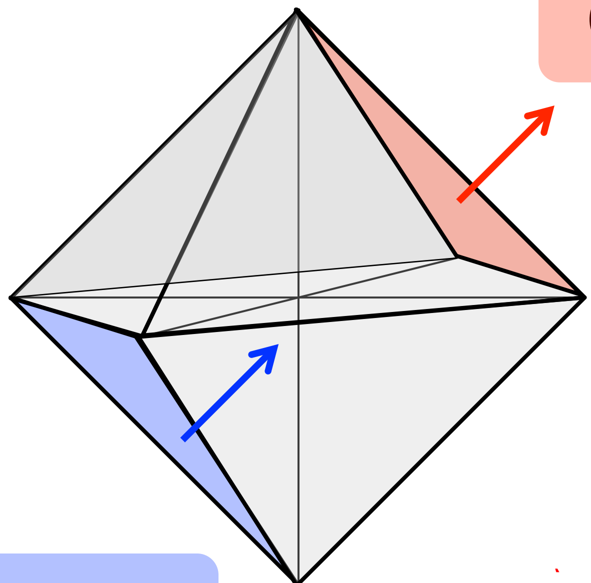
  - Quantized Kerr/Faraday rotation (*)
  - Topological magnetoelectric effect
  - Chiral hinge states

(*) L. Wu, M. Salehi, N. Koirala, J. Moon, S. Oh, and N.P. Armitage, Science **354**, 1124 (2016).

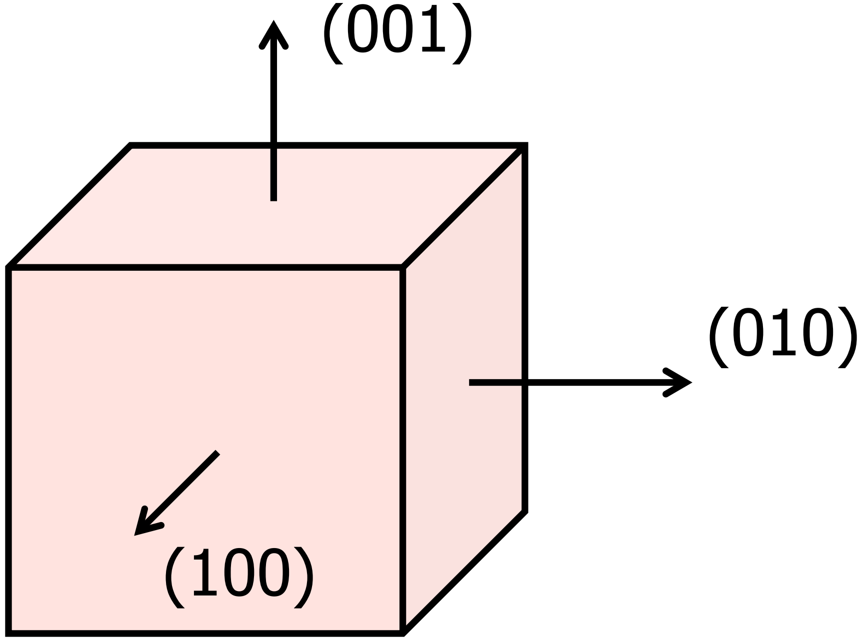
Convention: Color by outward-normal AHC

(111) : $\sigma_{xy}^{\text{surf}}$ = + e^2/2h



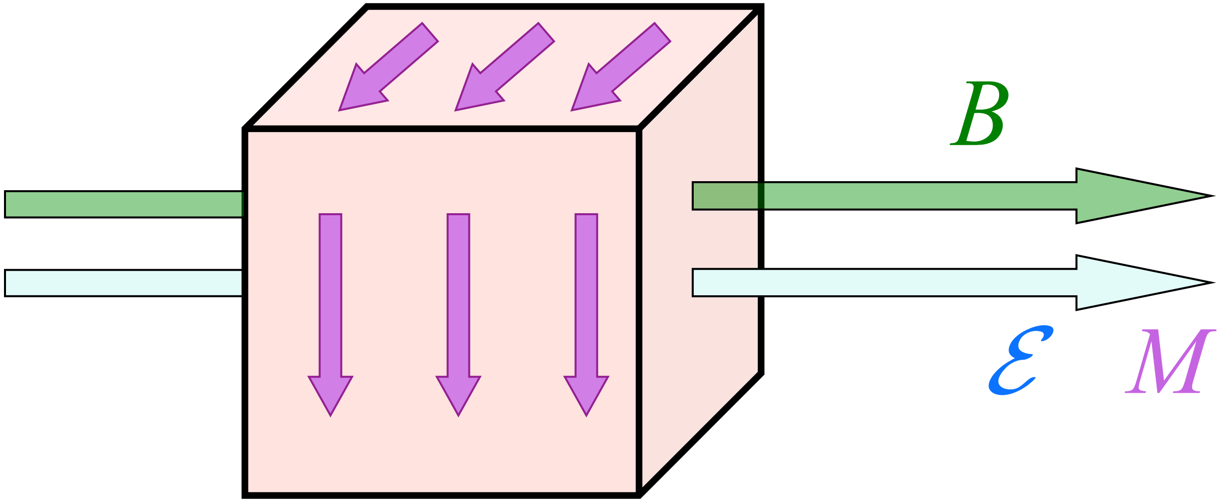
(111) : $\sigma_{xy}^{\text{surf}}$ = − e^2/2h

Topological ME effect



(Engineer surfaces to get consistent sign of AHC)

Topological ME effect



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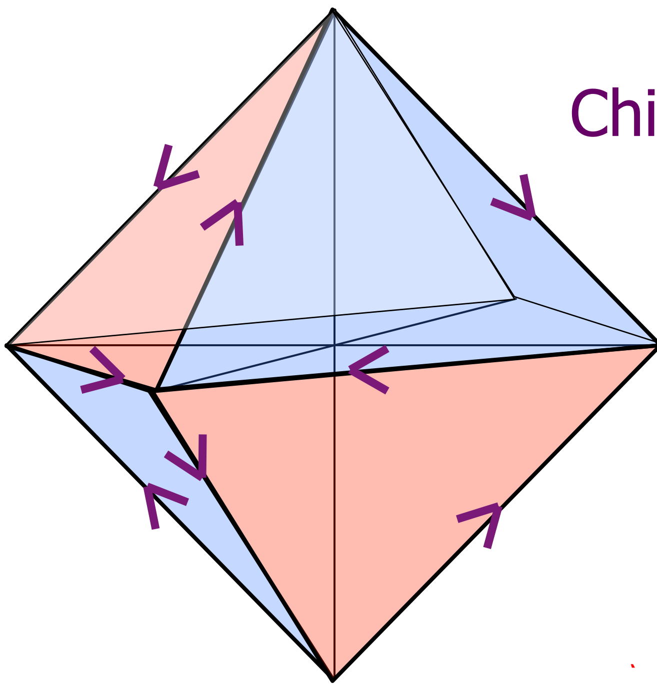
Chiral hinge states



Chiral hinge states

Real pyrochlore

From Wikipedia, the free encyclopedia

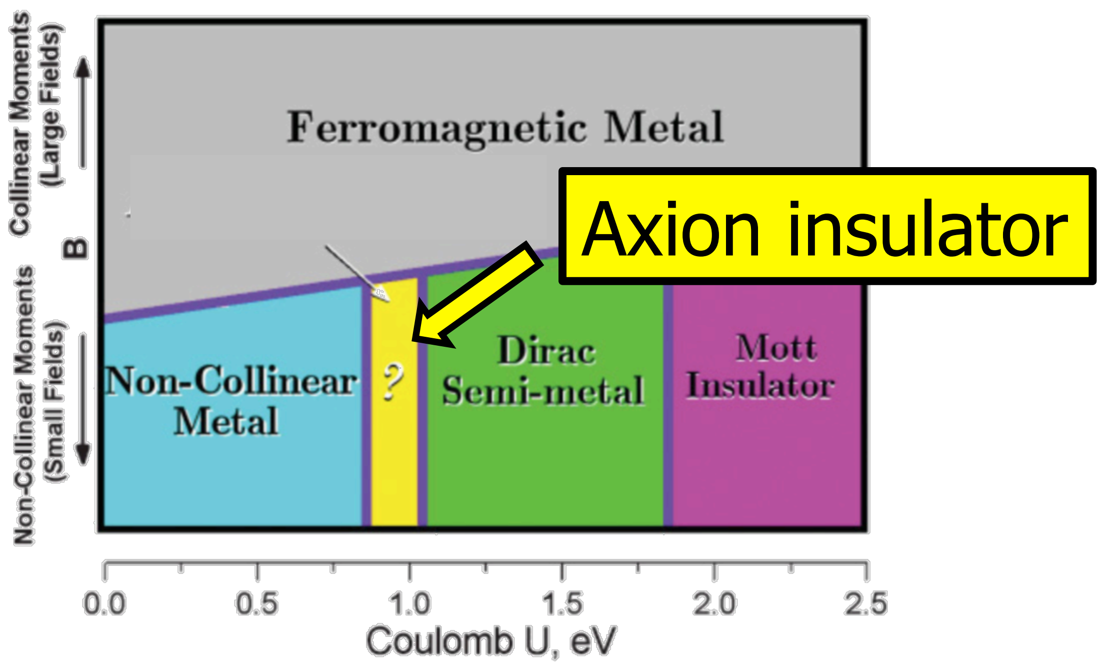
Pyrochlore from Russia

2011 theory of pyrochlore iridates

PHYSICAL REVIEW B **83**, 205101 (2011)

Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan,[1] Ari M. Turner,[2] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[1,4]
[1]*National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China*
[2]*Department of Physics, University of California, Berkeley, California 94720, USA*
[3]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[4]*Department of Physics, University of California, Davis, One Shields Avenue, Davis, California 95616, USA*



Updated theory: 2017

PRL 118, 026404 (2017) PHYSICAL REVIEW LETTERS week ending 13 JANUARY 2017

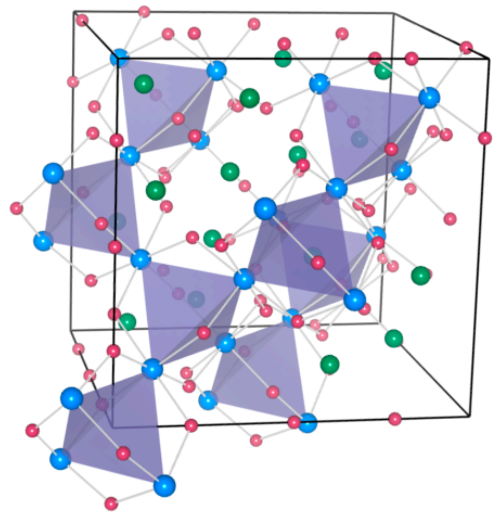
Metal-Insulator Transition and Topological Properties of Pyrochlore Iridates

Hongbin Zhang,[1,2] Kristjan Haule,[1] and David Vanderbilt[1]

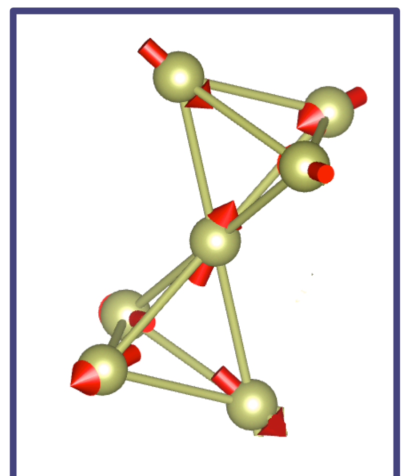
Conclusion:
AIAO phase is
topologically trivial

Minimal TB model of pyrochlore iridates

Nicodemus Varnava



Witczak-Krempa



All-in-all-out (AIAO) magnetic insulator

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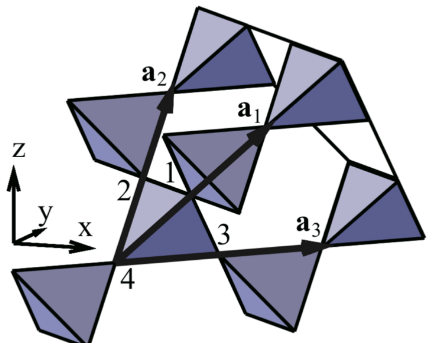
Tight binding Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.)$$

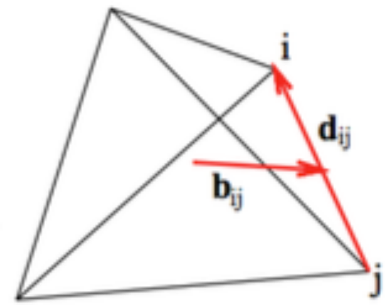
Real n.n hop.



J. Phys. Soc. Jpn. 80, 044708 (2011)

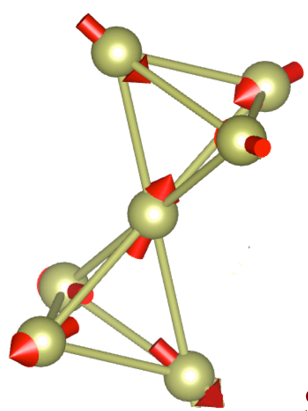
$$+ \sqrt{2}\lambda \sum_{\langle ij \rangle \alpha\beta} (i c_{i\alpha}^{\dagger} \hat{\boldsymbol{b}}_{ij} \times \hat{\boldsymbol{d}}_{ij} \cdot \boldsymbol{\sigma}_{\boldsymbol{\alpha\beta}} c_{j\beta} + h.c.)$$

SOC $(\boldsymbol{p} \times \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V)$

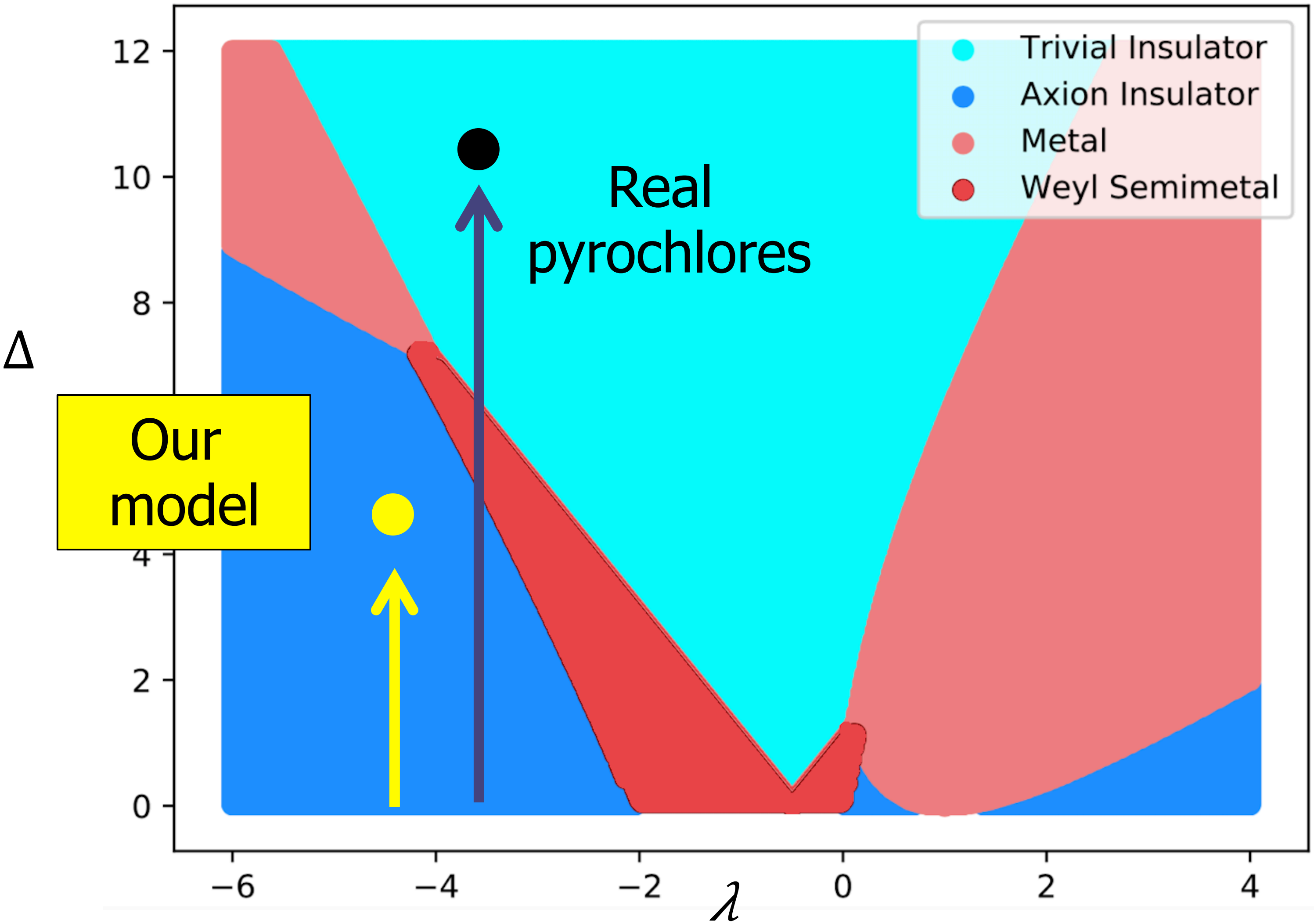


$$+ \Delta \sum_{i} \hat{\boldsymbol{n}}_i \cdot \boldsymbol{\sigma} c_i^{\dagger} c_i$$

On-site Zeeman fields



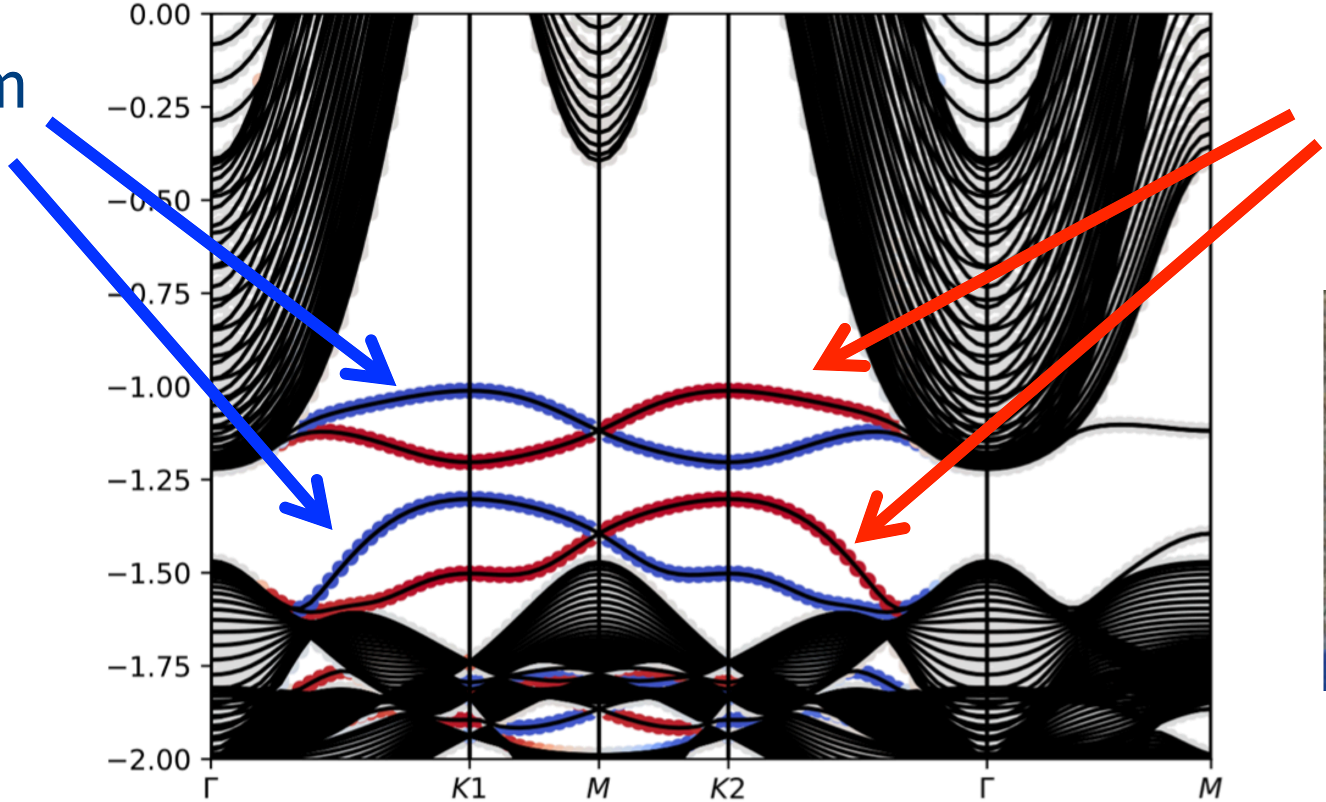
Phase diagram of TB model



Surface band structure: (111) slab

Bottom surf.

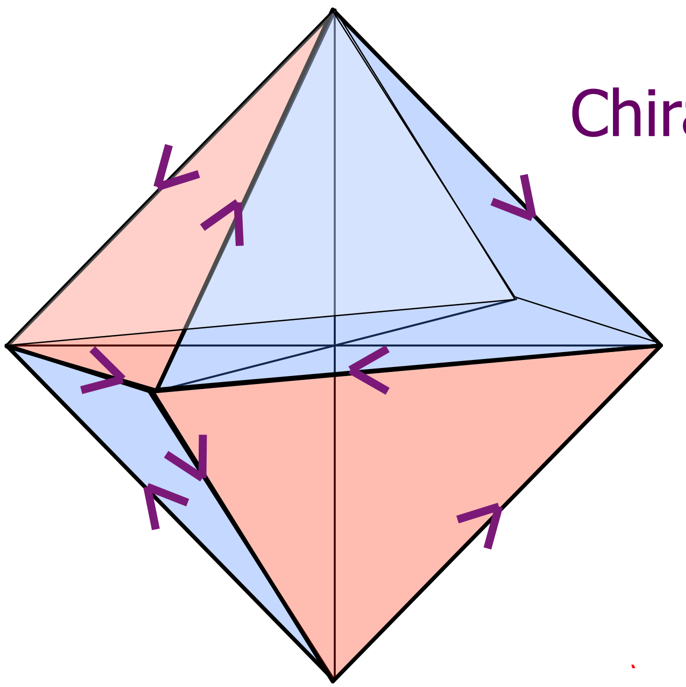
Top surf.



Axion phase with gapped surfaces

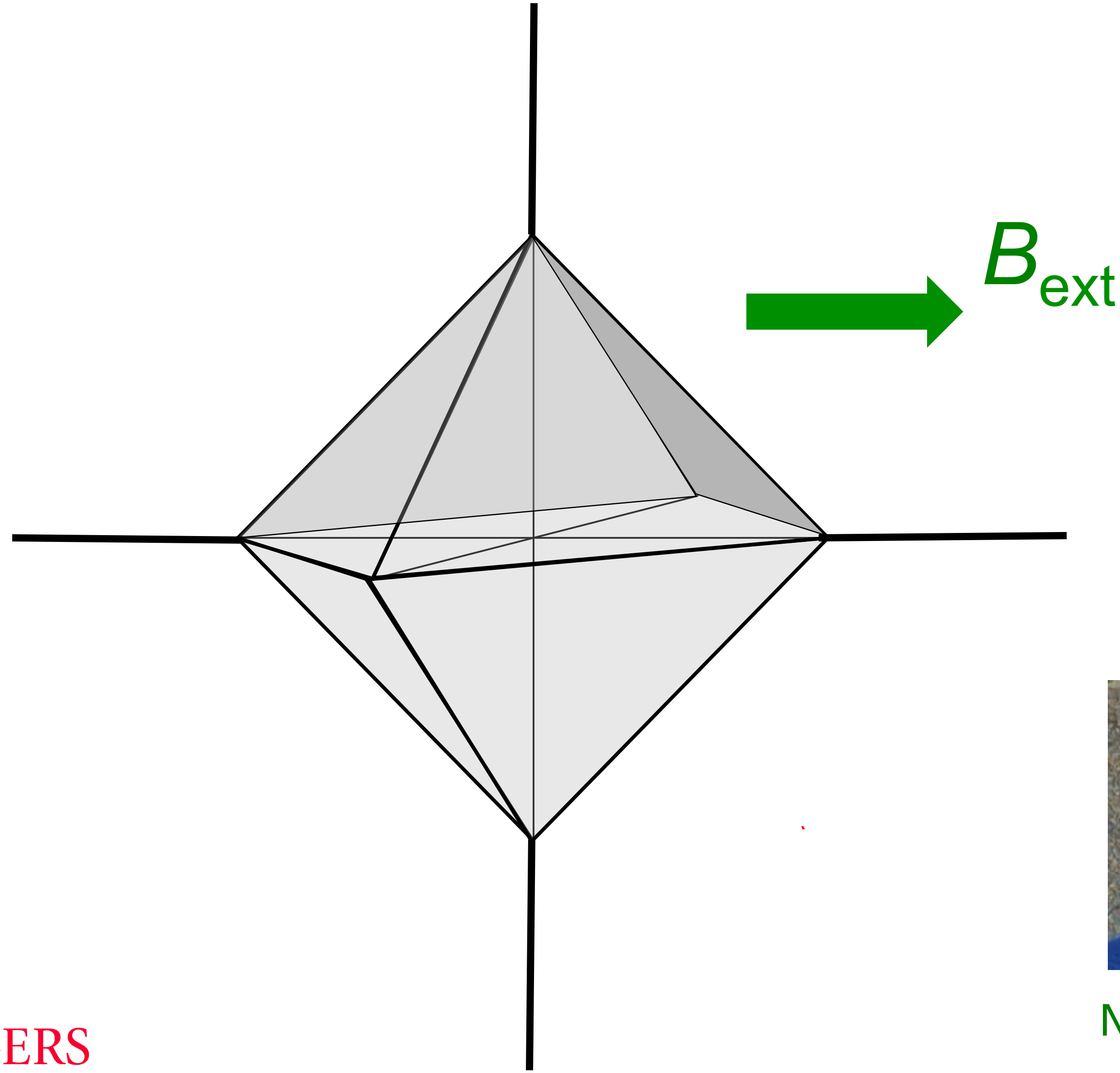
Nicodemus Varnava

All-in-all-out magnetic order



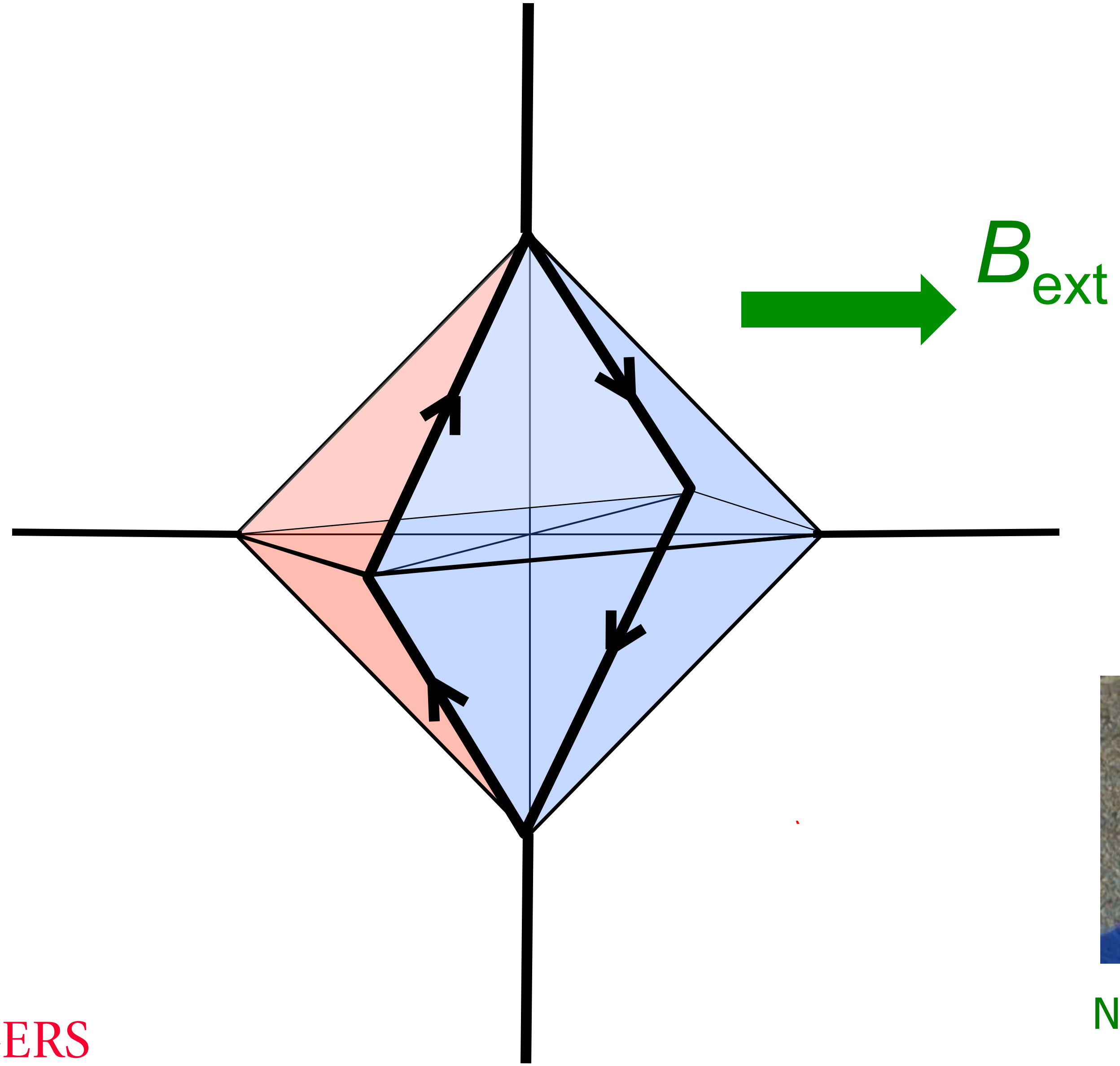
Chiral hinge states

FM order: Chiral hinge circuits



Nico Varnava

FM order: Chiral hinge circuits



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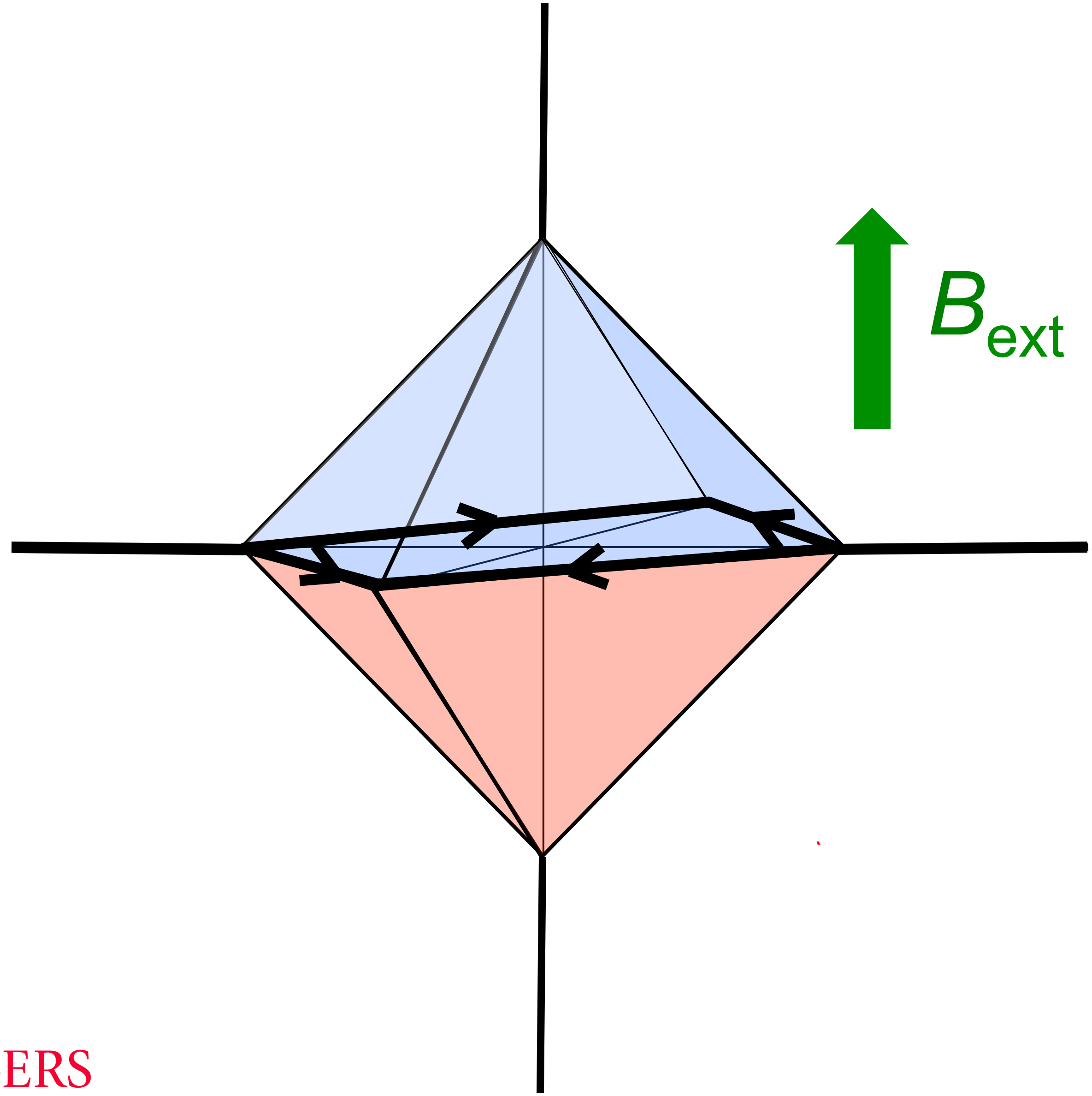
FM order: Chiral hinge circuits



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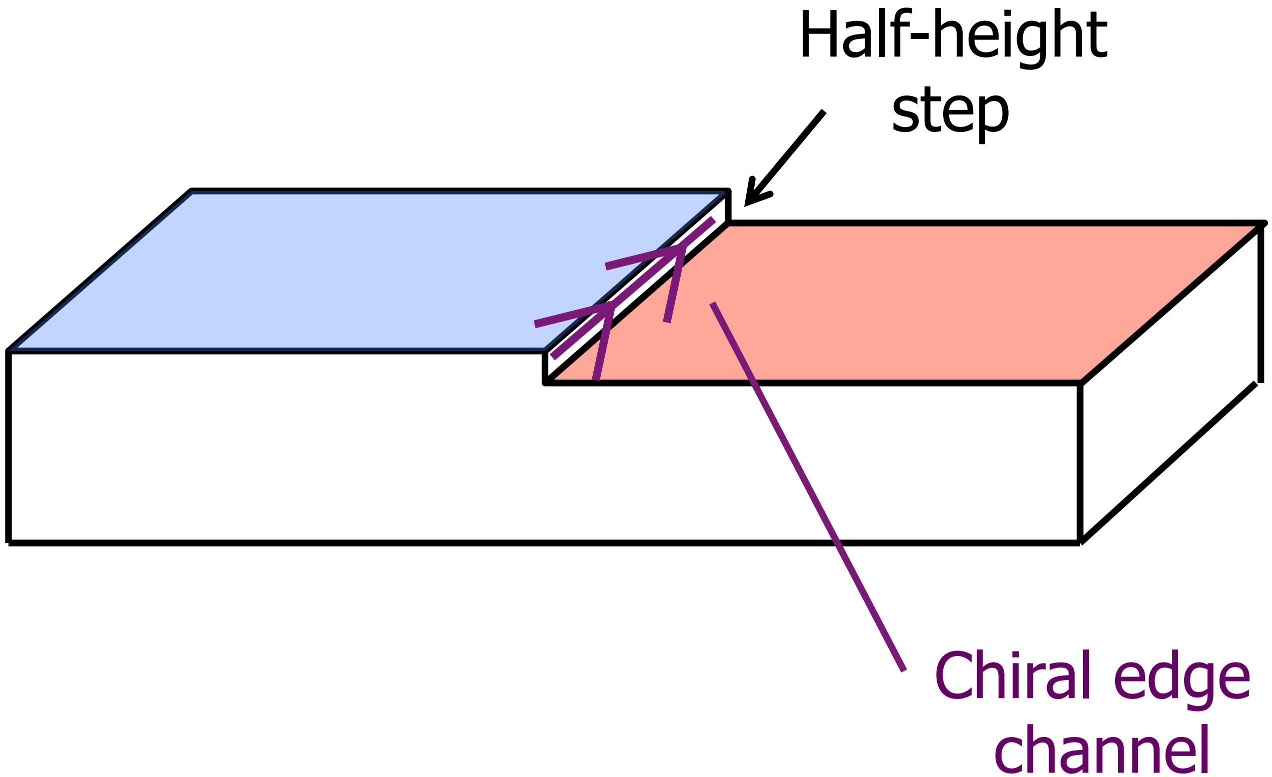
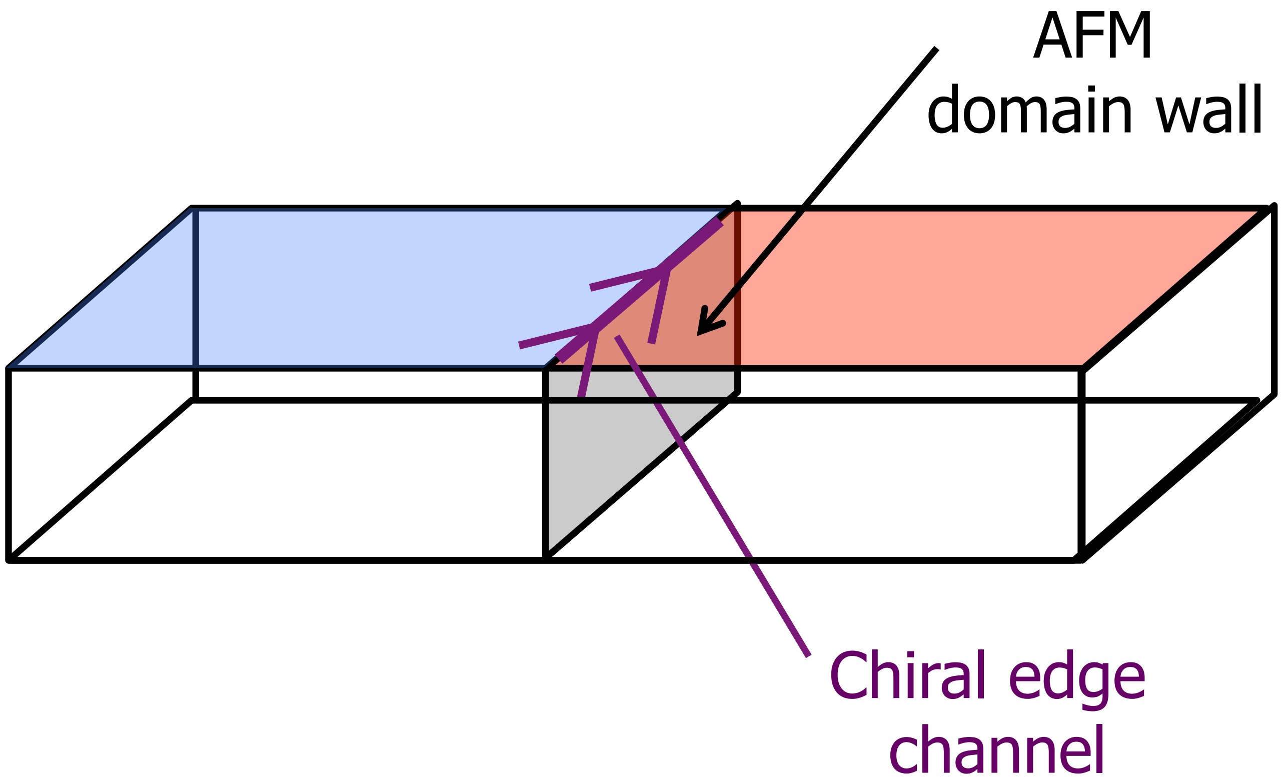
Stepped surface



See also Mong, Essin & Moore, PRB 81, 245209 (2010).

AFM domain wall



Summary: Axion insulators

- Topology protected by inversion
- Surfaces are naturally gapped
- Surfaces display half-integer quantum anomalous Hall effect
- 3D crystallites can show
  - Topological ME effect (if consistently terminated)
  - Chiral hinge modes (if not)
- *Materials realizations are missing!*

Collaborators & Grants

Maryam Taherinejad | Thomas Olsen | Ivo Souza | Nico Varnava








Sinisa Coh | Andrei Malashevich | Andrew Essin | Joel Moore | Ari Turner

NSF DMR-1408838

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