Topological insulators and the quantum anomalous Hall state

David Vanderbilt
Rutgers University

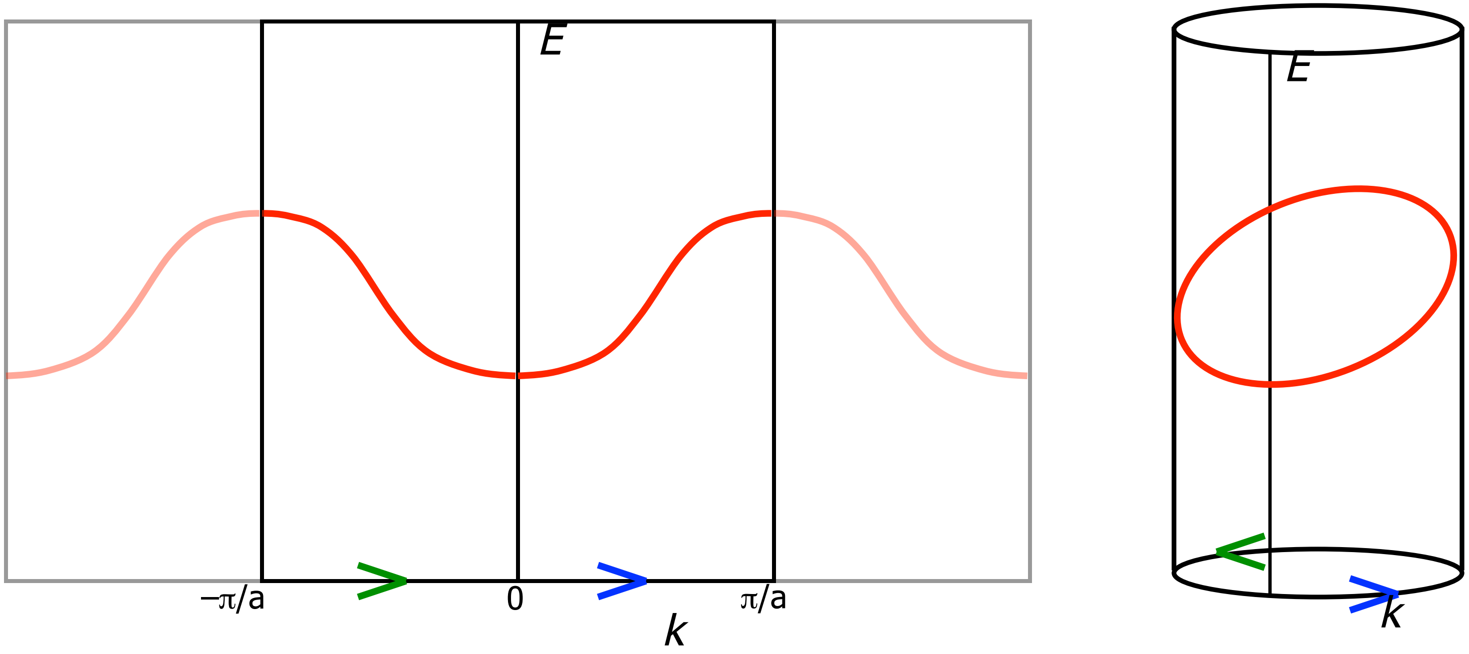
MASTANI School, Pune, India, July 10 2014

Outline

- Berry curvature and topology
- 2D quantum anomalous Hall (QAH) insulator
- TR-invariant insulators (Z_2)
  - 2D ("Quantum spin Hall") insulator
  - 3D topological insulators
- QAH strategies
  - Heavy-atom adlayers on magnetic substrates
  - Other ideas
- Summary

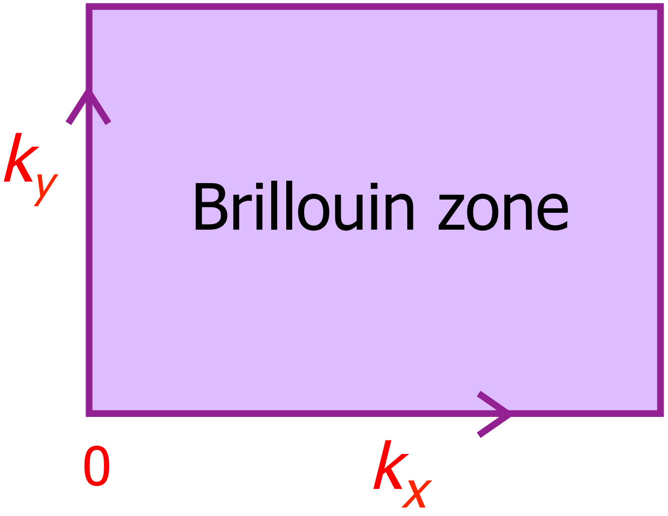
1D: BZ is really a loop

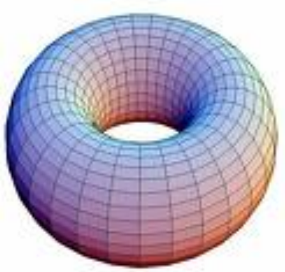
- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop



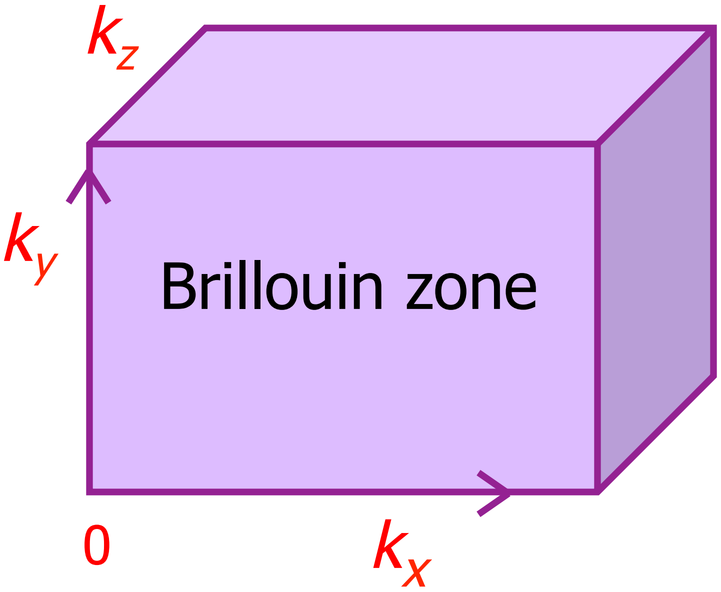
2D, 3D: BZ is a closed manifold

2-D Crystal





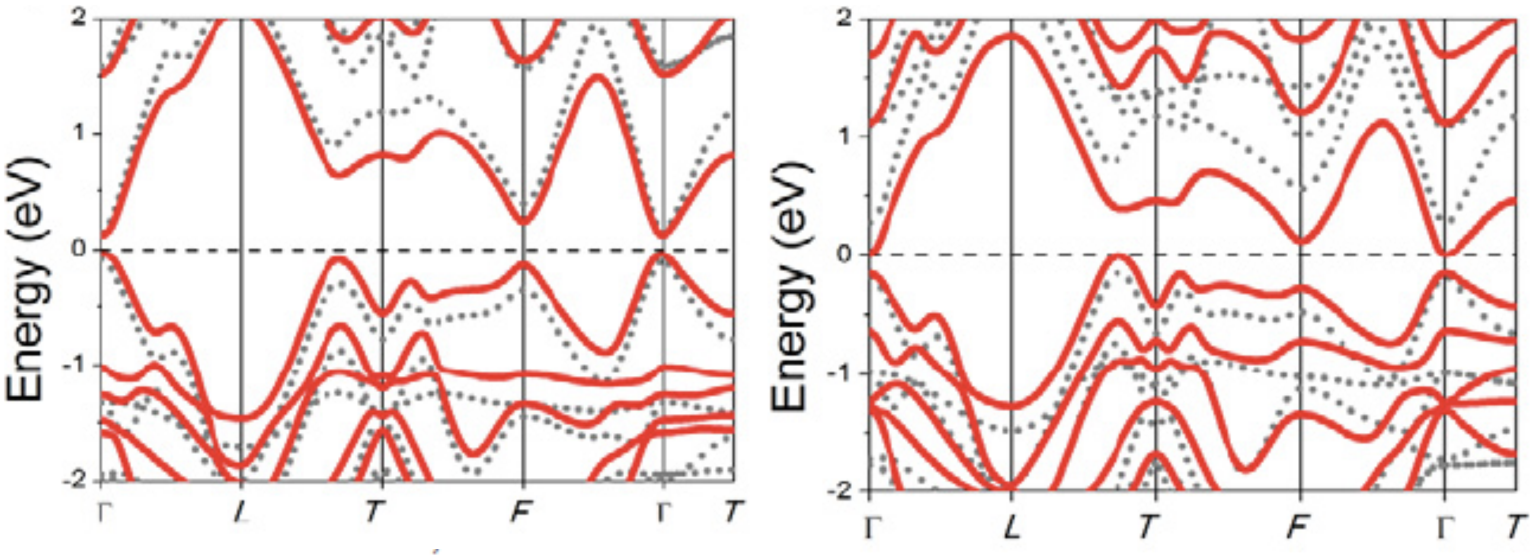
3-D Crystal



(3-torus)

Invisible information: Topology

.... Without spin-orbit coupling



$TlBiSe_2$ $TlBiTe_2$

BINGHAI YAN[1], CHAO-XING LIU[2], HAI-JUN ZHANG[3,4], CHI-YUNG YAM[1], XIAO-LIANG QI[4,5],
THOMAS FRAUENHEIM[1] and SHOU-CHENG ZHANG[4]

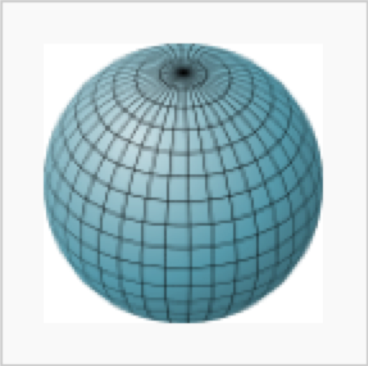
EPL, **90** (2010) 37002

Reds are topologically equivalent

Greys are topologically equivalent

Reds and greys are **inequivalent**

Topology of closed surfaces

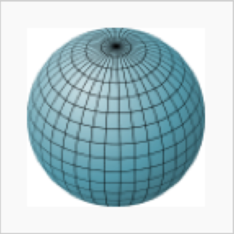


genus 0

genus 1

Compare: Two contexts for topology

Geometric topology



genus 0

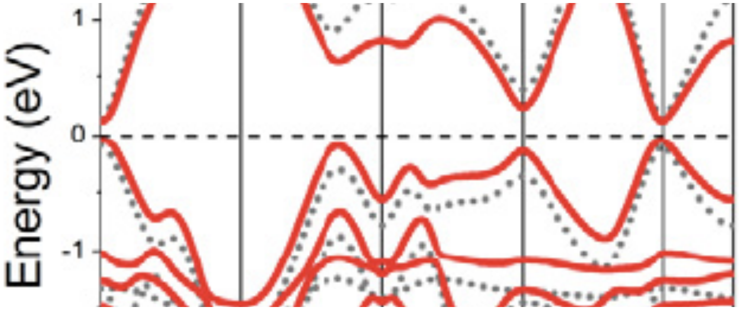
genus 1

genus 2

genus 3

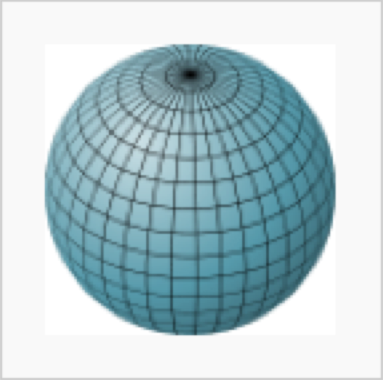
"Same" if can be deformed without singularity (pinch, rip, etc.)

Band structure topology



"Same" if can be adiabatically perturbed without gap closure

Compare: Gauss-Bonnet Theorem


genus 0


genus 1


genus 2

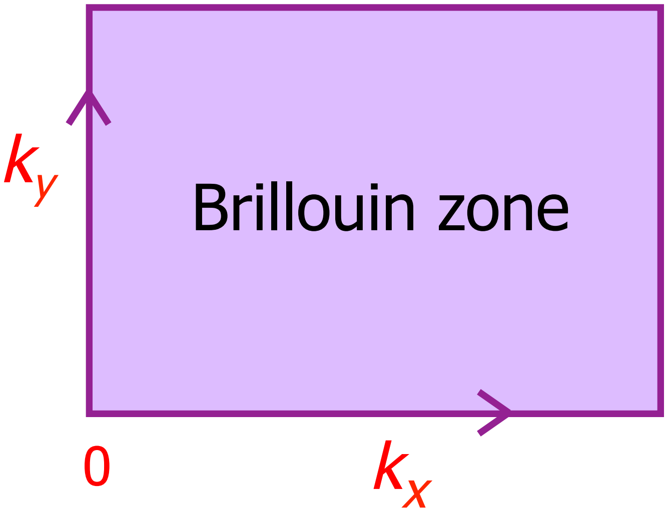

genus 3

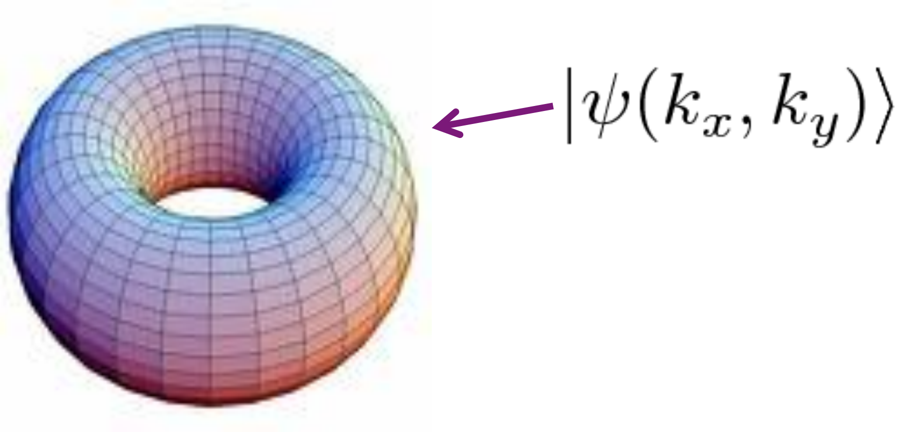
$$\boxed{\int_S K\, d\sigma = 2\pi\ \chi}$$

Gaussian
(geometrical)
curvature

Euler characteristic
= 2(1-genus)

Compare: Chern theorem





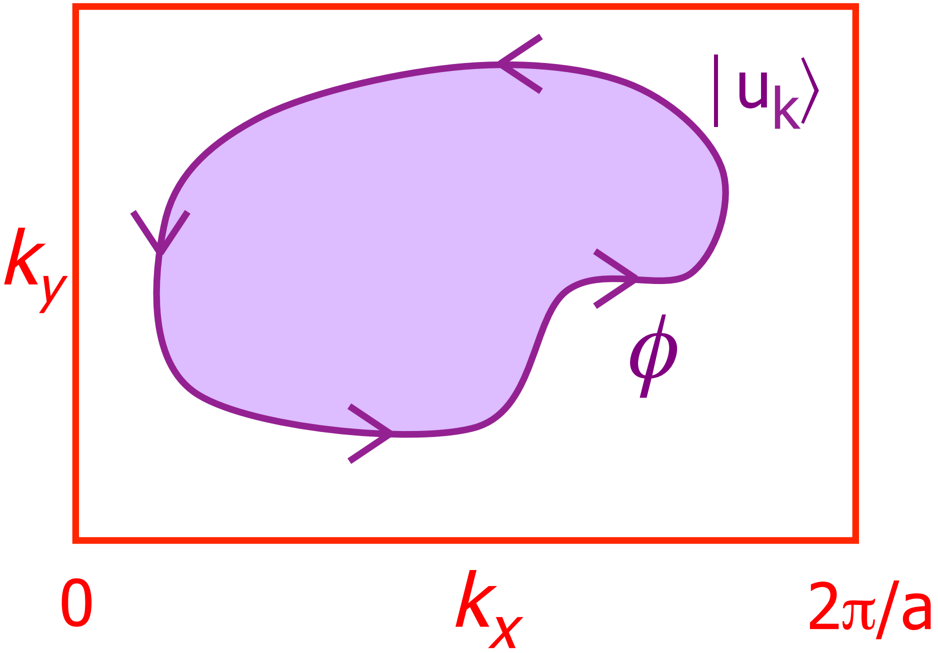
$$\boxed{\int_S F \, d\sigma = 2\pi \, C}$$

$(F \equiv \Omega)$

Berry curvature

Chern number

Berry phase and curvature in the BZ



$$u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}} \underbrace{\psi_{\mathbf{k}}(\mathbf{r})}_{\text{Bloch function}}$$

Berry potential:

$$\mathbf{A}(\mathbf{k}) = -\mathrm{Im}\,\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle$$

Berry phase:

$$\phi = \oint \mathbf{A}(\mathbf{k})\cdot d\mathbf{k}$$

Berry curvature:

$$\Omega(\mathbf{k}) = \nabla \times \mathbf{A}$$

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

Stoke's theorem:

$$\phi = \int \Omega_z(\mathbf{k})\, d^2k$$

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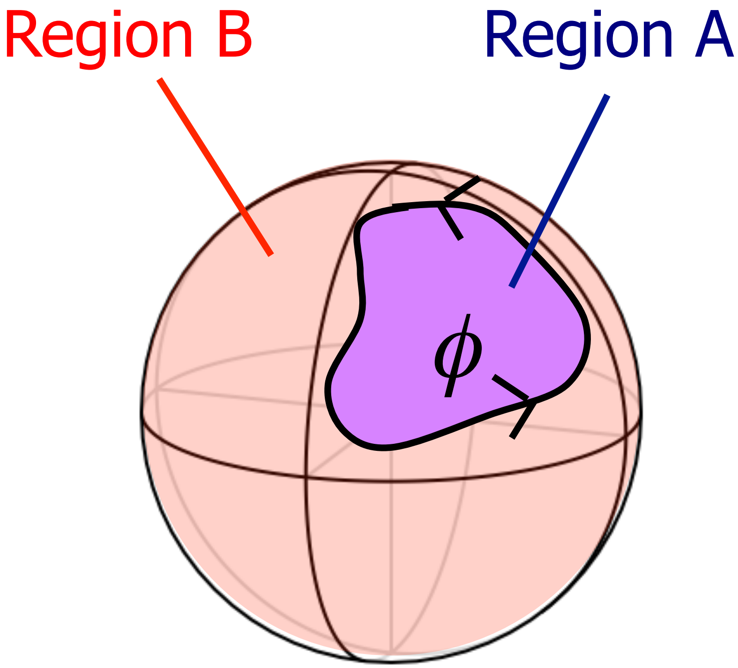
Chern Theorem



Stokes applied to A:

$$\phi = \int_A \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Stokes applied to B:

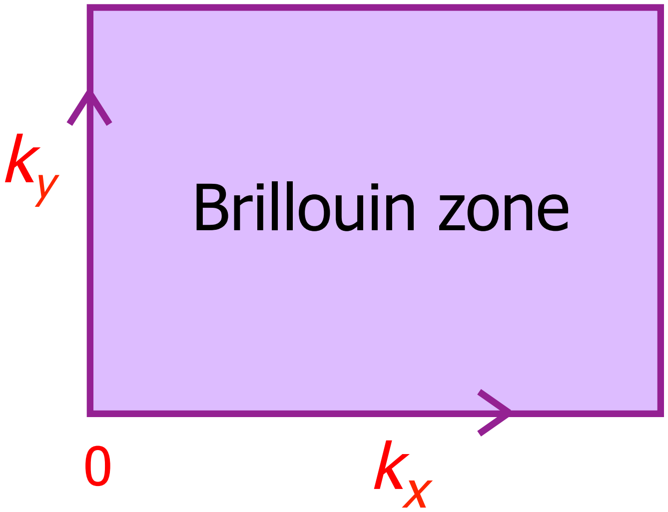
$$\phi = -\int_B \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

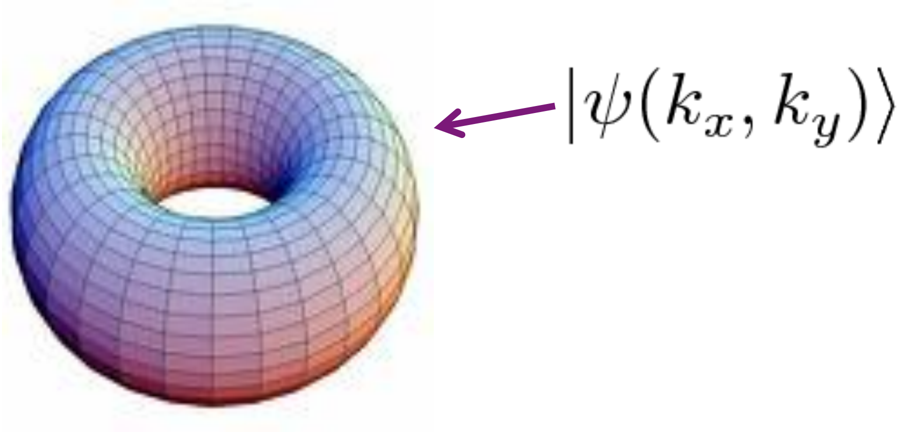
Subtract:

$$0 = \oint \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Chern theorem: $\oint \mathcal{F}(\lambda)\, dS_\lambda = 2\pi\, C$

Chern theorem





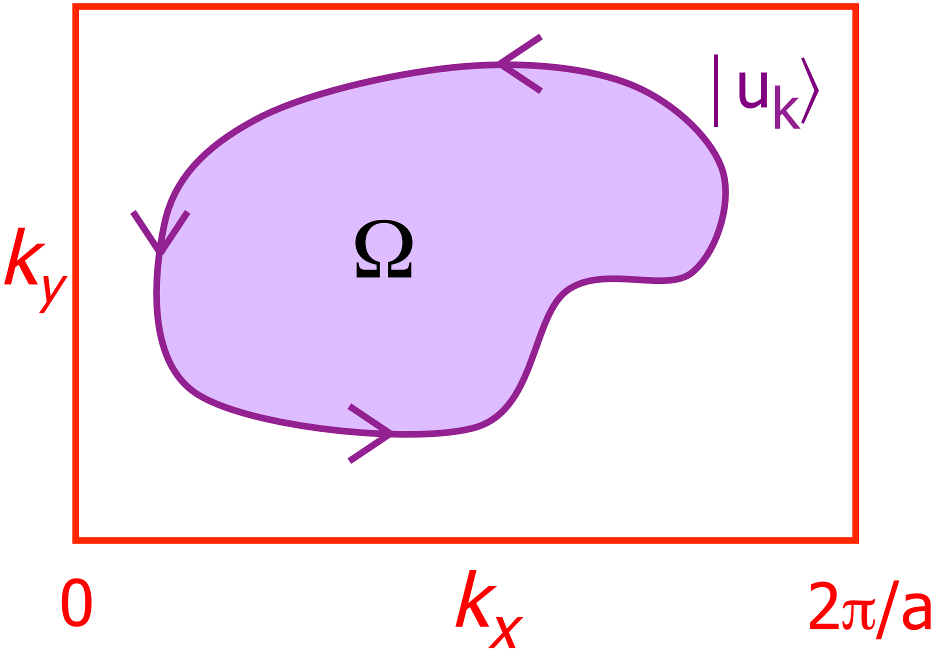
$$\boxed{\int_S F\, d\sigma = 2\pi\, C}$$

$(F \equiv \Omega)$

Berry curvature

Chern number

Berry curvature in the Brillouin zone



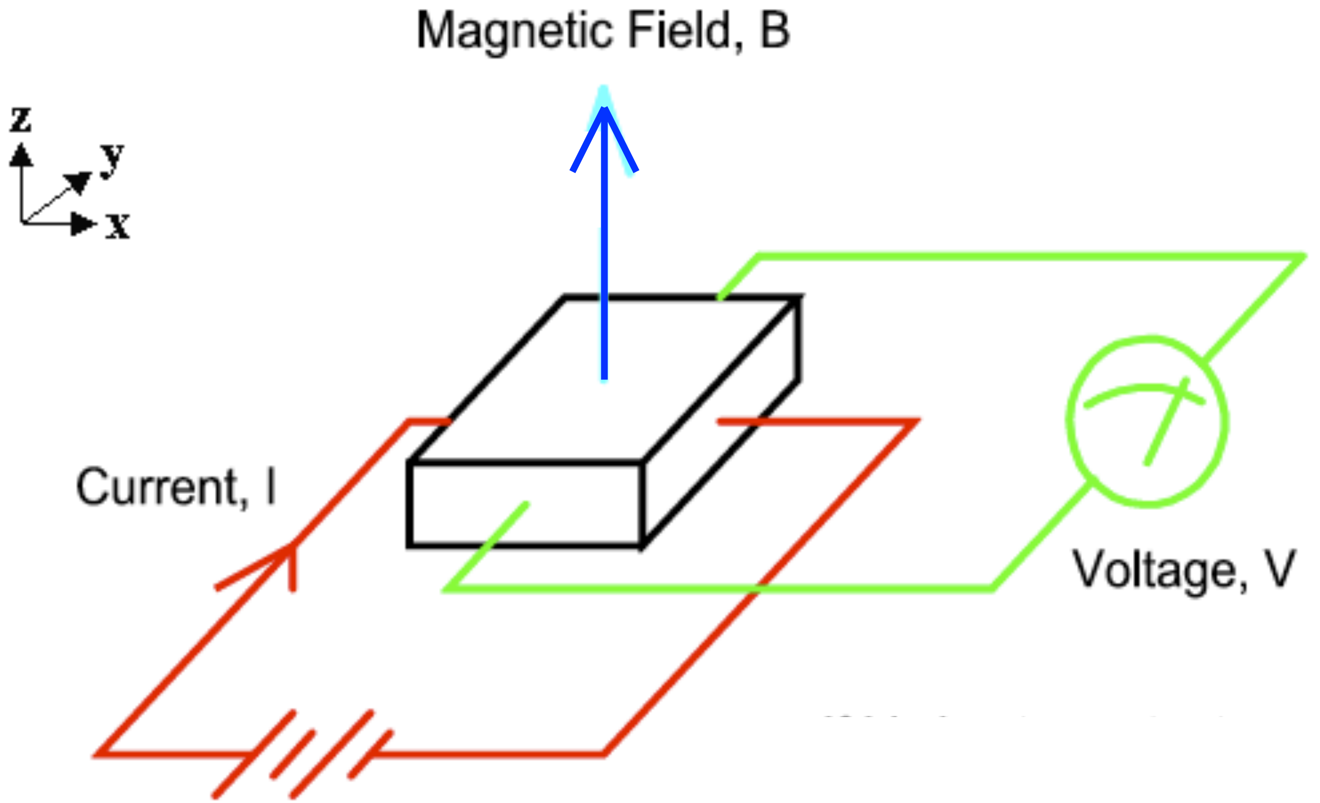
$$\boxed{\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle}$$

$$\phi = \int_{FS} \Omega_z(\mathbf{k})\, d^2k$$

Anomalous Hall conductivity:

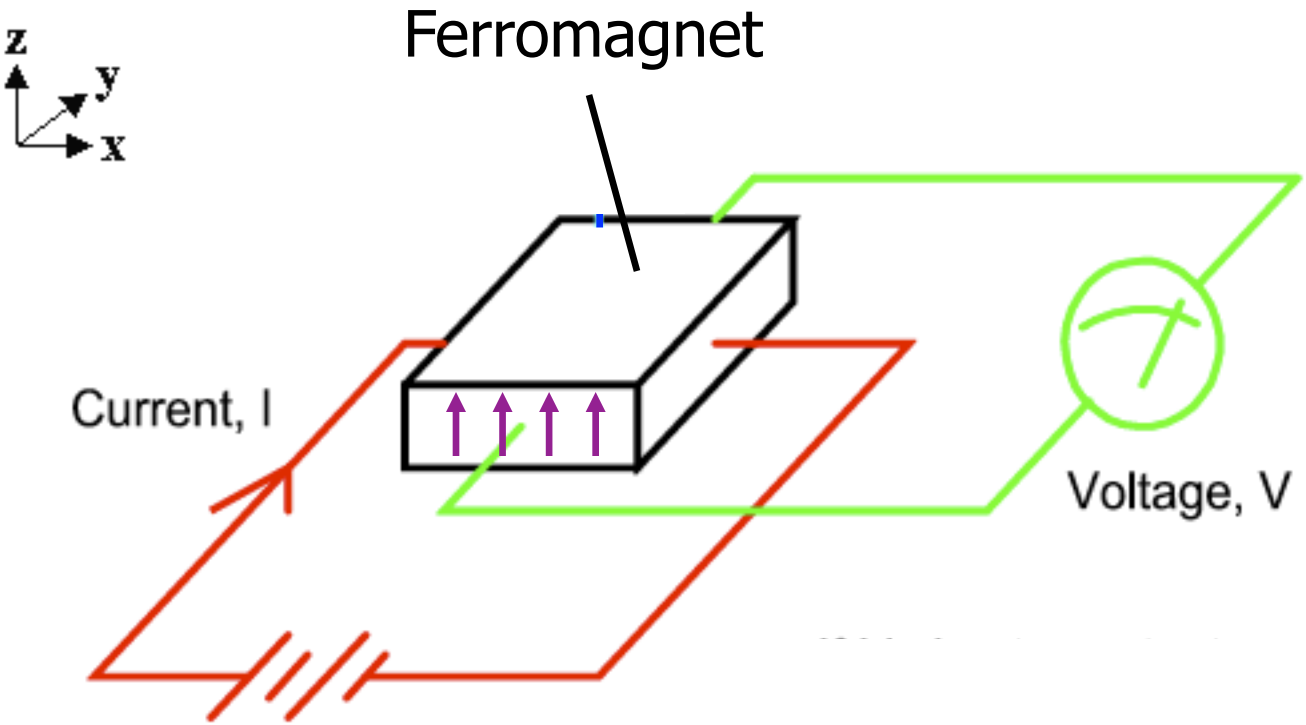
$$\boxed{\sigma_{xy} = \frac{-e^2}{2\pi h}\phi}$$

Ordinary Hall conductivity



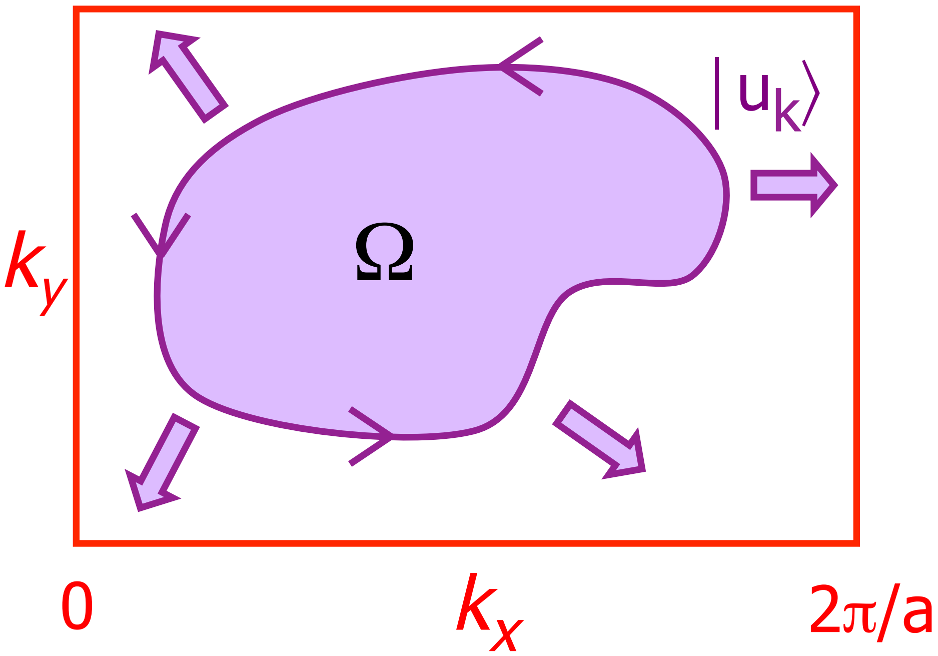
Measure σ_{xy} in presence of *B*-field

Anomalous Hall conductivity (AHC)



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

Berry curvature in the Brillouin zone



$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\phi = \int_{FS} \Omega_z(\mathbf{k})\, d^2k$$

Anomalous Hall conductivity:

$$\sigma_{xy} = \frac{-e^2}{2\pi h}\phi$$

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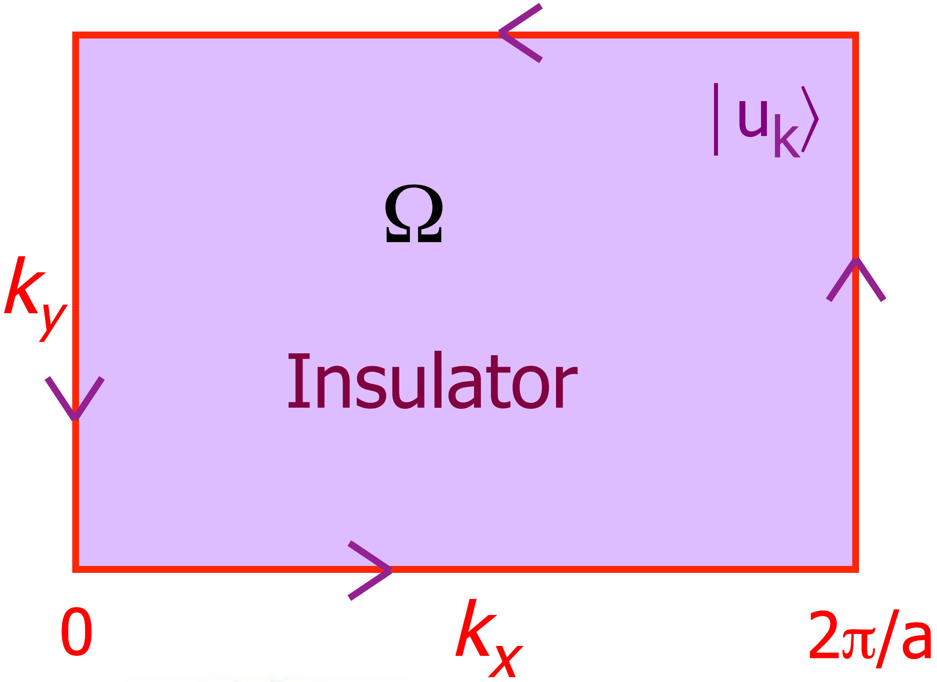
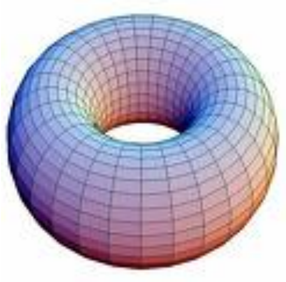
Berry curvature in the Brillouin zone



$$\boxed{\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle}$$

$$\phi = \int_{BZ} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$



Quantum Anomalous Hall: $\boxed{\sigma_{xy} = \frac{-e^2}{h} C}$

"Chern number" or "TKNN invariant"

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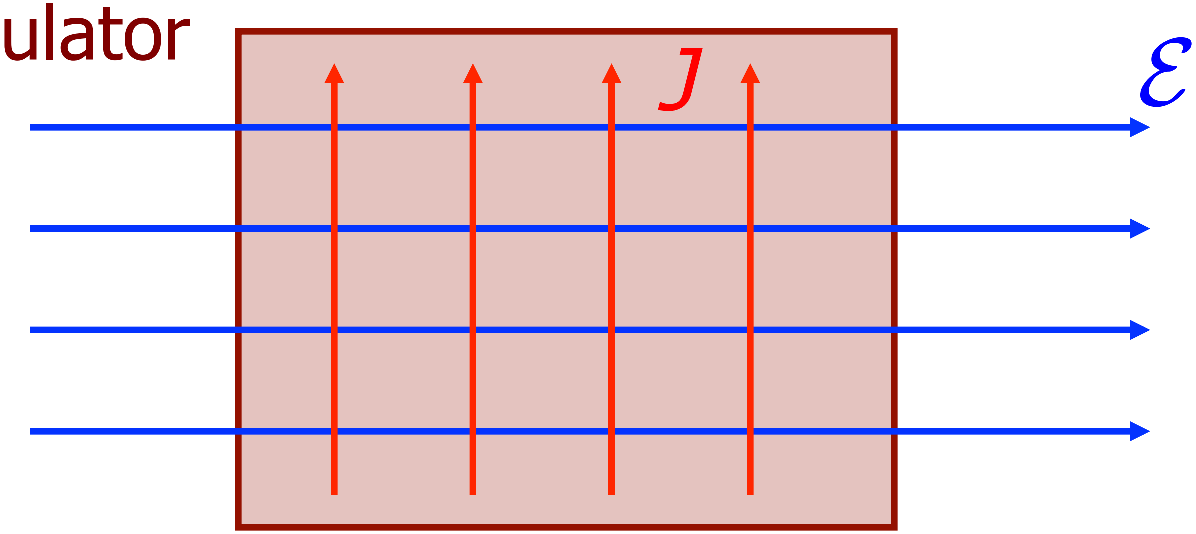
Quantum anomalous Hall effect

Ferromagnetic insulator



$\sigma_{xy} = e^2/h$

Like integer quantum Hall, but no B_{ext}

Outline

- Berry curvature and topology
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  - 2D ("Quantum spin Hall") insulator
  - 3D topological insulators
- QAH strategies
  - Heavy-atom adlayers on magnetic substrates
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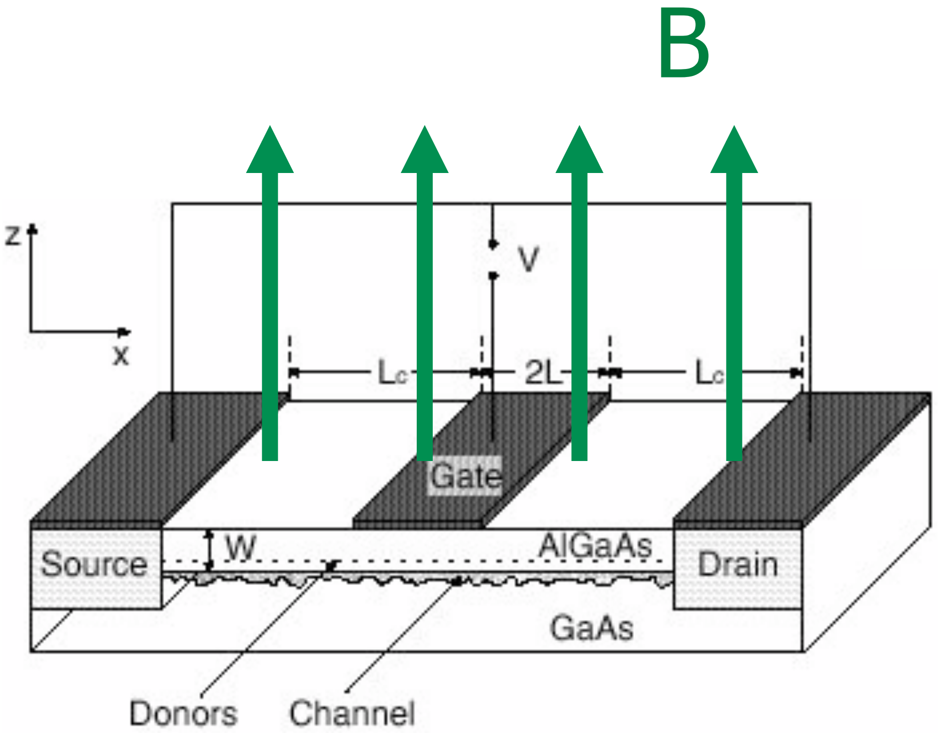
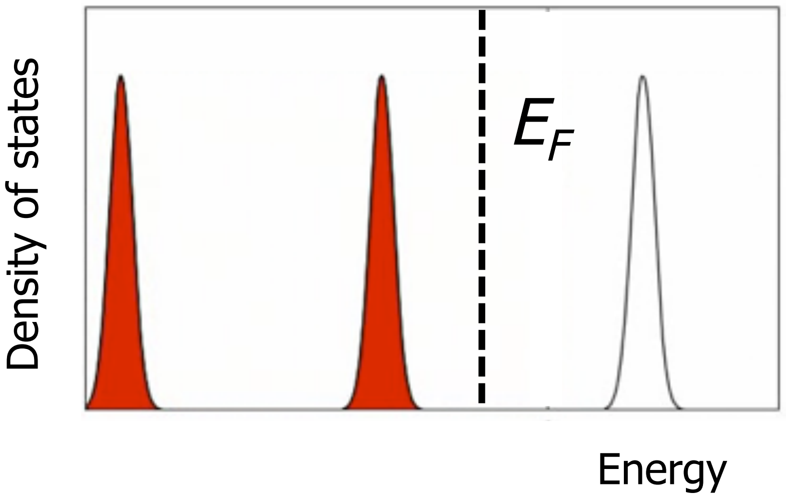
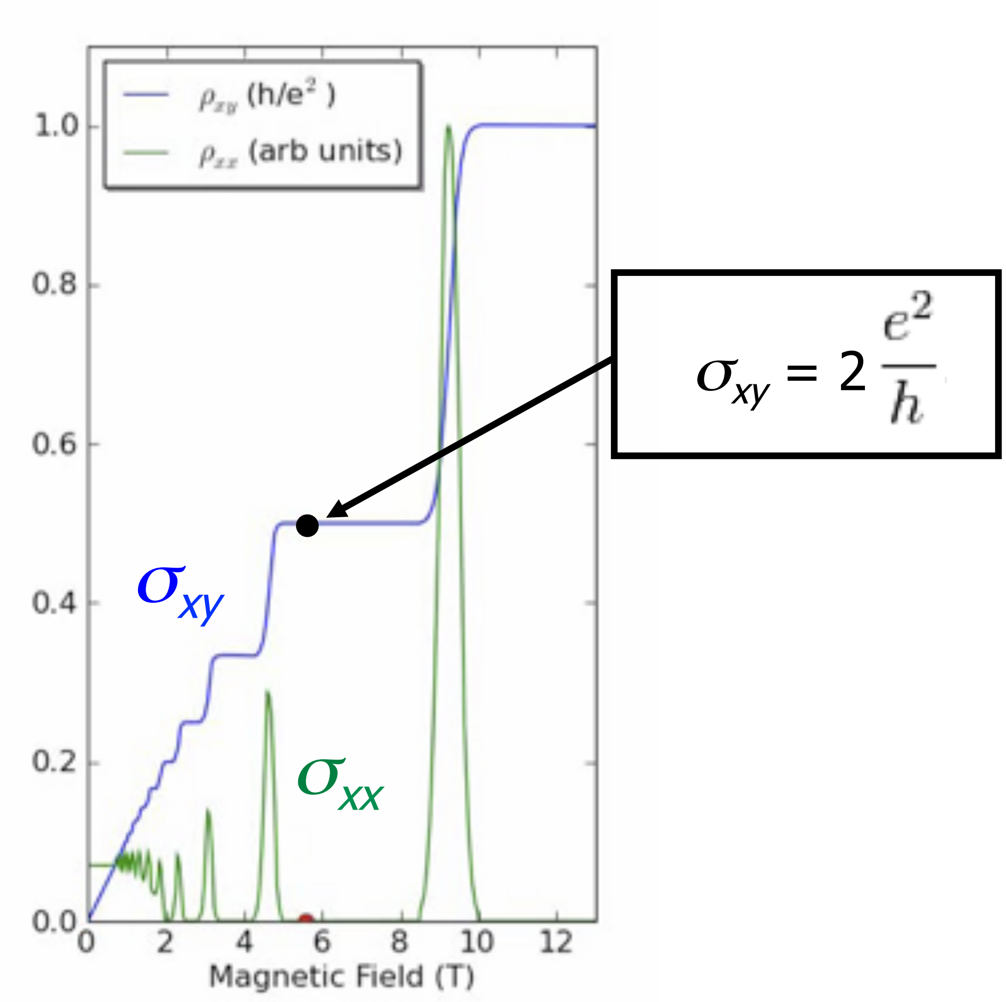
Quantum Hall effect



Quantum Hall effect



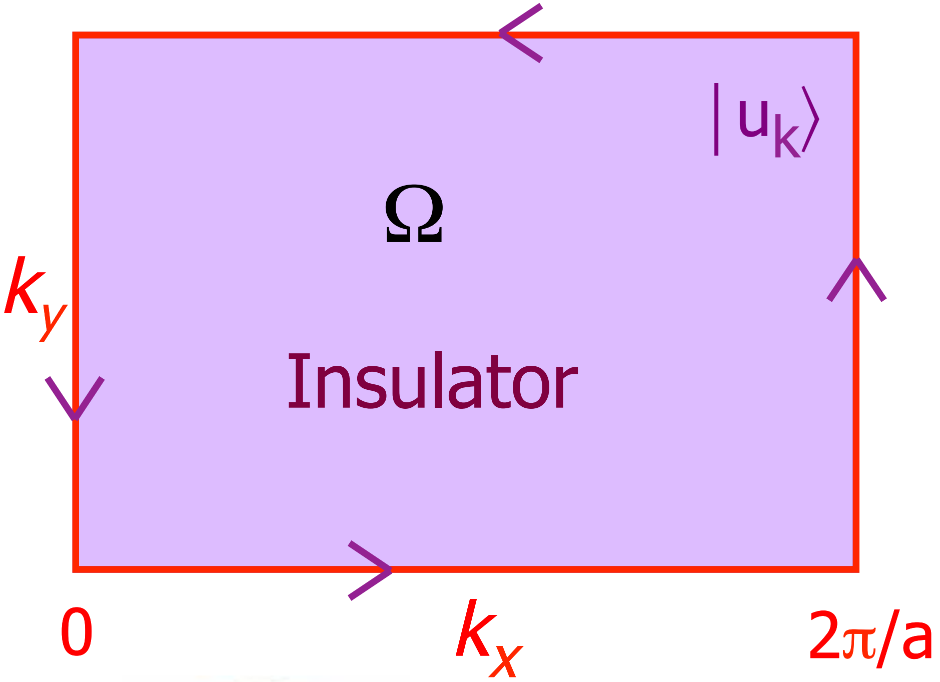


$$\sigma_{xy} = 2\,\frac{e^2}{h}$$

Hall effects: The big picture

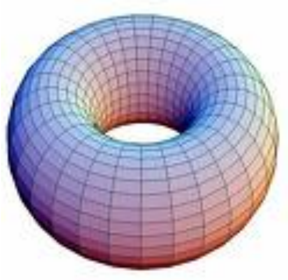
	Induced by B-field	Ferromagnetic sample
Metal	Ordinary Hall (1879)	Anomalous Hall (1881)
Topological insulator	Quantum Hall (1980)	Quantum Anomalous Hall ?

QAH insulator



$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x}\middle|\frac{du}{dk_y}\right\rangle$$

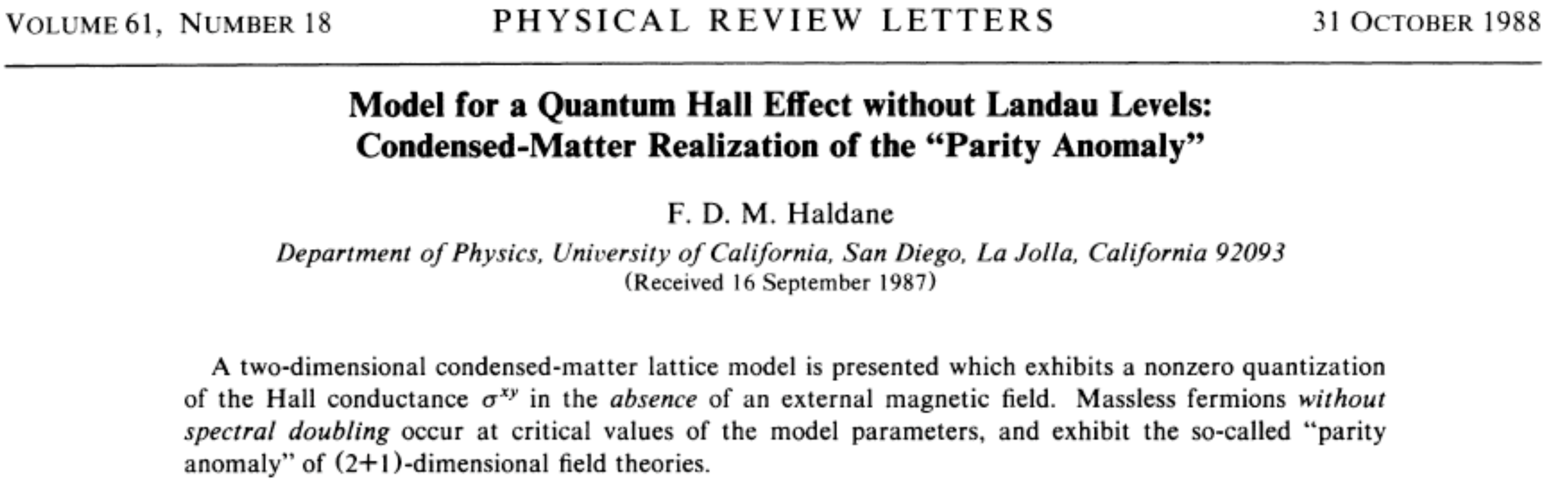
$$\int_{\mathrm{BZ}} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$



Quantum Anomalous Hall: $$\sigma_{xy} = \frac{-e^2}{h} C$$

Chern number

Proof of principle: QAH insulators



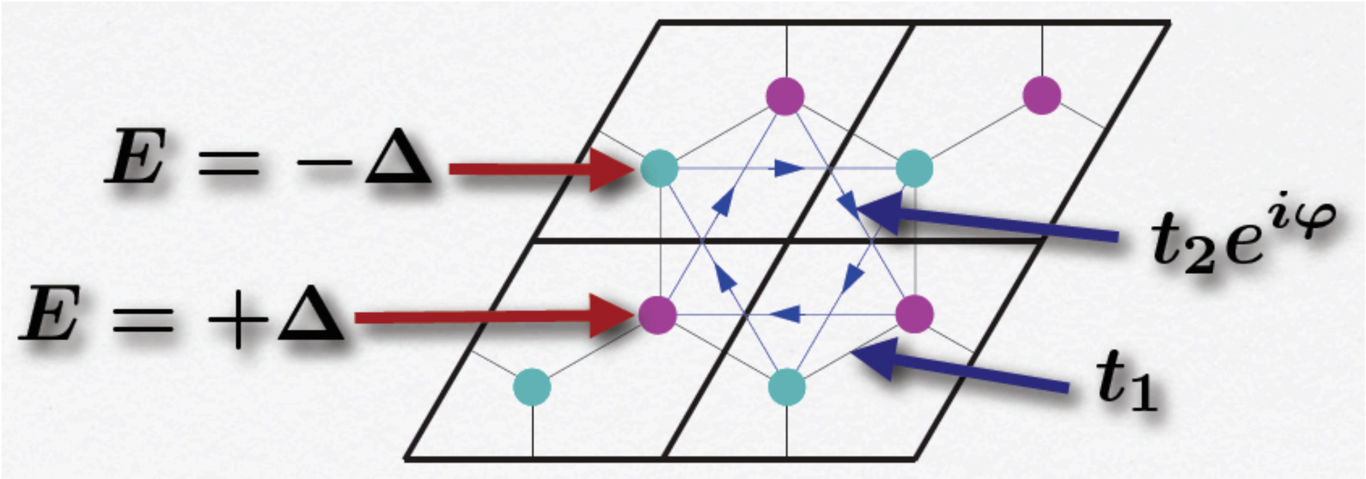
VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

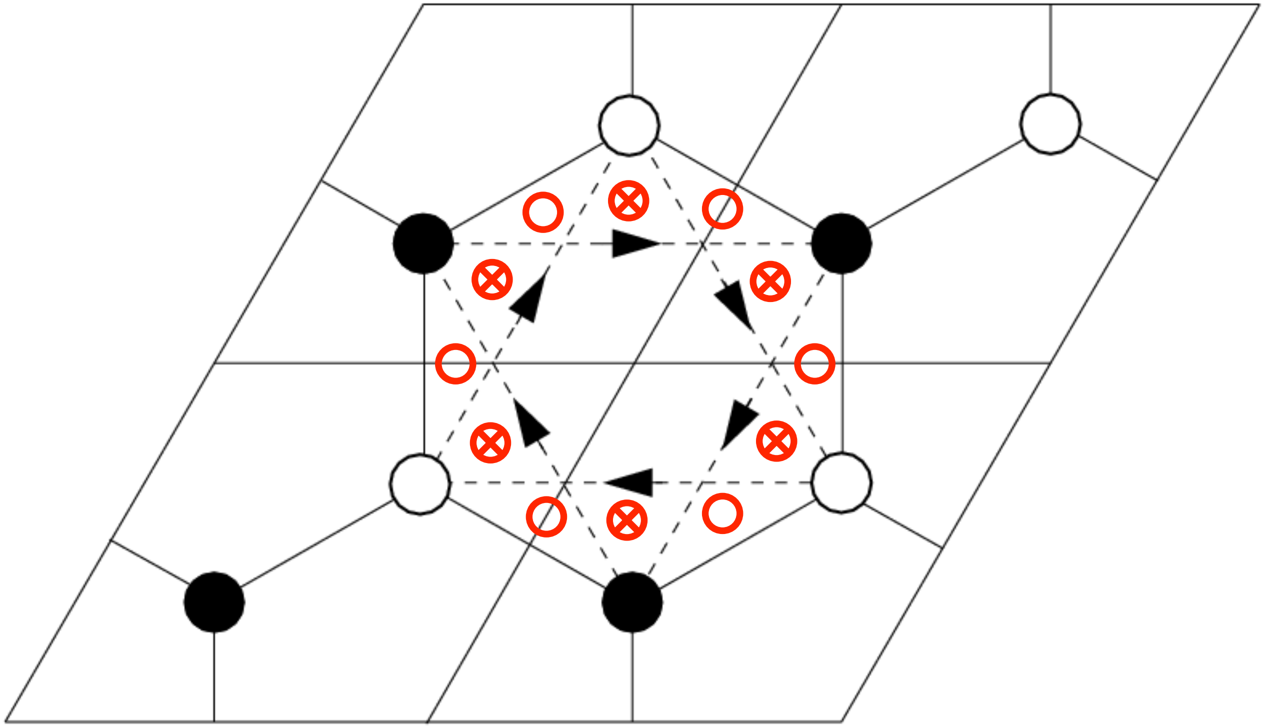
F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.



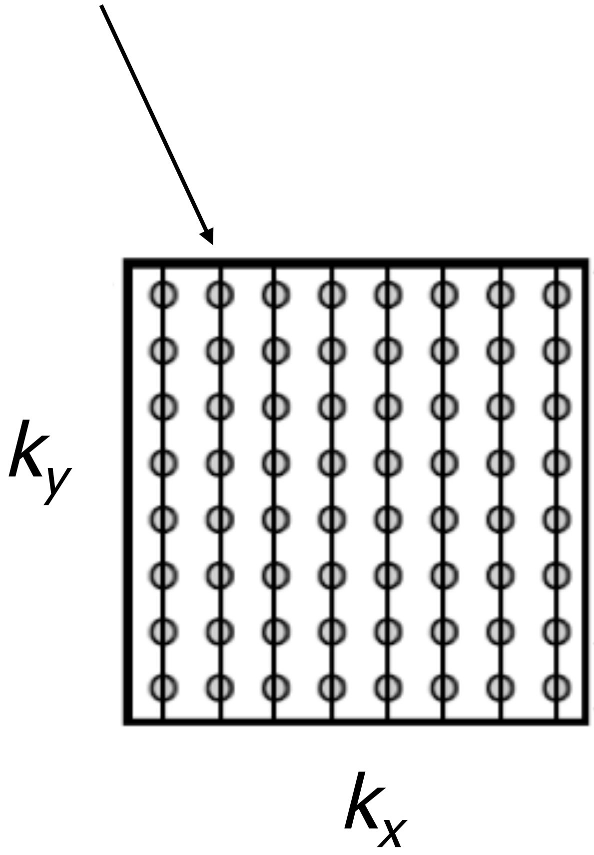
Flux tubes in Haldane model

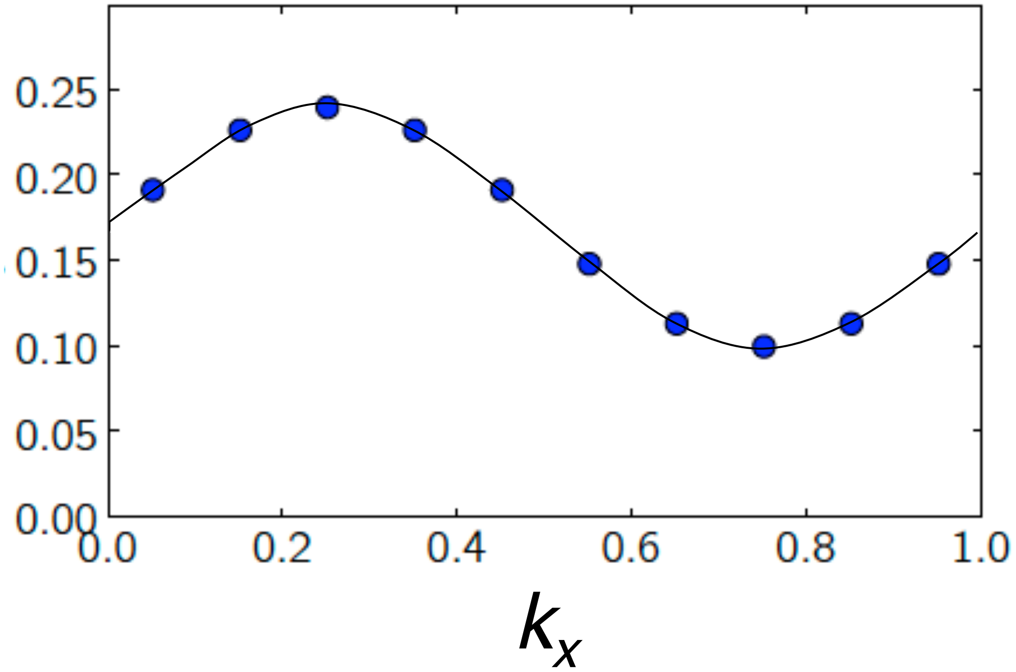


(Real materials: spin-orbit interaction gives similar effects)

String Berry phases for normal band

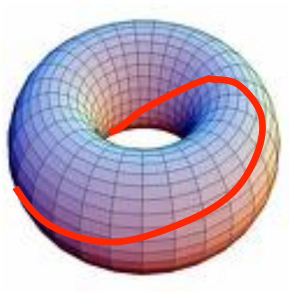
$$\phi\left(k_x\right) = -\mathrm{Im}\,\ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\,\right]$$

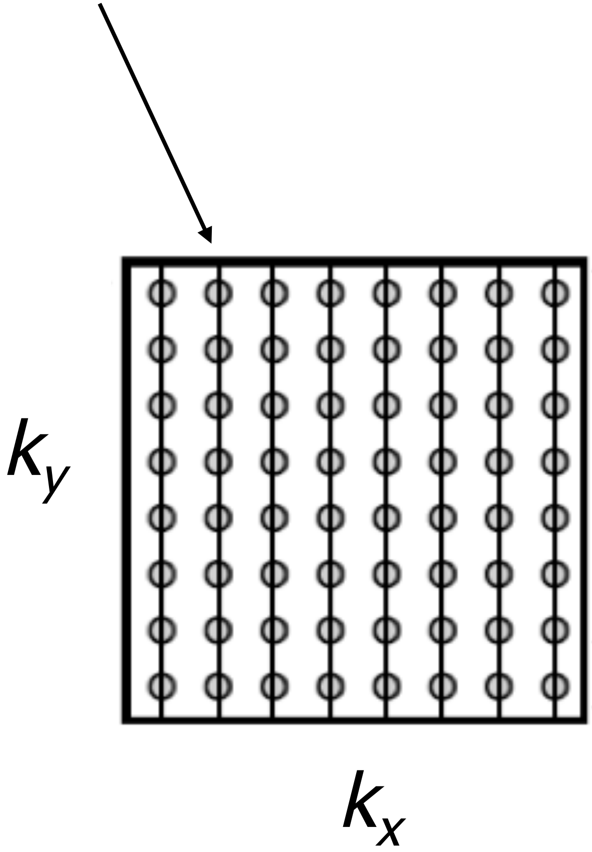


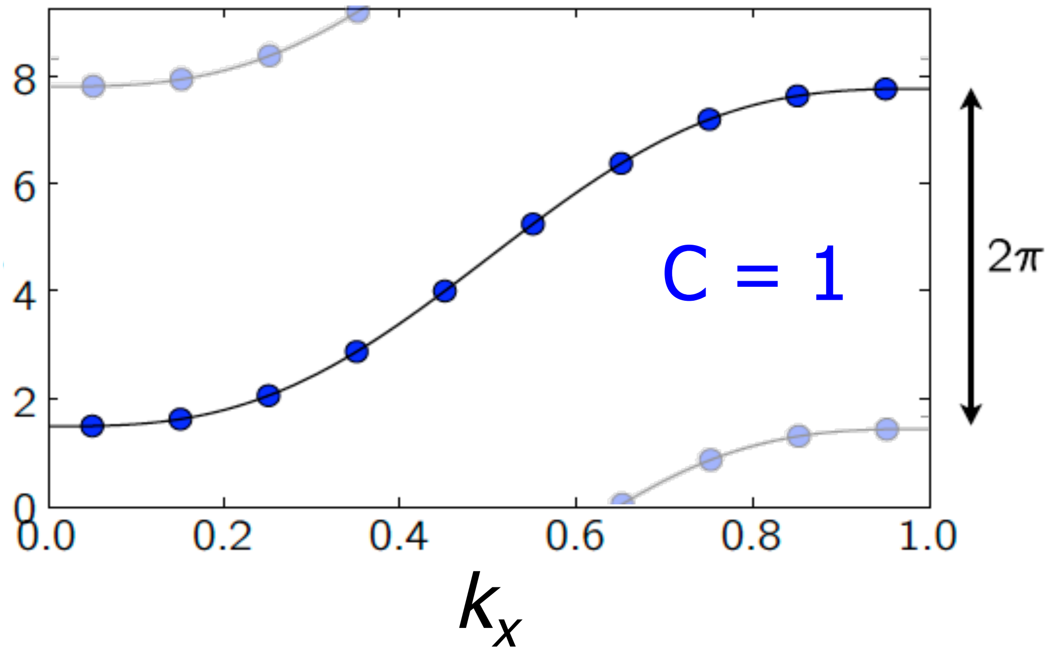


String Berry phases in QAH band

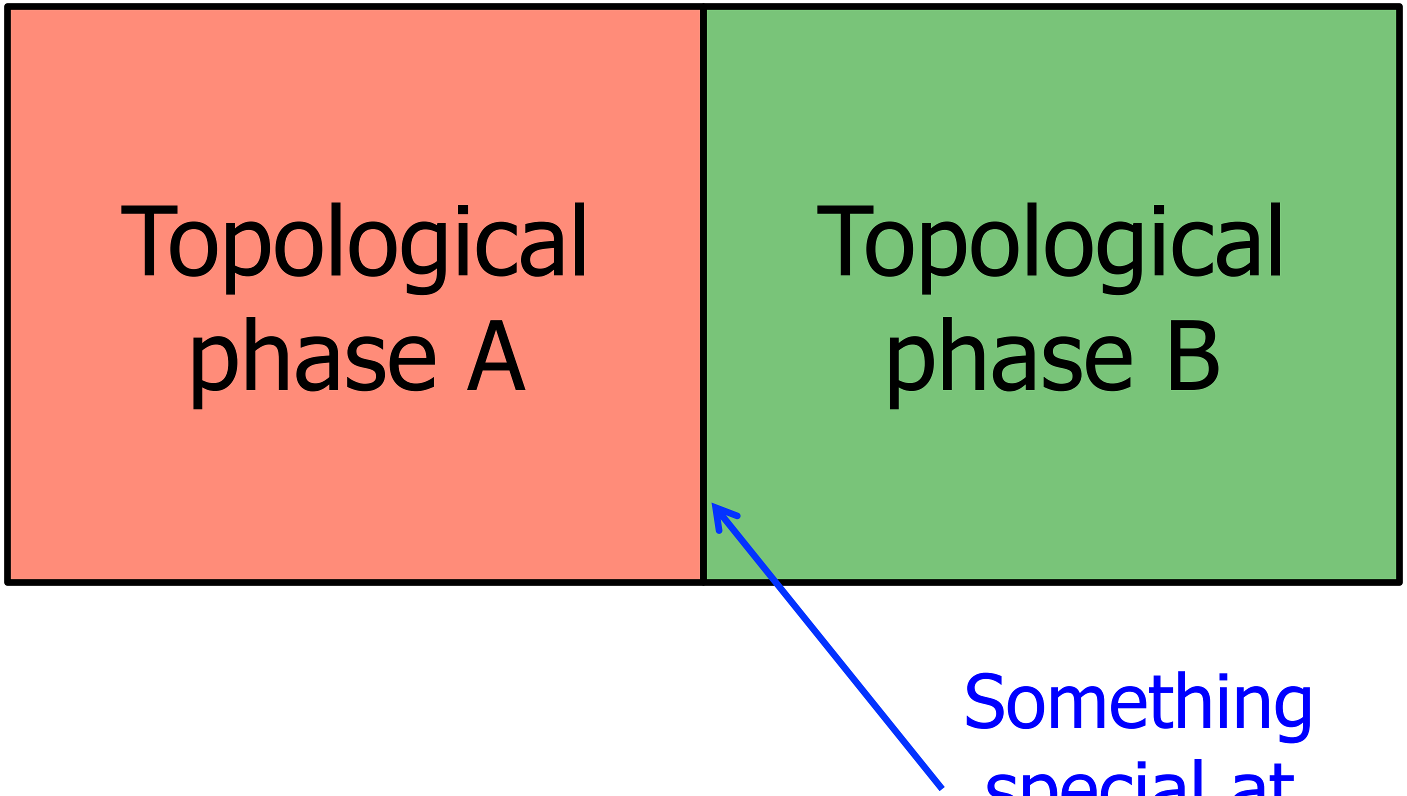
$$\phi\left(k_x\right) = -\mathrm{Im}\,\ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\,\right]$$







Bulk-boundary correspondence

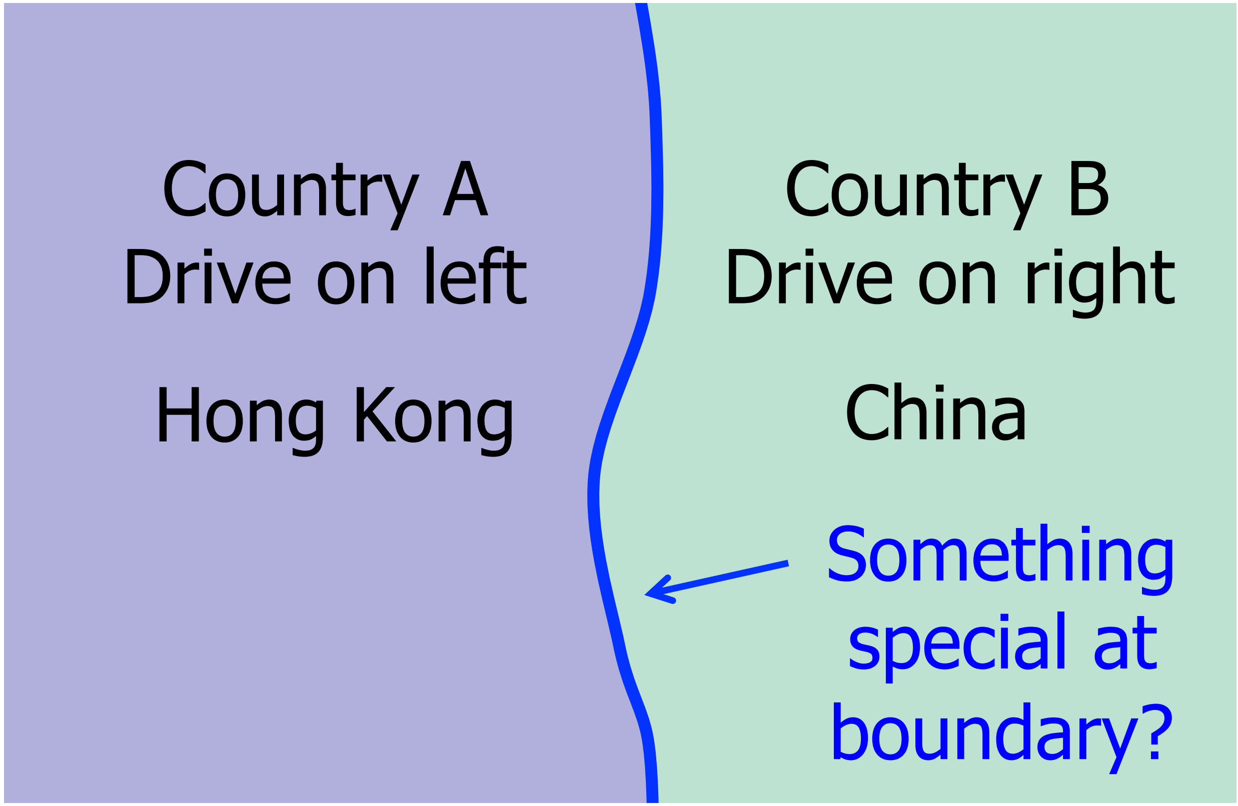


Topological phase A

Topological phase B

Something special at boundary

Bulk-boundary correspondence



Country A
Drive on left

Hong Kong

Country B
Drive on right

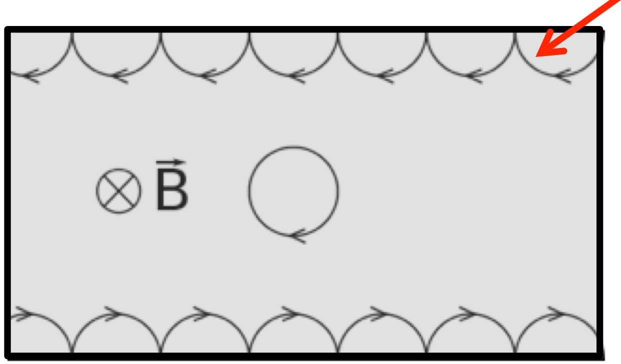
China

Something special at boundary?

Bulk-boundary correspondence

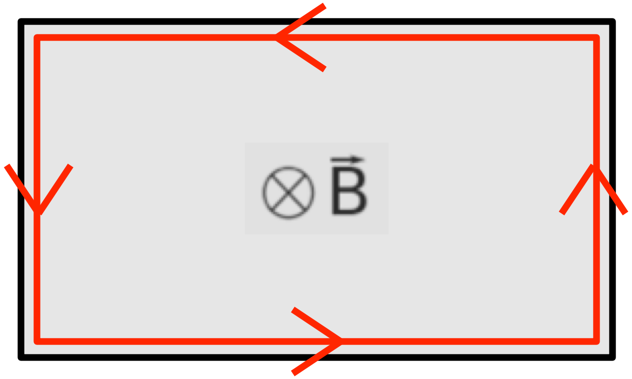
Quantum Hall effect

- Semiclassical picture:



Skipping orbits
(edge states)

- Quantum picture:



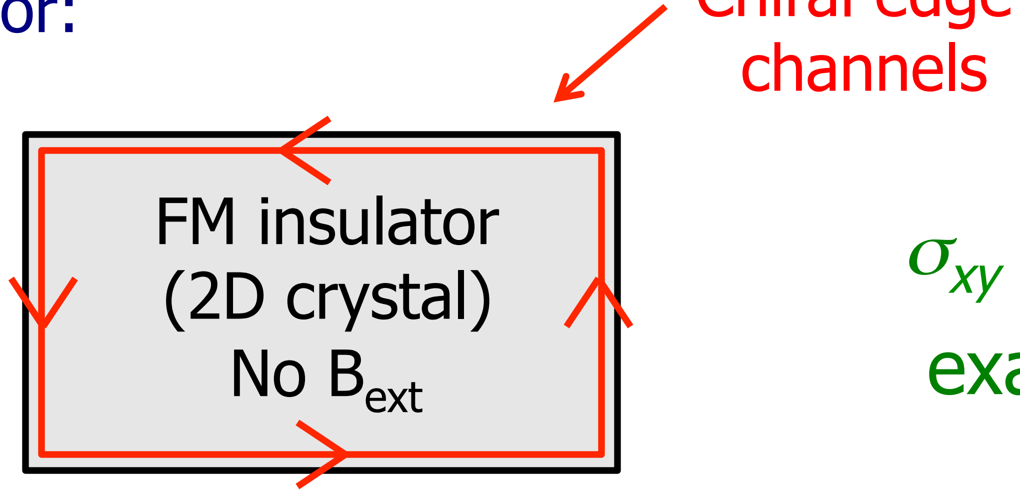
Chiral edge
channels

σ_{xy} = e^2/h

exactly !

Quantum anomalous Hall effect

- QAH insulator:

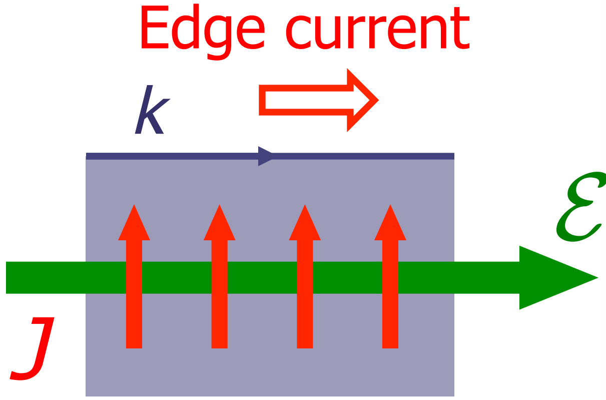


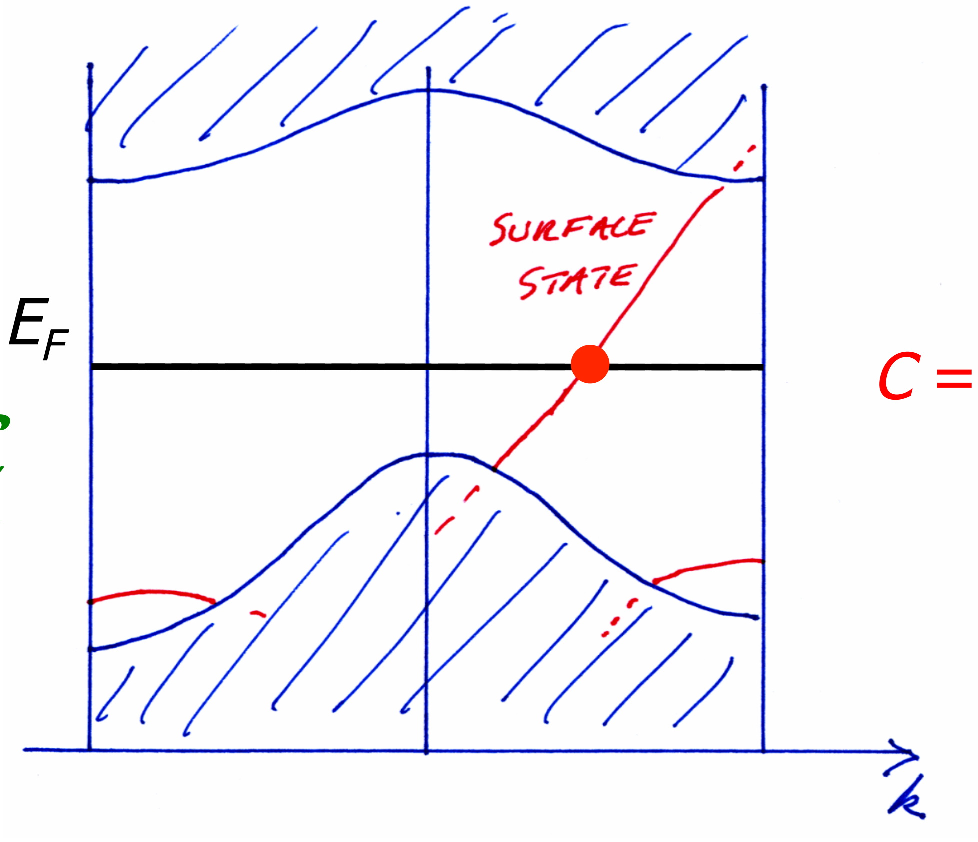
FM insulator
(2D crystal)
No B_{ext}

$\sigma_{xy} = e^2/h$

exactly !

Edge states: 2D QAH insulator





$C = +1$

Conservation of charge ⇒ chiral surface state

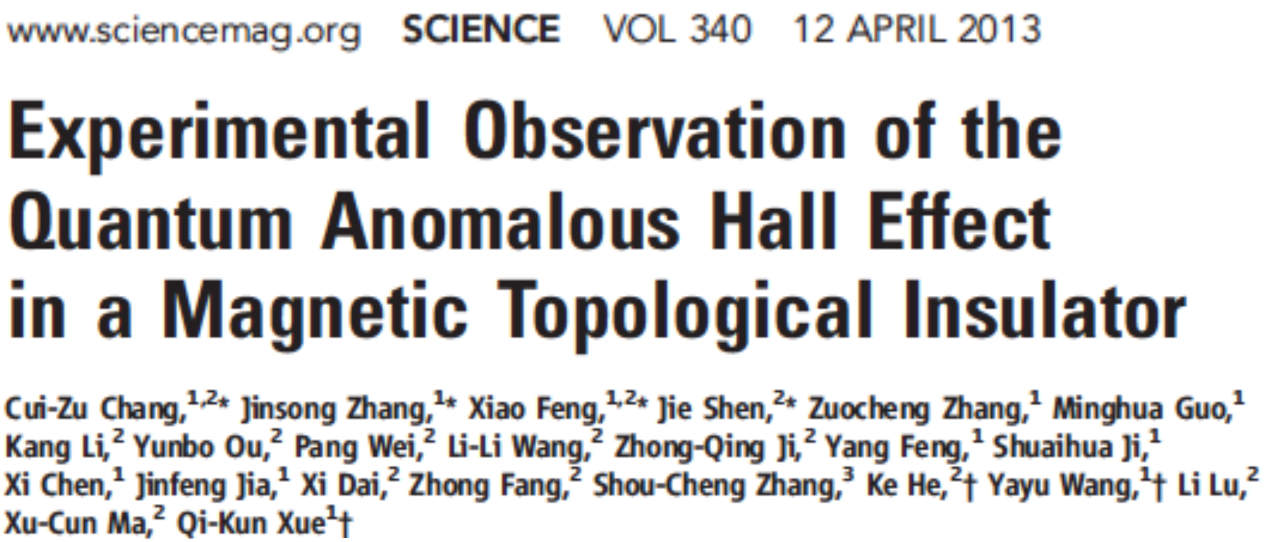
QAH insulators

- “QAH insulator” = “Chern insulator”
- Quantized Hall conductance even in the absence of macroscopic magnetic fields
- Quite possibly at room temperature
- Usefulness:
  - Precision measurement?
  - Dissipationless “wires” for microelectronics?
  - Magnetoelectric coupling?

Can QAH insulators be found?

- Requirements
  - Spontaneously broken TR (FM or FiM)
  - Insulator
  - Strong spin-orbit coupling (heavy atoms)
- Prefer gap > 0.2 eV (Q Hall at T_{room})
- Proposals
  - Magnetically doped TR-invariant TI's
  - Magnetic adatoms on graphene
  - 2D adlayer on a magnetic insulator

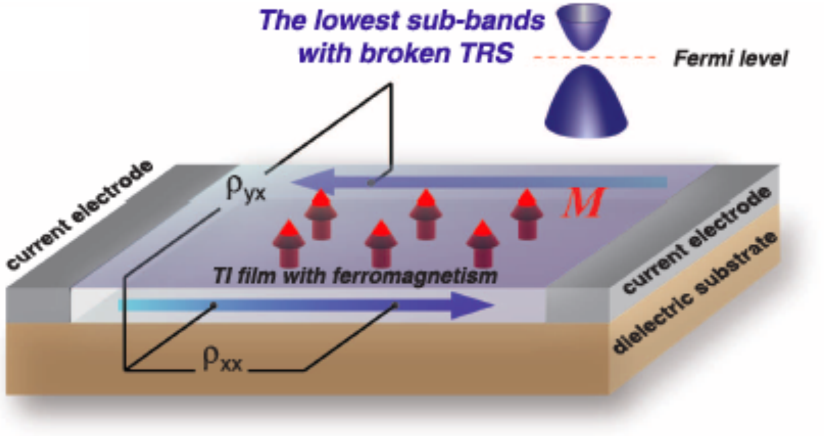
Magnetic doping: Claim for QAH



www.sciencemag.org SCIENCE VOL 340 12 APRIL 2013

Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator

Cui-Zu Chang,[1,2]* Jinsong Zhang,[1]* Xiao Feng,[1,2]* Jie Shen,[2]* Zuocheng Zhang,[1] Minghua Guo,[1] Kang Li,[2] Yunbo Ou,[2] Pang Wei,[2] Li-Li Wang,[2] Zhong-Qing Ji,[2] Yang Feng,[1] Shuaihua Ji,[1] Xi Chen,[1] Jinfeng Jia,[1] Xi Dai,[2] Zhong Fang,[2] Shou-Cheng Zhang,[3] Ke He,[2]† Yayu Wang,[1]† Li Lu,[2] Xu-Cun Ma,[2] Qi-Kun Xue[1]†



Observed below ~1K

Hall effects: The big picture

	Induced by B-field	Ferromagnetic sample
Metal	Ordinary Hall (1879)	Anomalous Hall (1881)
Topological insulator	Quantum Hall (1980)	Quantum Anomalous Hall (2013)

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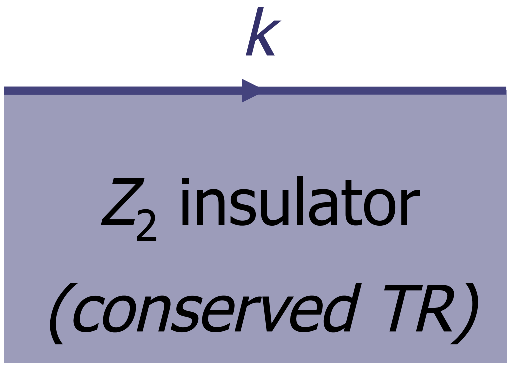
2D Z_2 topological insulator (QSH)

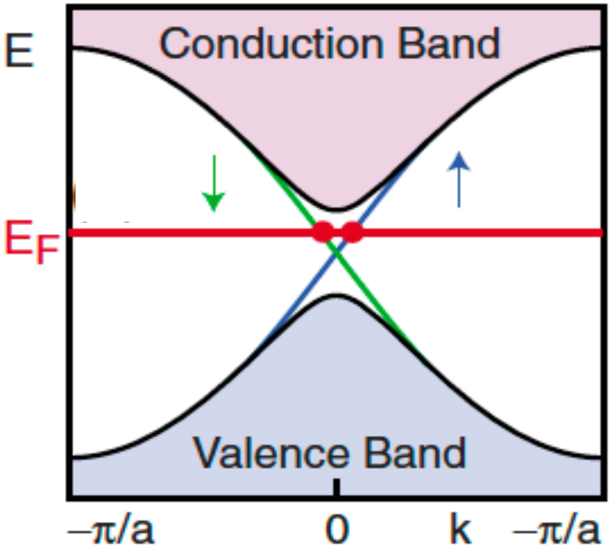
QSH = Quantum spin Hall



k

Z_2 insulator

(conserved TR)



Reviews of Modern Physics

***Colloquium*: Topological insulators**

M. Z. Hasan*

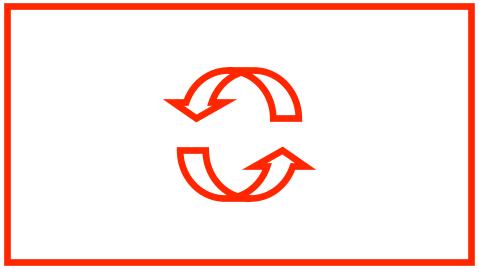
Joseph Henry Laboratories, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

C. L. Kane†

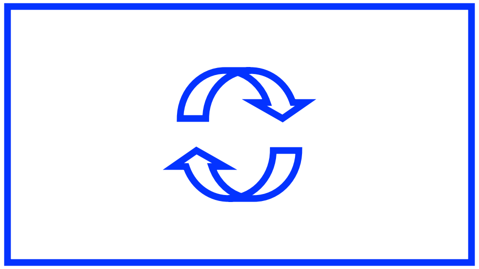
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Published 8 November 2010)

Z_2 Topological Insulator ("Quantum spin Hall")

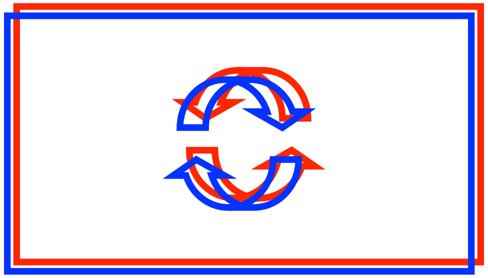


Spin up, $C = +1$



Spin down, $C = -1$

Z_2 Topological Insulator ("Quantum spin Hall")



Spin up, $C = +1$

Spin down, $C = -1$

Then turn on spin-orbit coupling (SOC):

- Obeys T symmetry
- Total $C = 0$
- Z_2 invariant is odd

Meaning of Z and Z_2

- Z = group of integers under addition

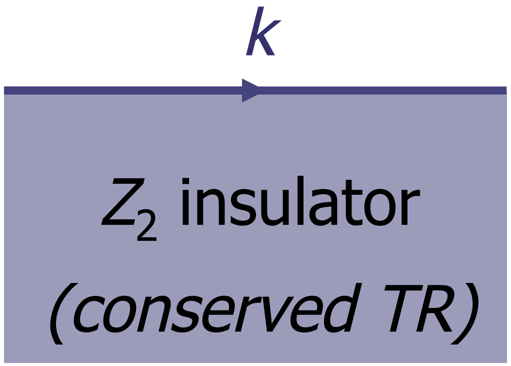
- $Z_2 = \{0,1\}$ under addition (mod 2)

Or equivalently,

- $Z_2 = \{+, -\}$ under multiplication

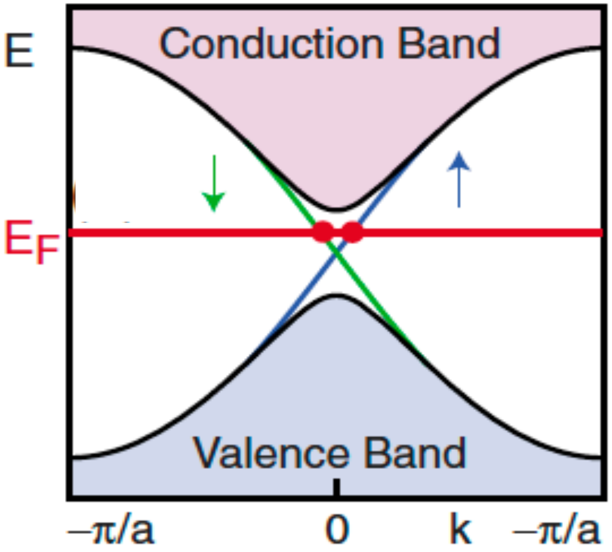
2D Z_2 topological insulator (QSH)

QSH = Quantum spin Hall



Z_2 insulator

(conserved TR)



Reviews of Modern Physics

***Colloquium*: Topological insulators**

M. Z. Hasan*

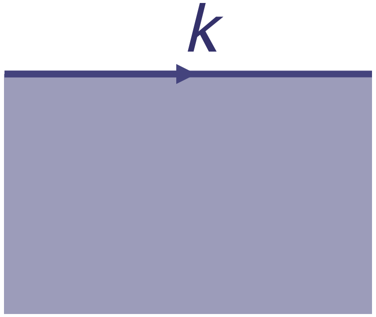
Joseph Henry Laboratories, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

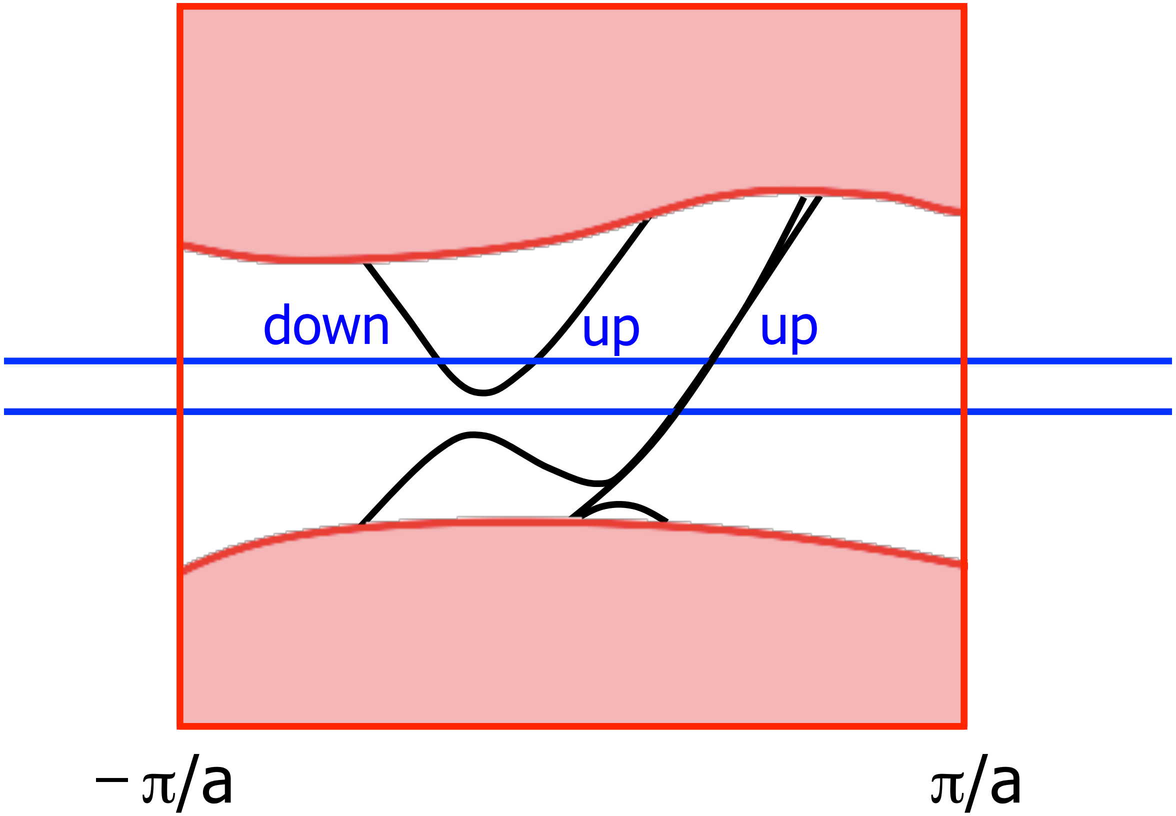
C. L. Kane†

Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Published 8 November 2010)

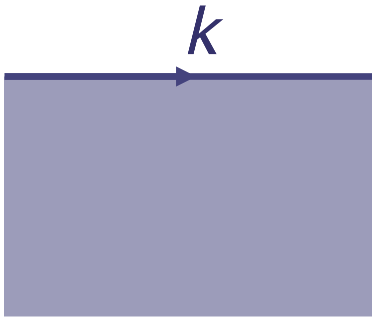
Edge states: 2D QAH insulator

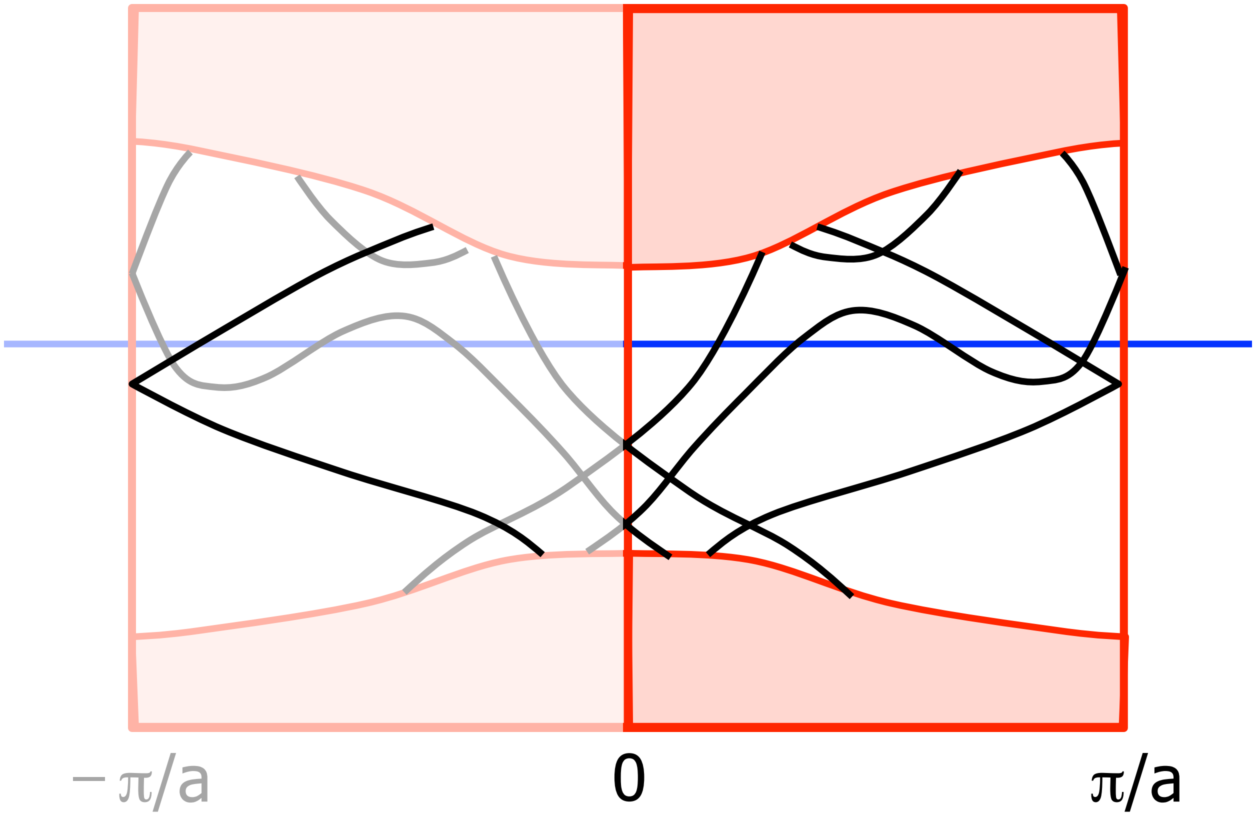




$$Z = N_{\text{up}} - N_{\text{down}} = \text{Invariant}$$

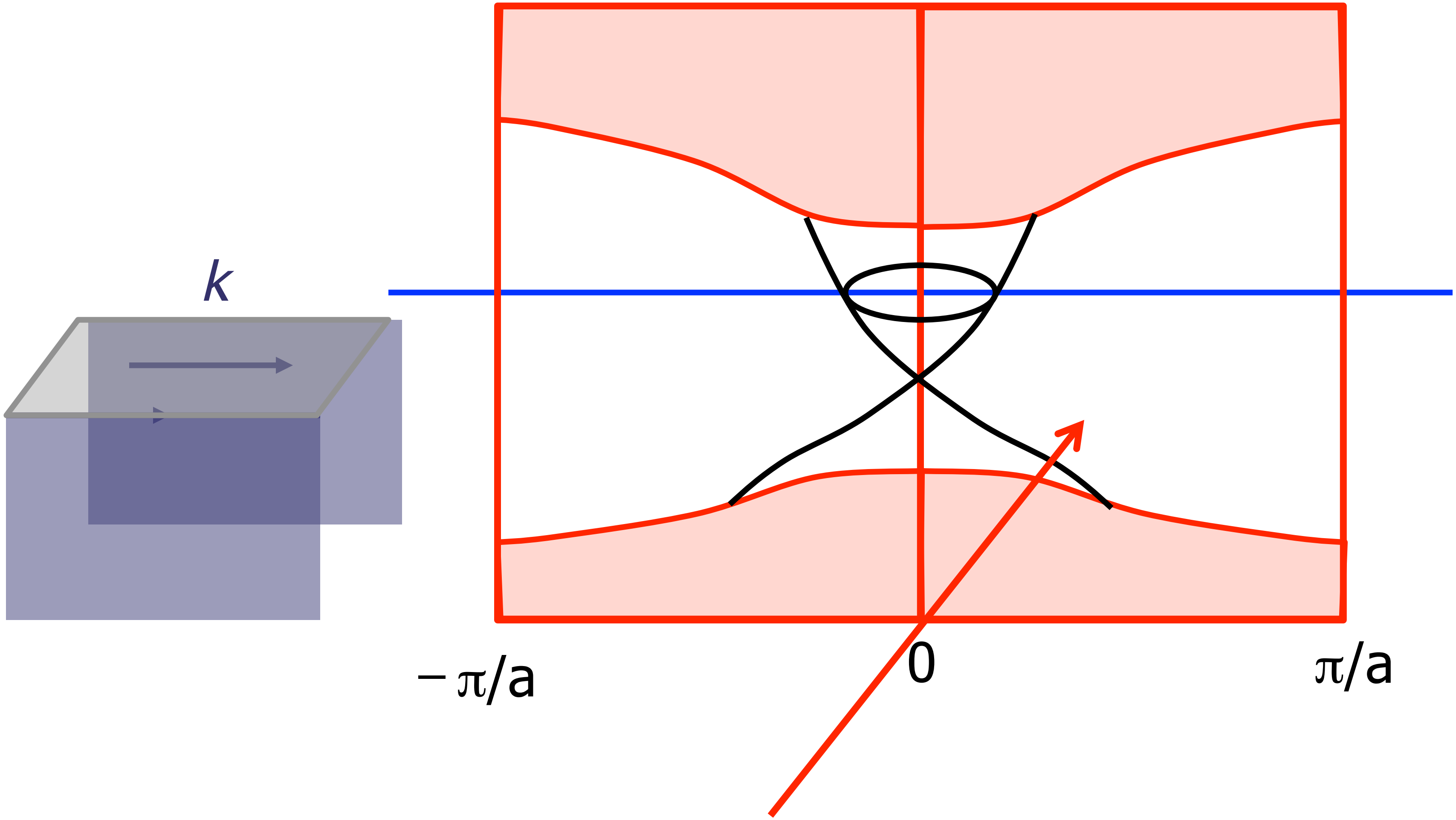
Edge states: 2D TR-invariant insulator



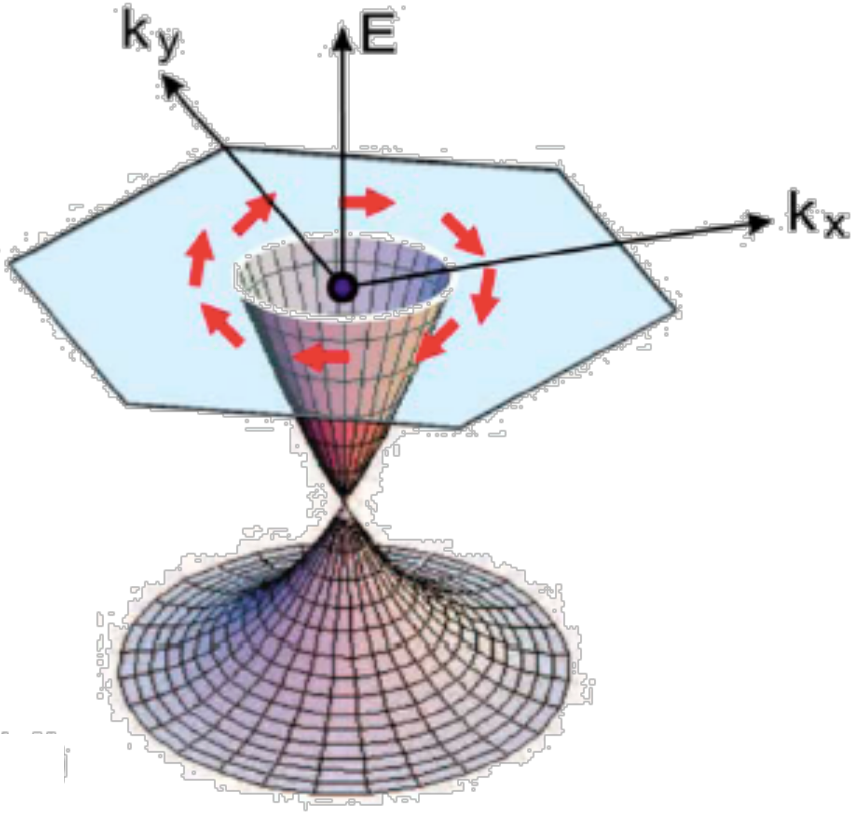


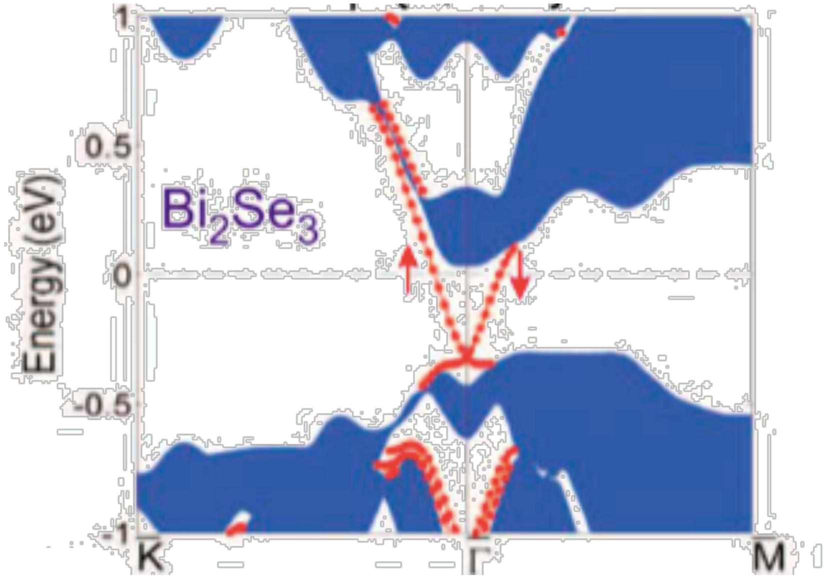
$Z_2 = N_{\text{cross}}$ (mod 2) = Invariant

3D TR-invariant topological insulator



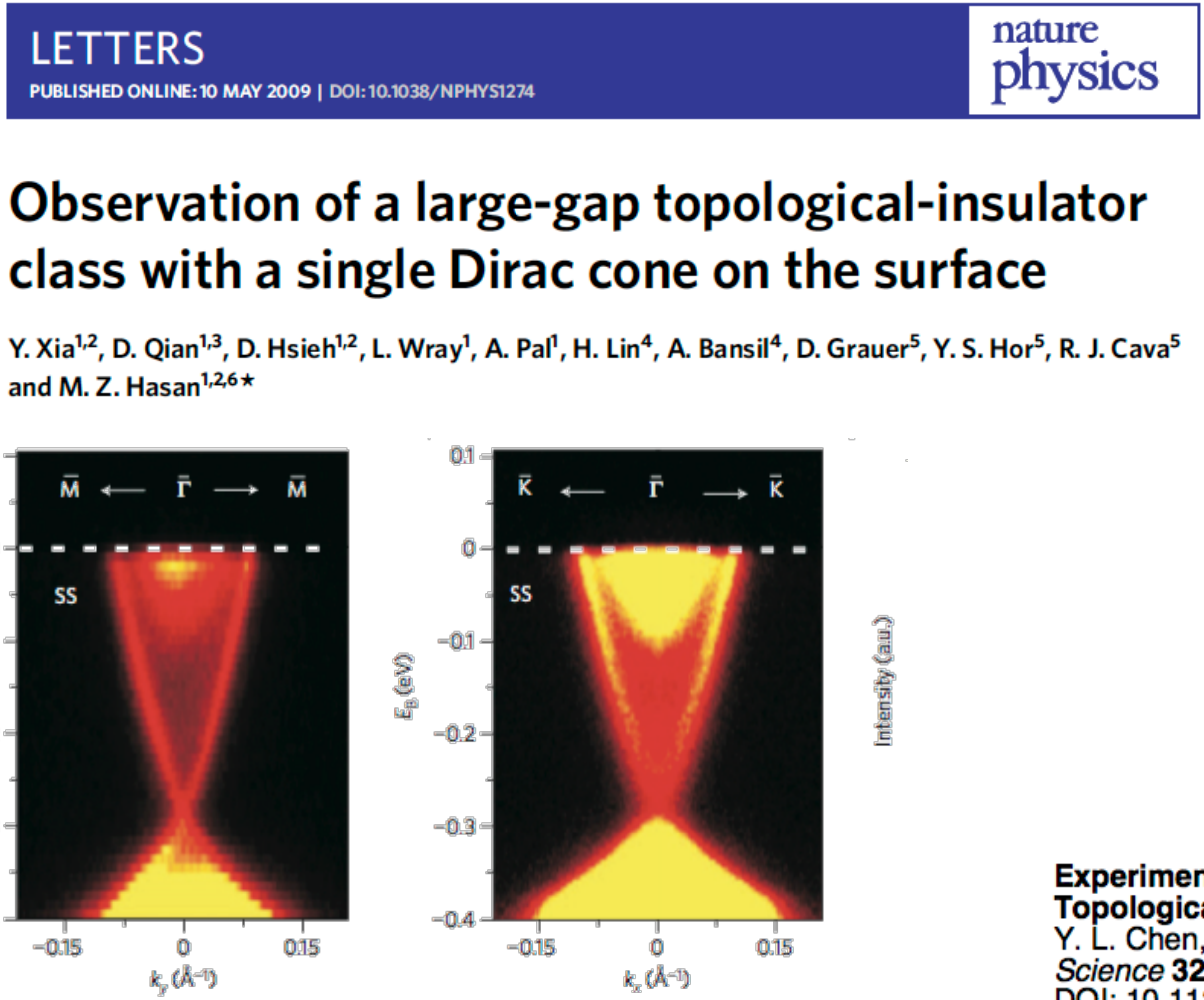
3D TR-invariant topological insulator





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)

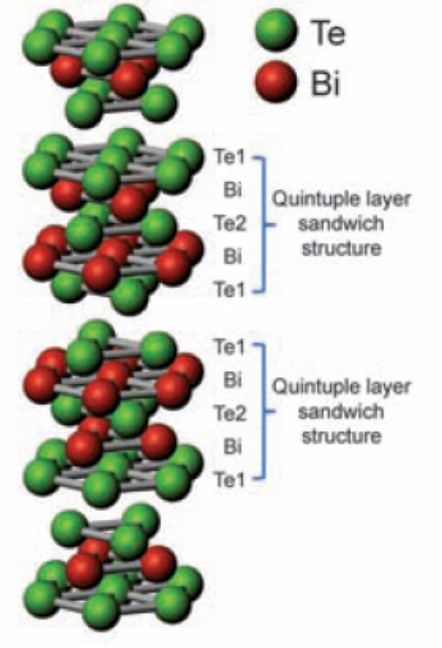
Bi_2Se_3 and Bi_2Te_3



LETTERS
PUBLISHED ONLINE: 10 MAY 2009 | DOI: 10.1038/NPHYS1274
nature physics

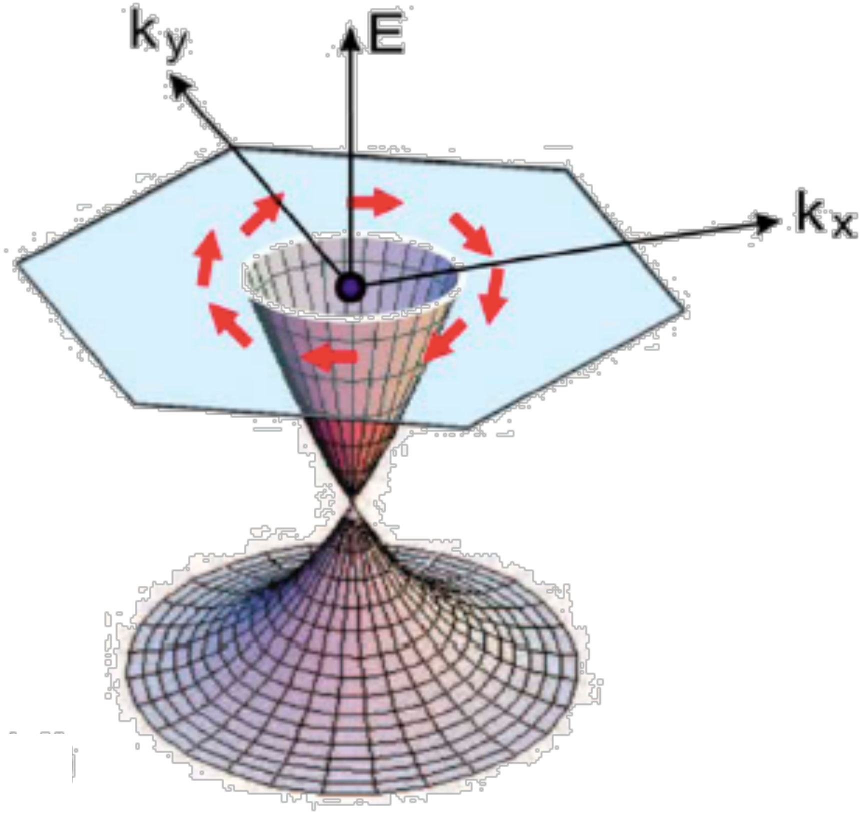
Observation of a large-gap topological-insulator class with a single Dirac cone on the surface

Y. Xia[1,2], D. Qian[1,3], D. Hsieh[1,2], L. Wray[1], A. Pal[1], H. Lin[4], A. Bansil[4], D. Grauer[5], Y. S. Hor[5], R. J. Cava[5] and M. Z. Hasan[1,2,6]★



Experimental Realization of a Three-Dimensional Topological Insulator, Bi 2Te3
Y. L. Chen, *et al.*
Science **325**, 178 (2009);
DOI: 10.1126/science.1173034

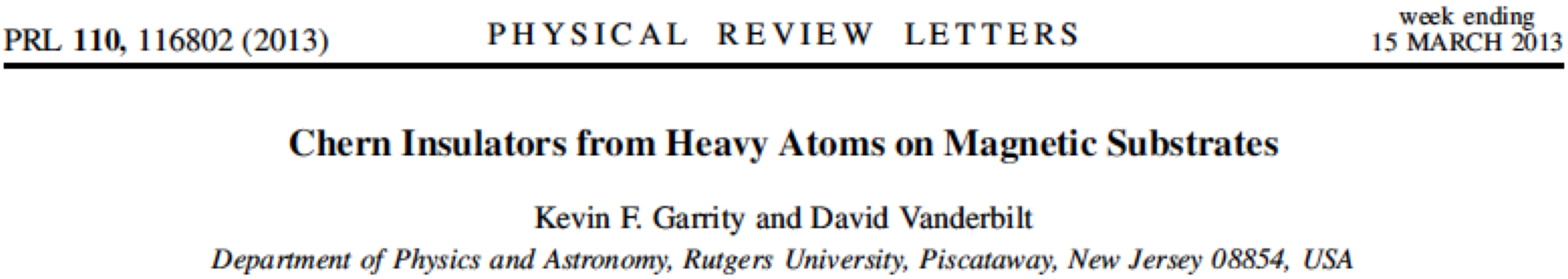
Spin chirality of surface states



Outline

- Berry curvature and topology
- 2D quantum anomalous Hall (QAH) insulator
- TR-invariant insulators (Z_2)
  - 2D ("Quantum spin Hall") insulator
  - 3D topological insulators
- **QAH strategies**
  - **Heavy-atom adlayers on magnetic substrates**
  - Other ideas
- Summary

Our strategy



PRL **110,** 116802 (2013) PHYSICAL REVIEW LETTERS week ending 15 MARCH 2013

Chern Insulators from Heavy Atoms on Magnetic Substrates

Kevin F. Garrity and David Vanderbilt

Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

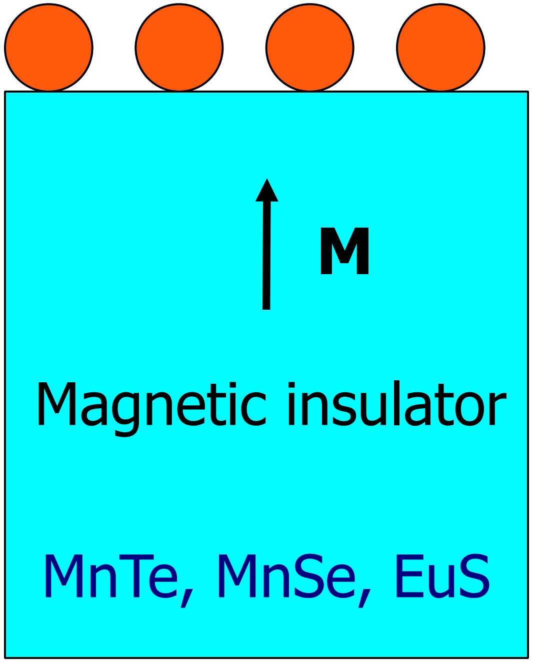
Our strategy

Heavy atoms
- -Large spin-orbit

Magnetic insulator
- -Breaks time reversal
- -FM or A-type AFM

Advantages:
- -Spins align automatically
- -No doping
- -Large gap insulators
- -Large spin-orbit

Disadvantages:
- -Preparing surfaces is difficult



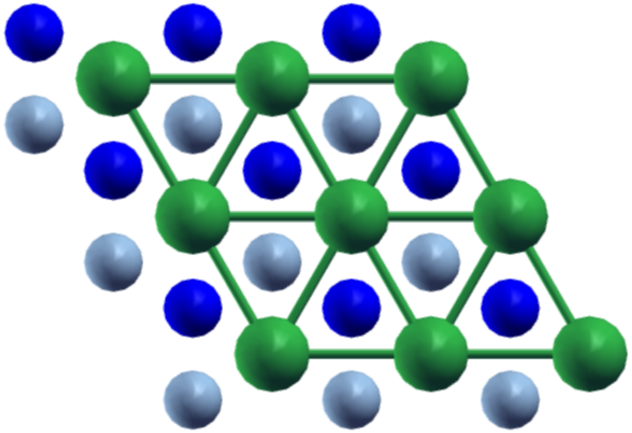
Au, Hg, Tl, Pb, Bi

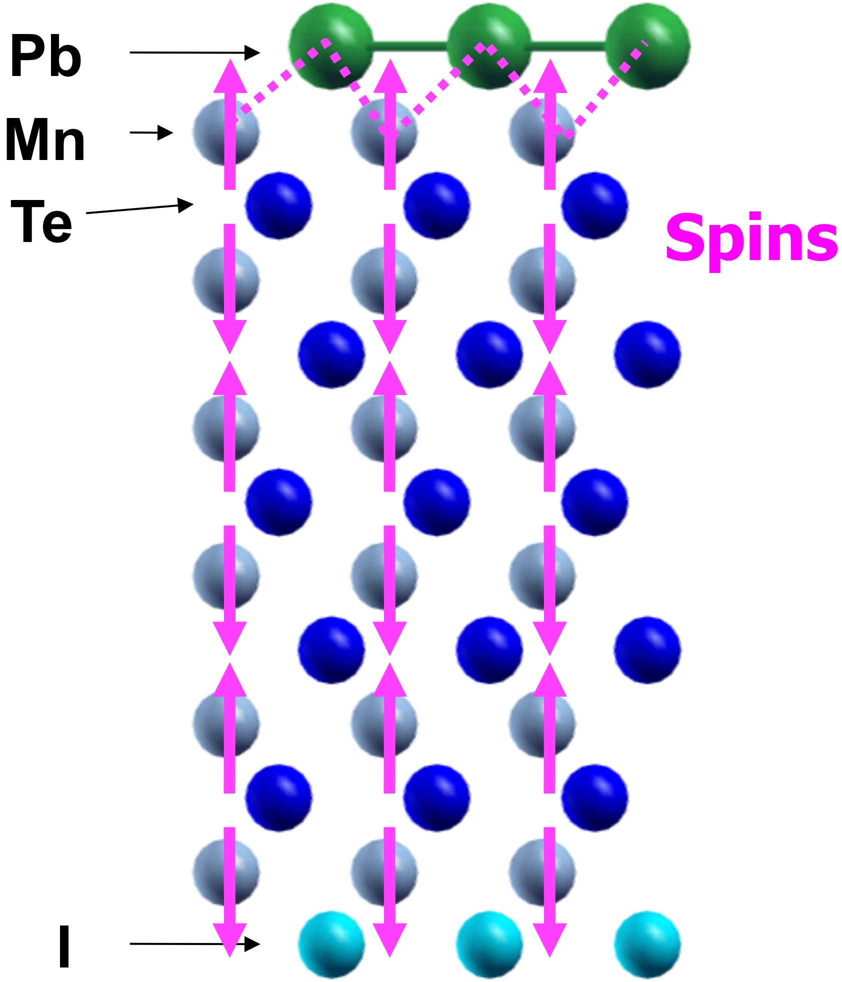
Magnetic insulator

MnTe, MnSe, EuS

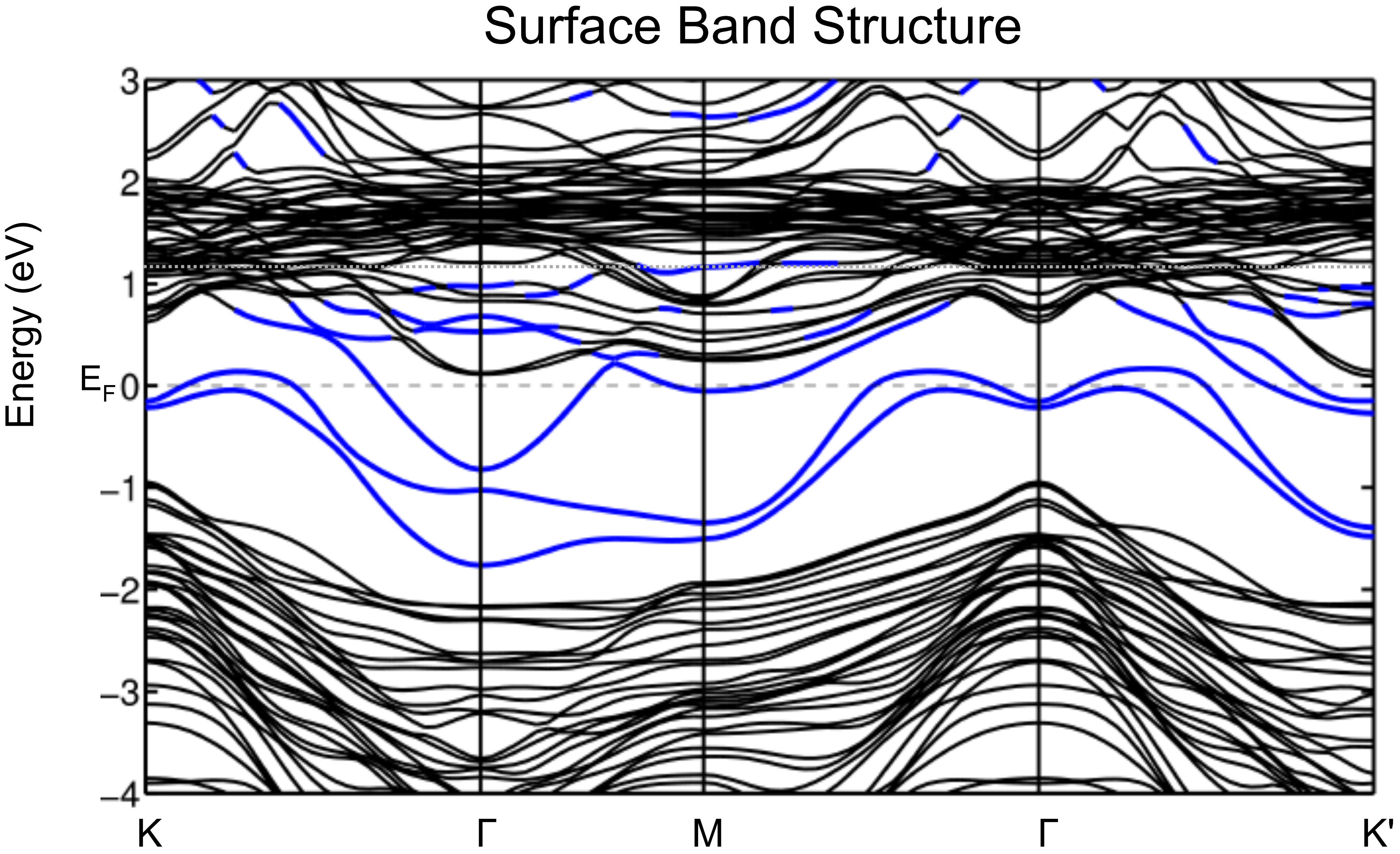
Attempt I: One ML heavy atoms

- 6 layers MnTe
- 1 ML heavy atom
  - Directly on Mn
- Polar surface
- (Bottom: 1 ML iodine)

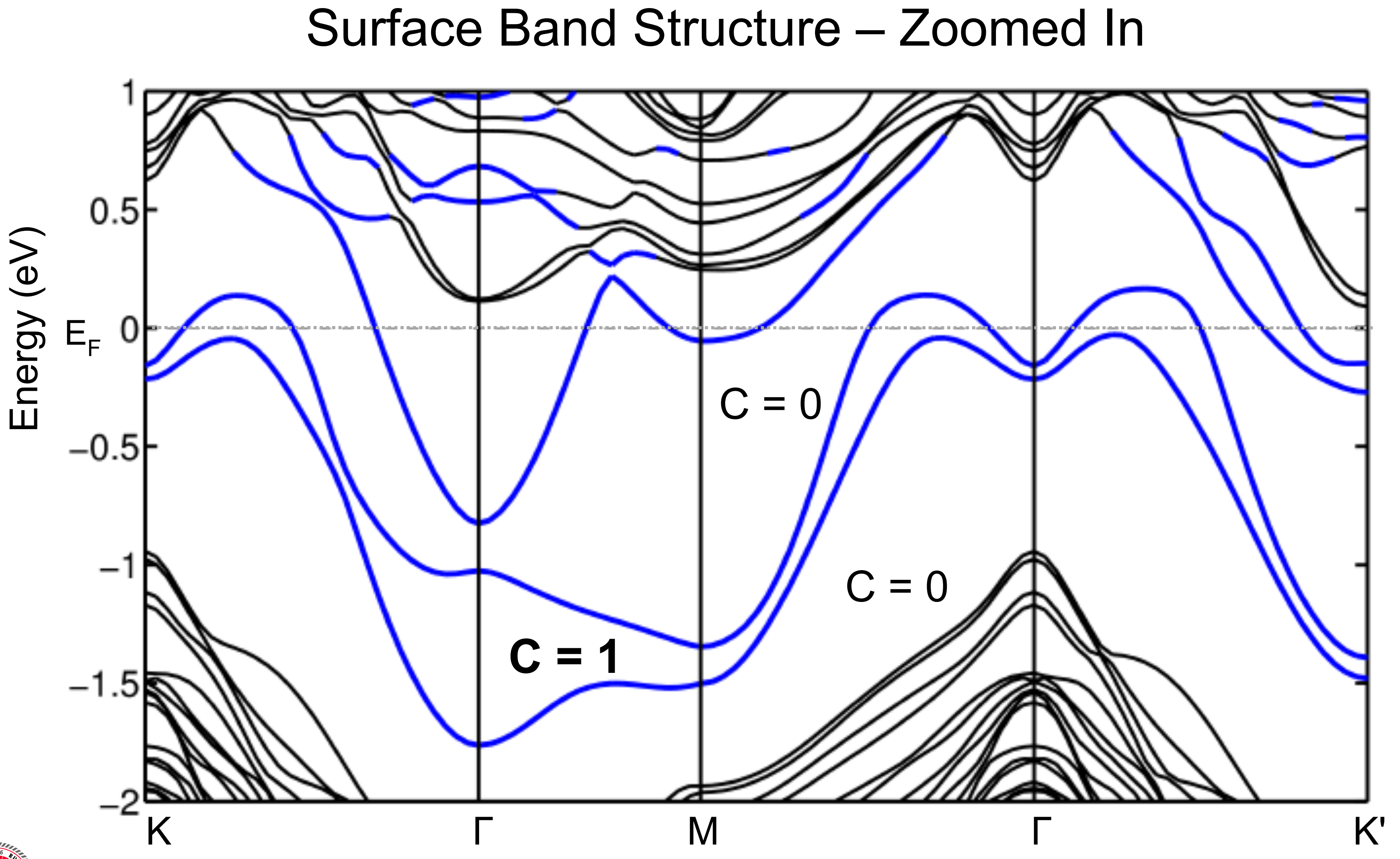




1 ML Tl on MnTe



1 ML Tl on MnTe

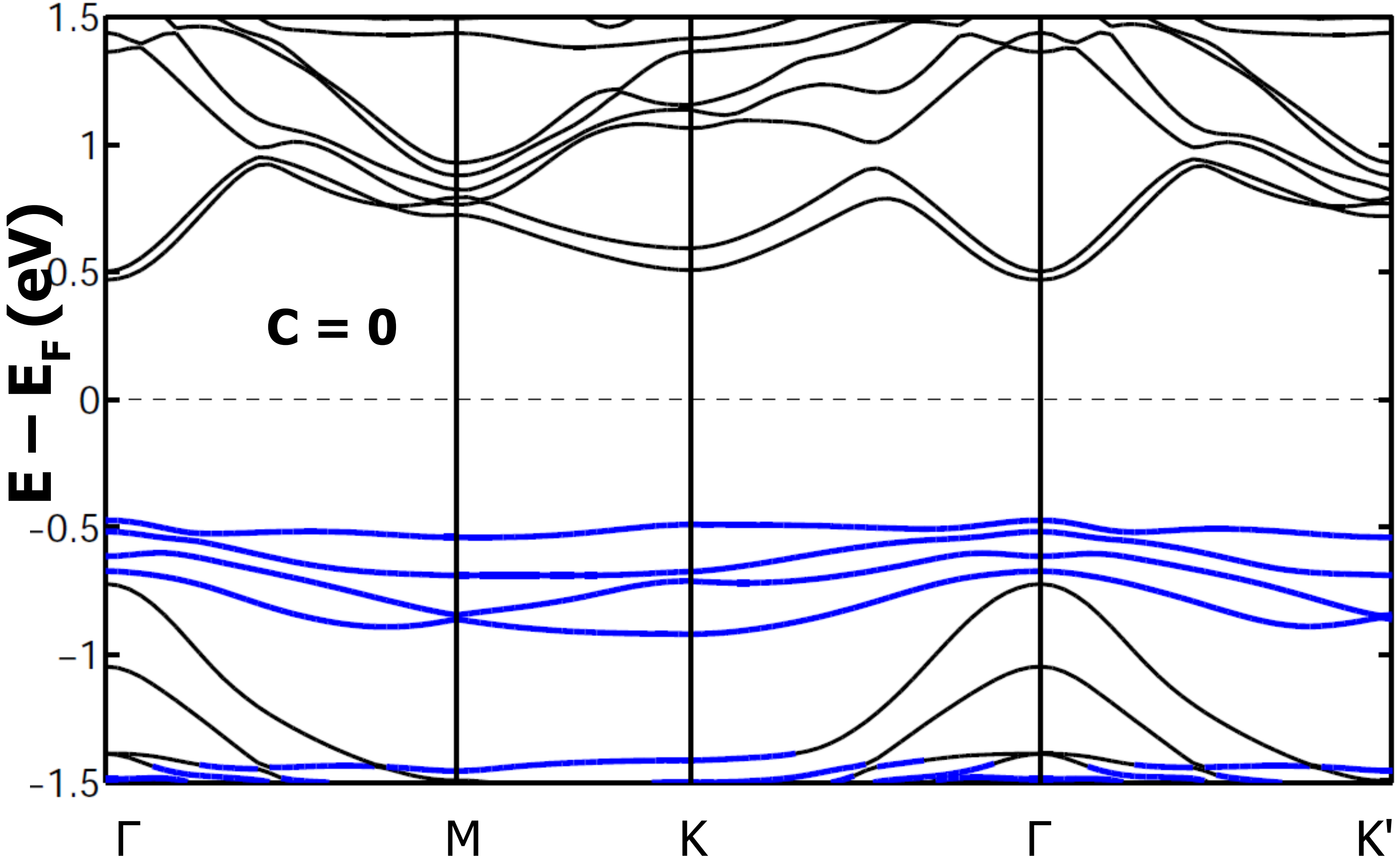


Three observations

- Non-zero Chern numbers are common
  - Provided E_{hop}, E_{SO} and E_{mag} are at similar scale
- Bands are generically isolated in 2D
  - No symmetry-induced degeneracies
  - No accidental degeneracies
- However, if E_{hop} is too large, there is no global gap

Attempt II: 1/3 ML heavy atoms

1/3 ML Bi on MnSe



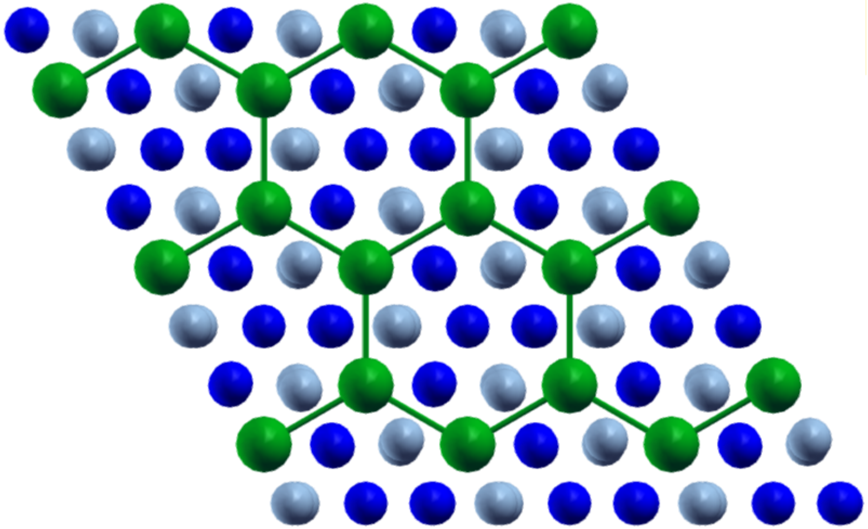
Attempt II: 1/3 ML heavy atoms

Result:

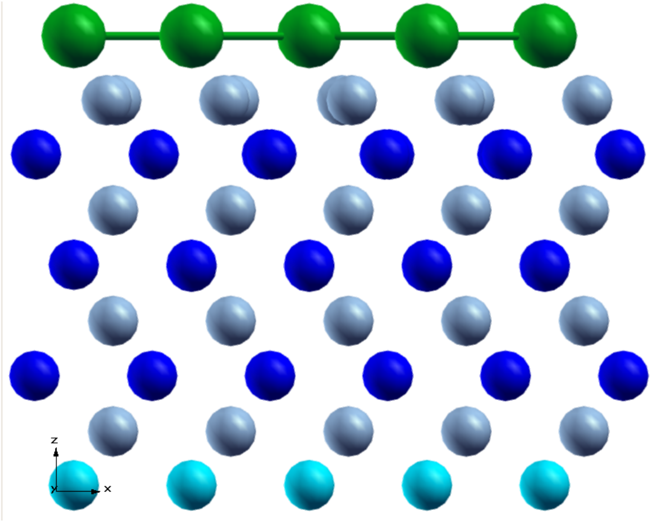
- Bands tend to be flatter
- Global band gaps are easier to find
- But Chern numbers are typically all zero

Attempt III: 2/3 ML honeycomb

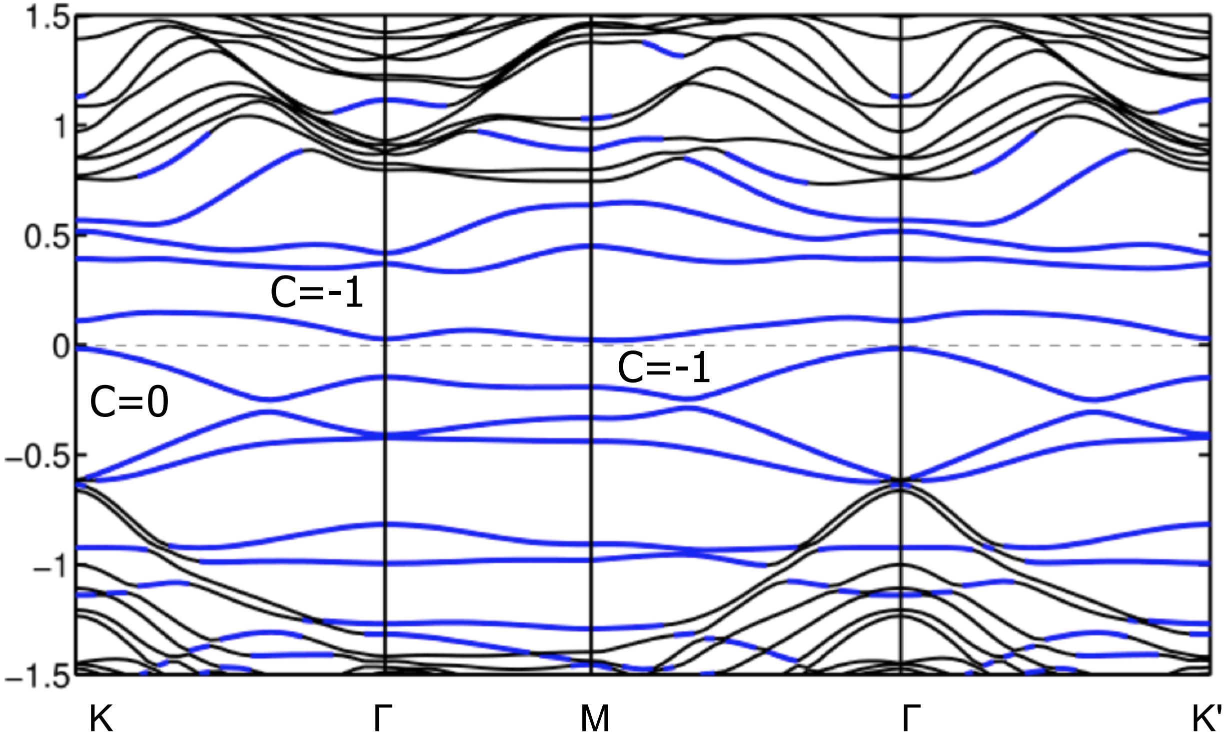
Top view



Side view

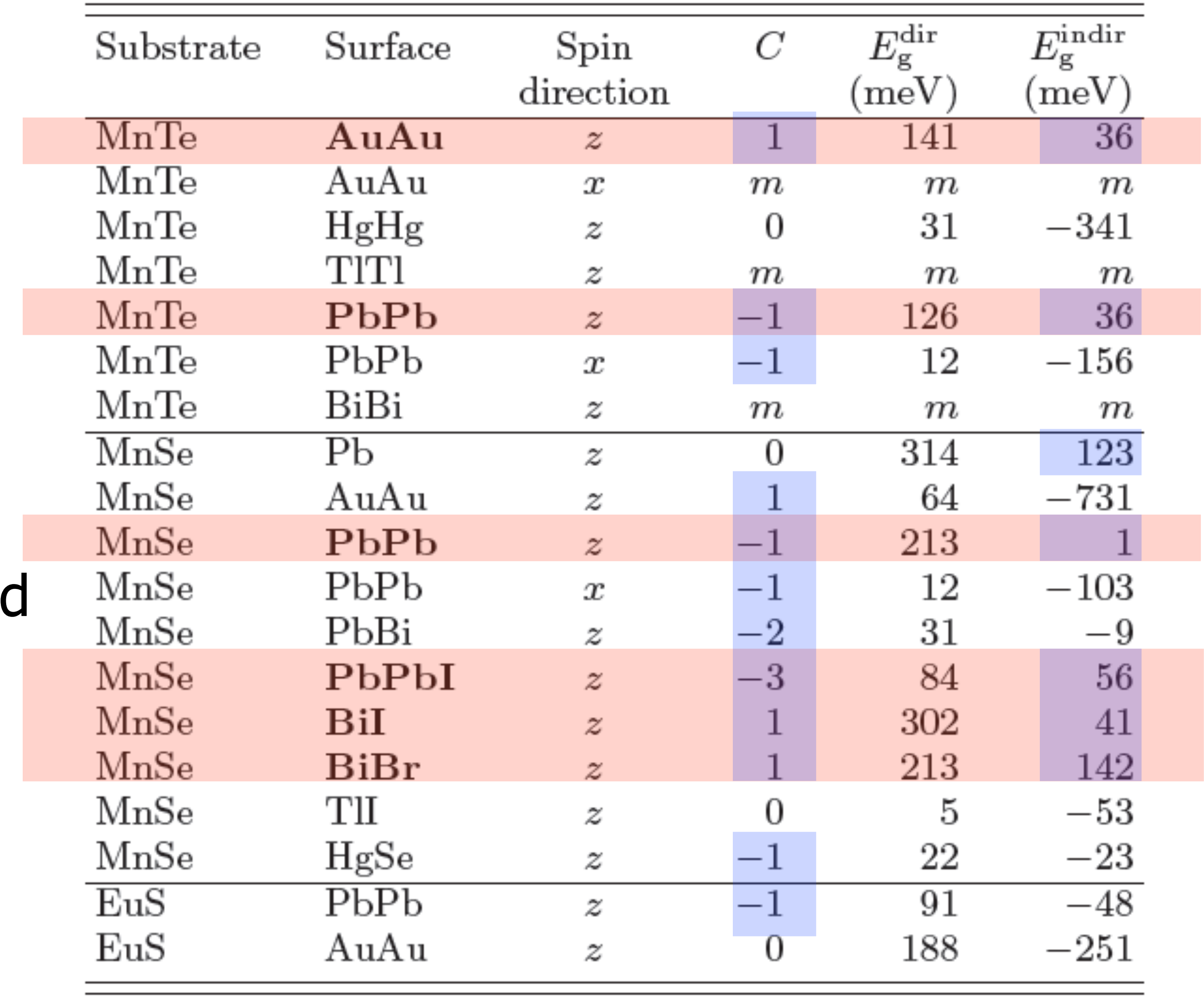


2/3 ML of Pb on MnTe



- E_F is in gap of 36 meV with C=-1
- This is a QAH insulator!
- Even larger minimum direct gap (>0.2eV above)

Search for Chern Insulators

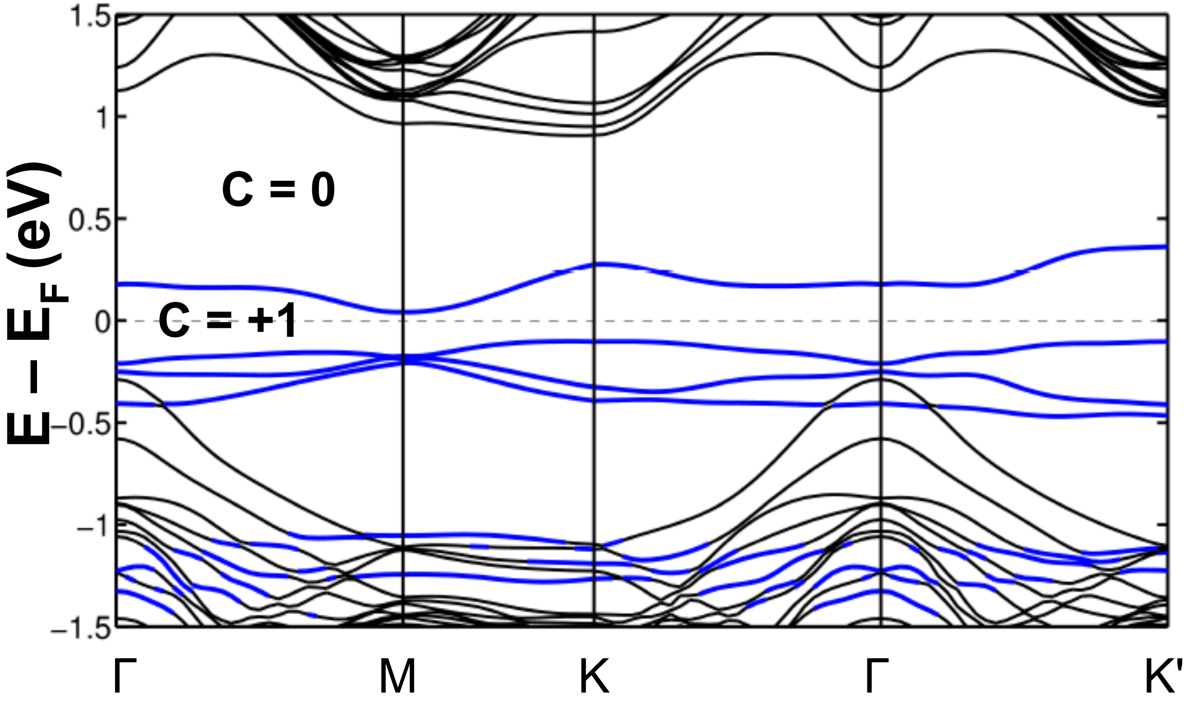


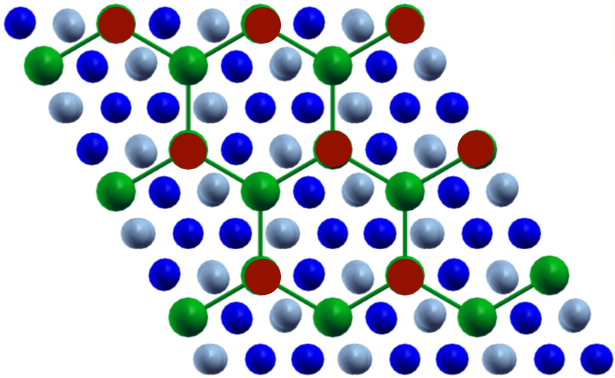
Substrate	Surface	Spin direction	C	$E_\mathrm{g}^\mathrm{dir}$ (meV)	$E_\mathrm{g}^\mathrm{indir}$ (meV)
MnTe	**AuAu**	z	1	141	36
MnTe	AuAu	x	m	m	m
MnTe	HgHg	z	0	31	−341
MnTe	TlTl	z	m	m	m
MnTe	**PbPb**	z	−1	126	36
MnTe	PbPb	x	−1	12	−156
MnTe	BiBi	z	m	m	m
MnSe	Pb	z	0	314	123
MnSe	AuAu	z	1	64	−731
MnSe	**PbPb**	z	−1	213	1
MnSe	PbPb	x	−1	12	−103
MnSe	PbBi	z	−2	31	−9
MnSe	**PbPbI**	z	−3	84	56
MnSe	**BiI**	z	1	302	41
MnSe	**BiBr**	z	1	213	142
MnSe	TlI	z	0	5	−53
MnSe	HgSe	z	−1	22	−23
EuS	PbPb	z	−1	91	−48
EuS	AuAu	z	0	188	−251

Strained
-2%

Our champion to date

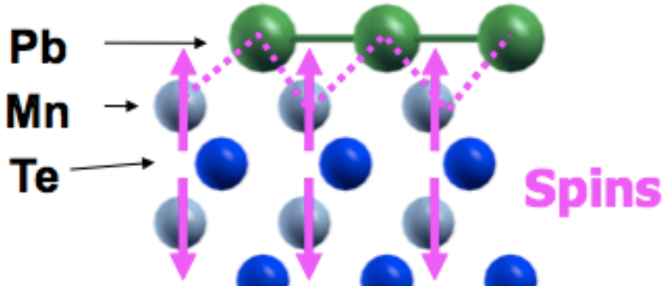
Bi/Br on MnSe: 142 meV gap





Status

- First principles proof of principle
  - Gaps can be as large as 0.14 eV
- Surfaces studied in current work are not experimentally realistic
  - Probably unstable



- Theory / experimental collaboration needed to find practical examples

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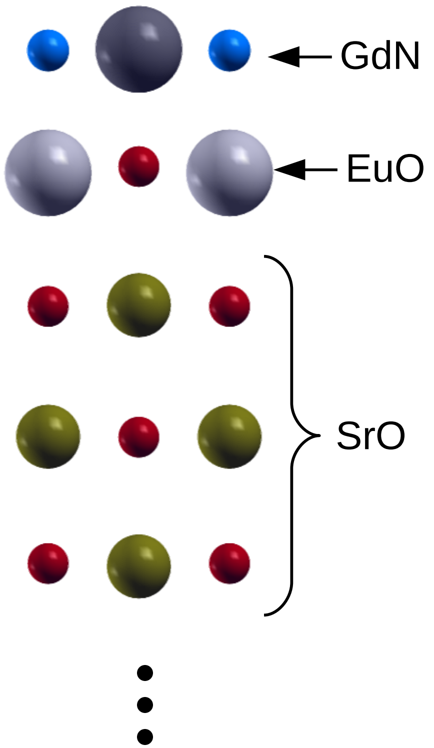
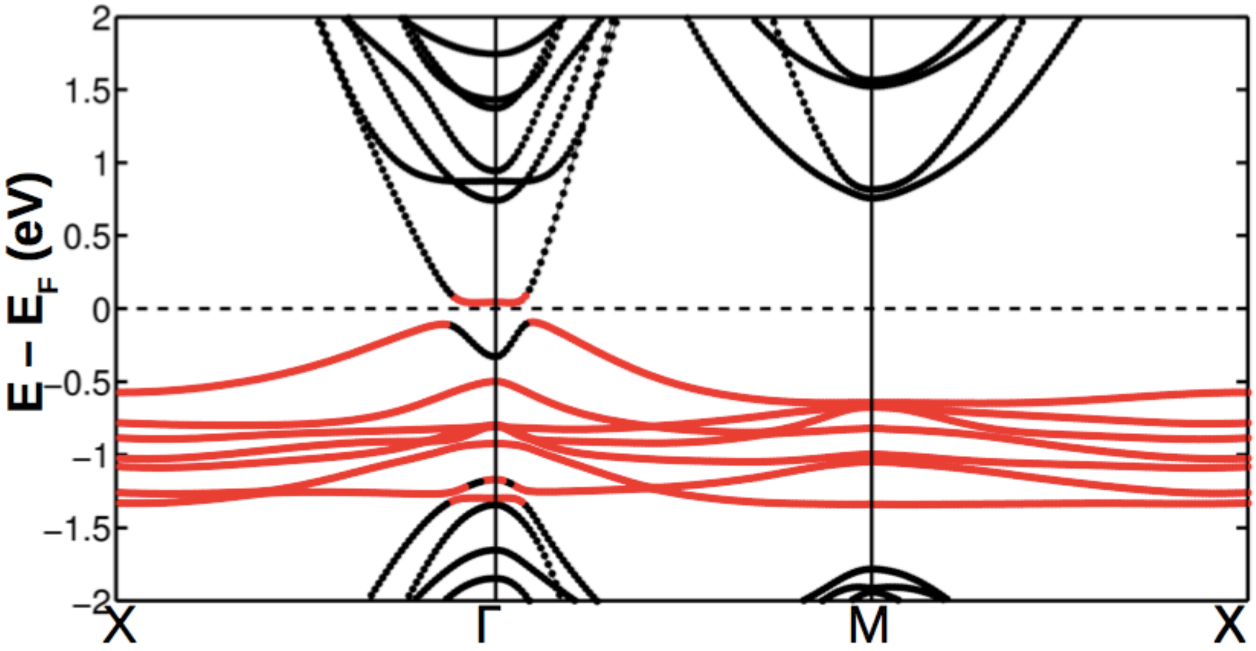
Another idea

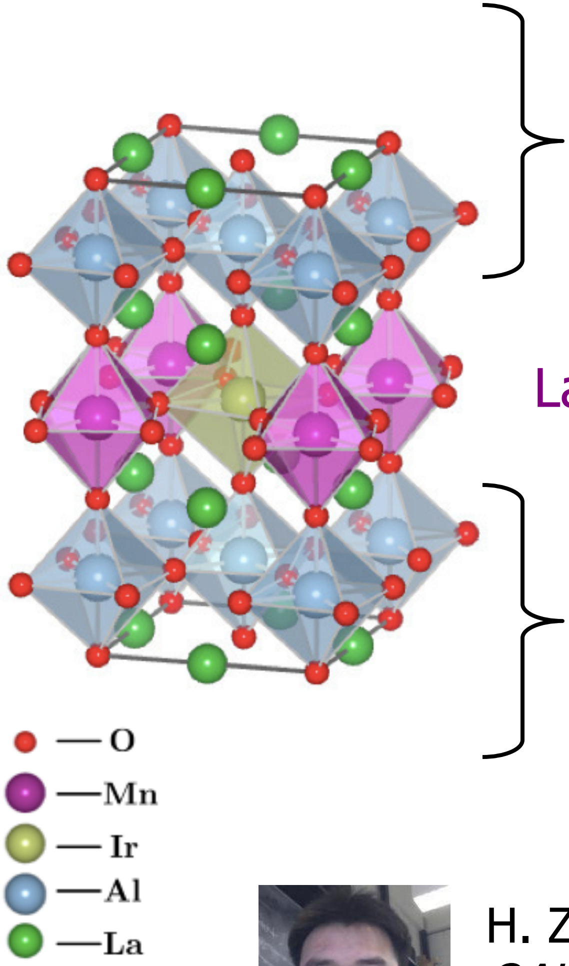




C = -1 Gap = 130 meV

Kevin Garrity and D.V.
Chern insulators from a magnetic rocksalt interface
arXiv:1404.0973

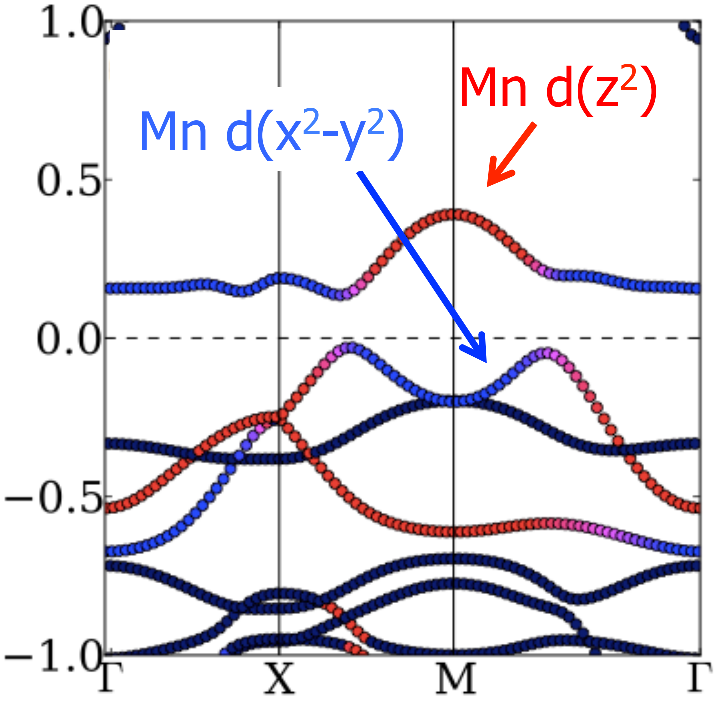
Another idea



$LaAlO_3$ host

La_2MnIrO_6 layer

$LaAlO_3$ host



C = 2 (unrelaxed)

H. Zhang, H. Huang, K. Haule, and D.V.
QAH phase in (001) double-perovskite monolayers via intersite spin-orbit coupling
arXiv:1404.0973

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