

Bulk-edge dualities in topological matter

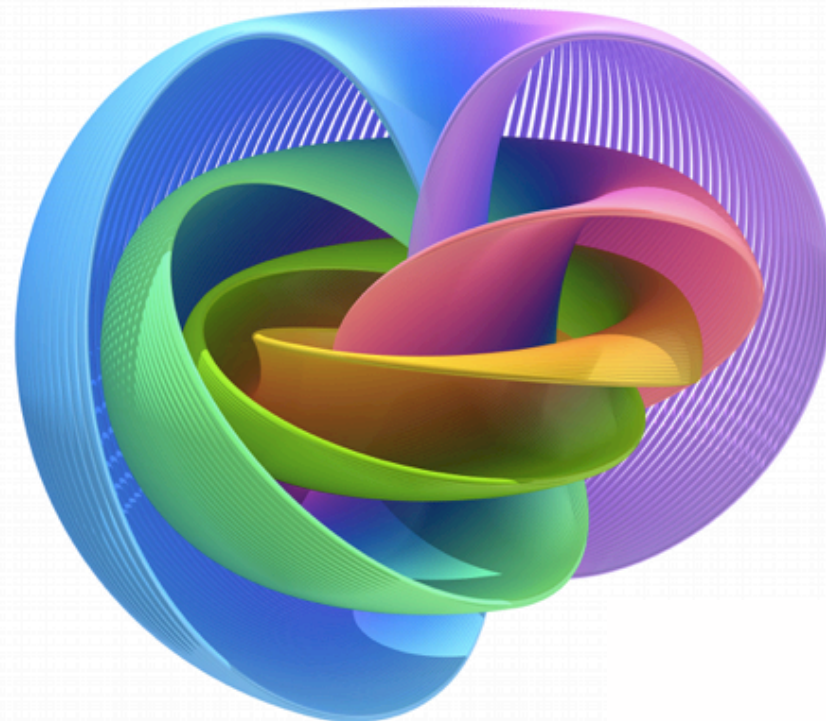
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CENTRO DE CIENCIAS
DE **BENASQUE**
PEDRO PASCUAL



PHYSICS & GEOMETRY - REMEMBERING GIUSEPPE MORANDI



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Density-matrix renormalization-group simulation of the $SU(3)$ antiferromagnetic Heisenberg model

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We analyze the antiferromagnetic $SU(3)$ Heisenberg chain by means of the density-matrix renormalization group. The results confirm that the model is critical and the computation of its central charge and the scaling dimensions of the first-excited states show that the underlying low-energy conformal field theory is the $SU(3)_1$ Wess-Zumino-Novikov-Witten model.

MONOGRAPHS AND TEXTBOOKS
IN PHYSICAL SCIENCE
LECTURE NOTES

GIUSEPPE MORANDI

QUANTUM HALL EFFECT

TOPOLOGICAL PROBLEMS
IN CONDENSED-MATTER PHYSICS



BIBLIOPOLIS

where $P_l(s) = P_l(R(s))$, and:

$$A(s) = \exp[iR(s)\hat{p}/\hbar] ; \hat{p} = \frac{\hbar}{i} \frac{d}{dx} \quad (8.42)$$

i.e. A is a translation operator. If we now choose the initial wave function as, say:

$$\psi(x, 0) = \sqrt{\frac{2}{\Delta}} \sin\left(\frac{\pi l}{\Delta}\right) \exp(i\delta x/\hbar) \theta(x) \theta(\Delta - x) \quad (8.43)$$

for some l , the Adiabatic Theorem yields:

$$\psi(x, t) = \sqrt{\frac{2}{\Delta}} \sin\left[\frac{\pi l}{\Delta} (x - R(s))\right] \exp[i\delta (x - R(s))/\hbar] \exp[-iE_l t/\hbar]. \quad (8.44)$$

The factor: $\exp[-i\delta R(s)/\hbar]$ is just Berry's phase. For a complete excursion, the wave function acquires then a phase:

$$\exp\left[-2\pi i \frac{\delta}{\hbar}\right] \equiv \exp\left[-2\pi i \frac{\Phi}{\Phi_0}\right] \quad (8.45)$$

where Φ is the magnetic flux of the Aharonov-Bohm solenoid, and: $\Phi_0 = hc/e$ is the elementary fluxon. As remarked by Berry, this establishes the link between the Aharonov-Bohm effect and the Quantum Adiabatic Phase.

We are now in the position to recast the results of Ch.6 in the language of fiber bundles and connections [21,59], and, in particular, of the Bott-Chern connection and Berry's phase. Recall that what has been eventually done in the last part of Ch.6 is a study of the changes of the ground-state wave function when the boundary conditions, represented by the parameters α and β defined there, are changed. α and β play then the rôle of adiabatically-changing parameters and; as the ground state is assumed to be nondegenerate, the conditions of the Adiabatic Theorem apply. Combining (5.39) and (5.46), we have:

$$\frac{\hbar}{e^2} \bar{\sigma}_H = \int_0^{2\pi} d\alpha \int_0^{2\pi} d\beta \frac{i}{2\pi} \left\{ \left\langle \frac{\partial \phi_0}{\partial \alpha} \middle| \frac{\partial \phi_0}{\partial \beta} \right\rangle - \left\langle \frac{\partial \phi_0}{\partial \beta} \middle| \frac{\partial \phi_0}{\partial \alpha} \right\rangle \right\}. \quad (8.46)$$

Comparing with (8.19) and (6.93), we see that this is just *the integral over a two-cycle of the first Chern class associated with the Bott-Chern connection* (or with Berry's phase). Some caution must be used as to how the manifold corresponding to the parameter space is defined. If we take:

$$M = \{\text{square of side } 2\pi \text{ in the } (\alpha, \beta) - \text{plane}\},$$

then M is a manifold with boundary, and both the curvature form Ω and the connection ω are well-defined. Therefore, Stokes' theorem applies, and:

$$\frac{\hbar}{e^2} \bar{\sigma}_H = \int_M \frac{i\Omega}{2\pi} = \int_{\partial M} \frac{i}{2\pi} \omega \quad (8.47)$$

which is just a way of rephrasing Eqns.(5.29) to (5.41) in the language of differential forms. On the other hand, α and β are actually angles, and hence the parameters space should actually be identified as: $M = T^2$, the two-torus. In such a case, however, the connection one-form ω is only locally defined (moving from, say, α to $\alpha + 2\pi$ it changes by an additive constant), and hence Ω is *closed but not exact*, and only the first of Eqns.(8.47) applies. In any event, the Hall conductivity (in units of e^2/h) is given by the integral over the parameters space of the first Chern class, and hence *is quantized according to integers as a consequence of the periods of the Chern classes* (with the appropriate normalization) *being integral*. Stated in more physical (but of course equivalent) terms, *we can also view integral quantization of the Hall conductivity as a manifestation of Berry's phase*.

The considerations of this Chapter should therefore clarify completely the *topological nature of the IQHE*: a (static) magnetic field induces a *nontrivial* $U(1)$ -bundle over the parametr space. *If* the ground state is nondegenerate, the curvature of the connection determines the Hall conductivity via the integral over the base manifold of its first Chern class.

Some further material related to the unusual features of electrons in a magnetic field is reviewed in Appendix A.

$$\frac{h}{e^2} \bar{\sigma}_H = \int_0^{2\pi} d\alpha \int_0^{2\pi} d\beta \frac{i}{2\pi} \left\{ \left\langle \frac{\partial \phi_0}{\partial \alpha} \middle| \frac{\partial \phi_0}{\partial \beta} \right\rangle - \left\langle \frac{\partial \phi_0}{\partial \beta} \middle| \frac{\partial \phi_0}{\partial \alpha} \right\rangle \right\}. \quad (8.46)$$

TKKN

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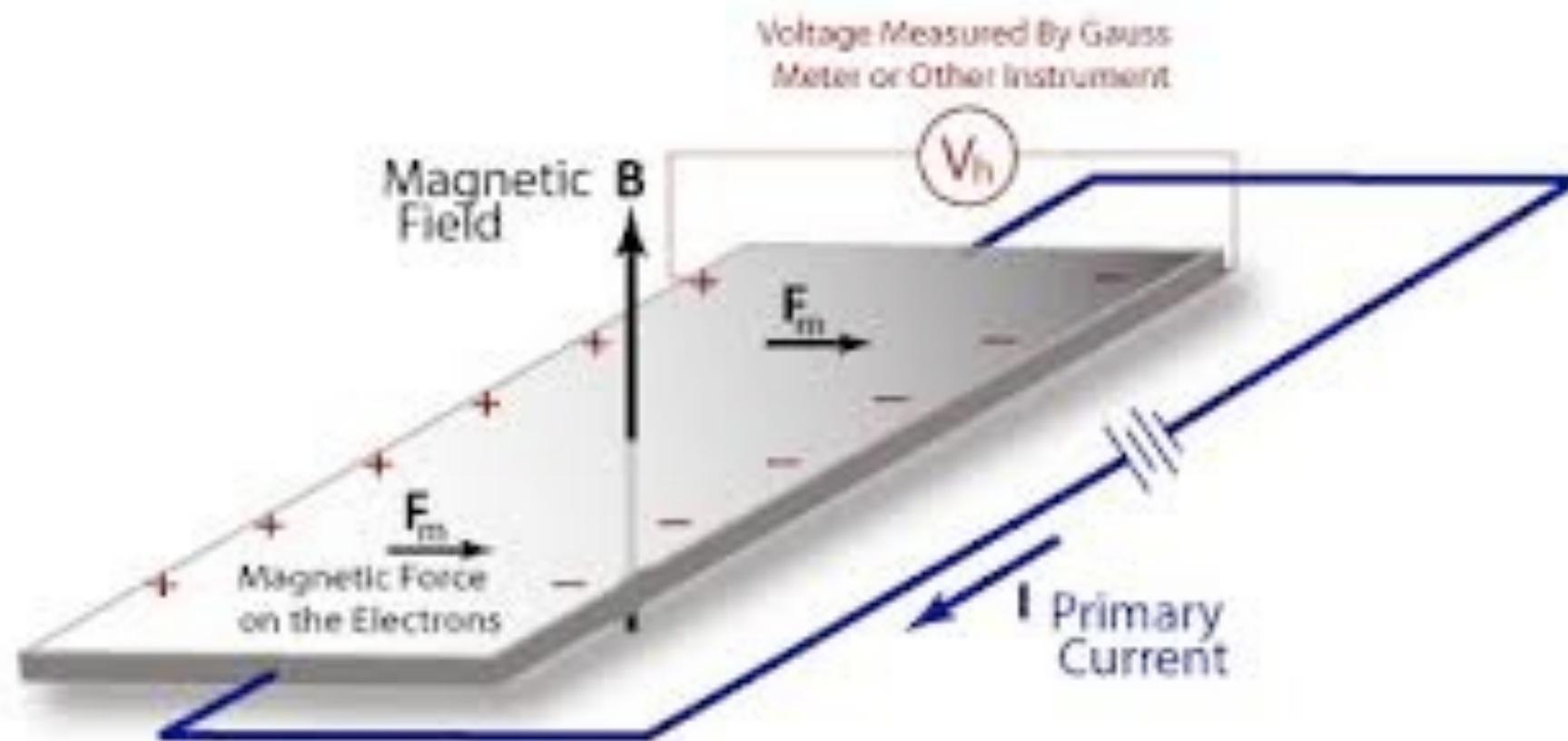
TOPOLOGICAL INSULATORS

- Bulk insulators
- Edge conductors
- Edge currents topologically protected
- Spin-momentum locking
- Time reversal protection

TOPOLOGICAL SEMIMETALS

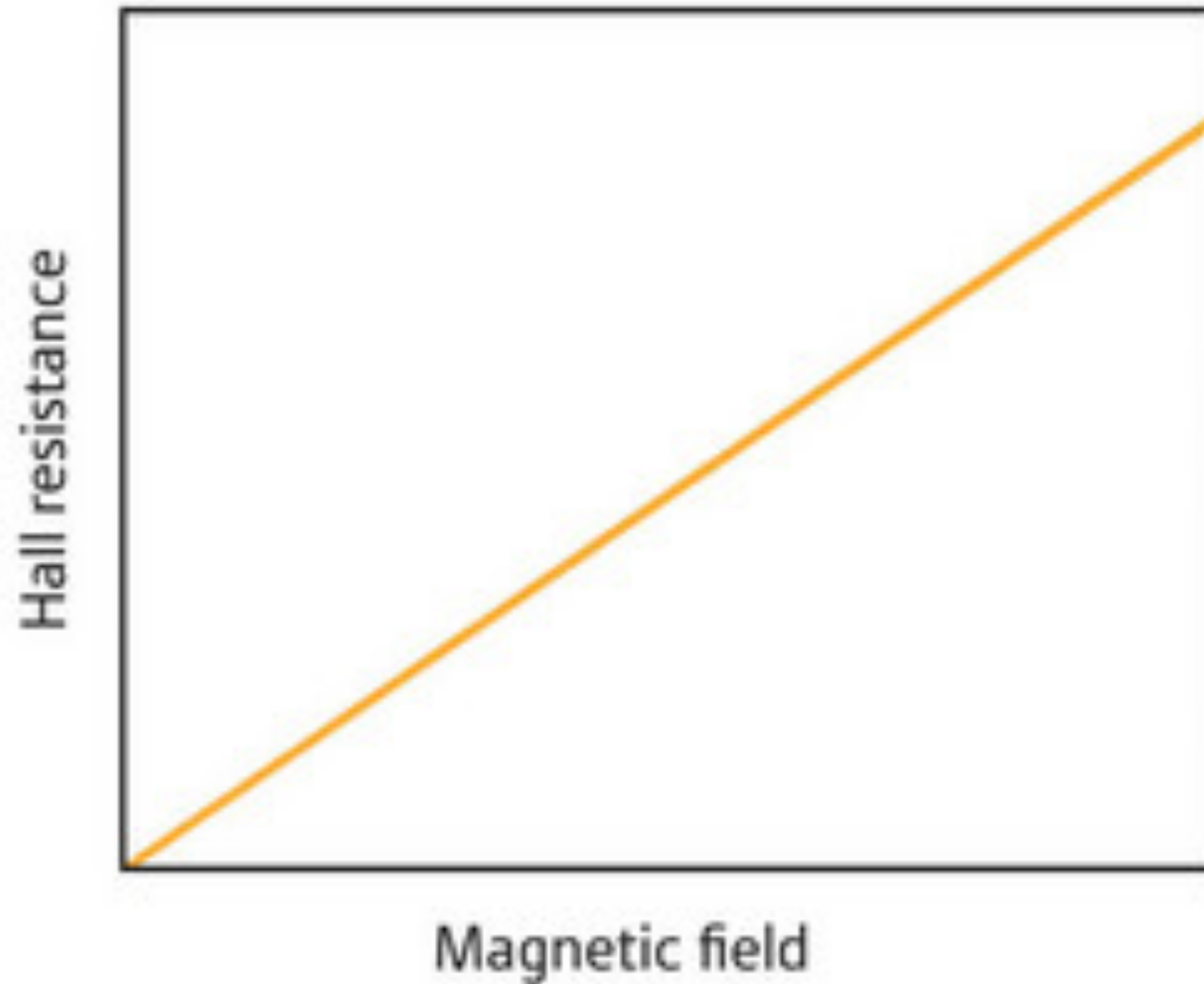
- Massless bulk states
- Special edge currents
- Topological protected

Hall effect

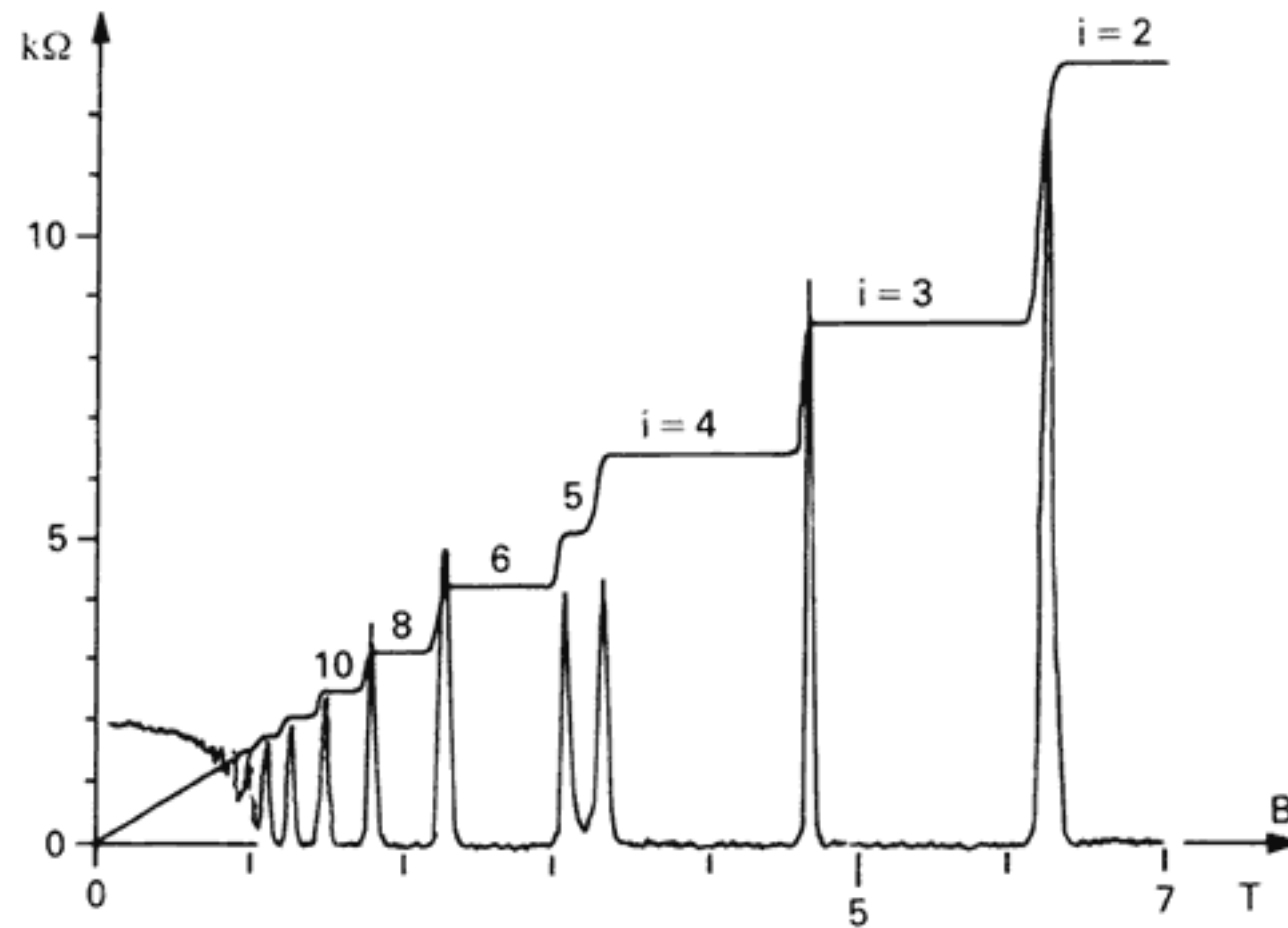


Magnetoresistance: Hall effect

Classical Hall effect



Integer Quantum Hall effect



[von Klitzing]

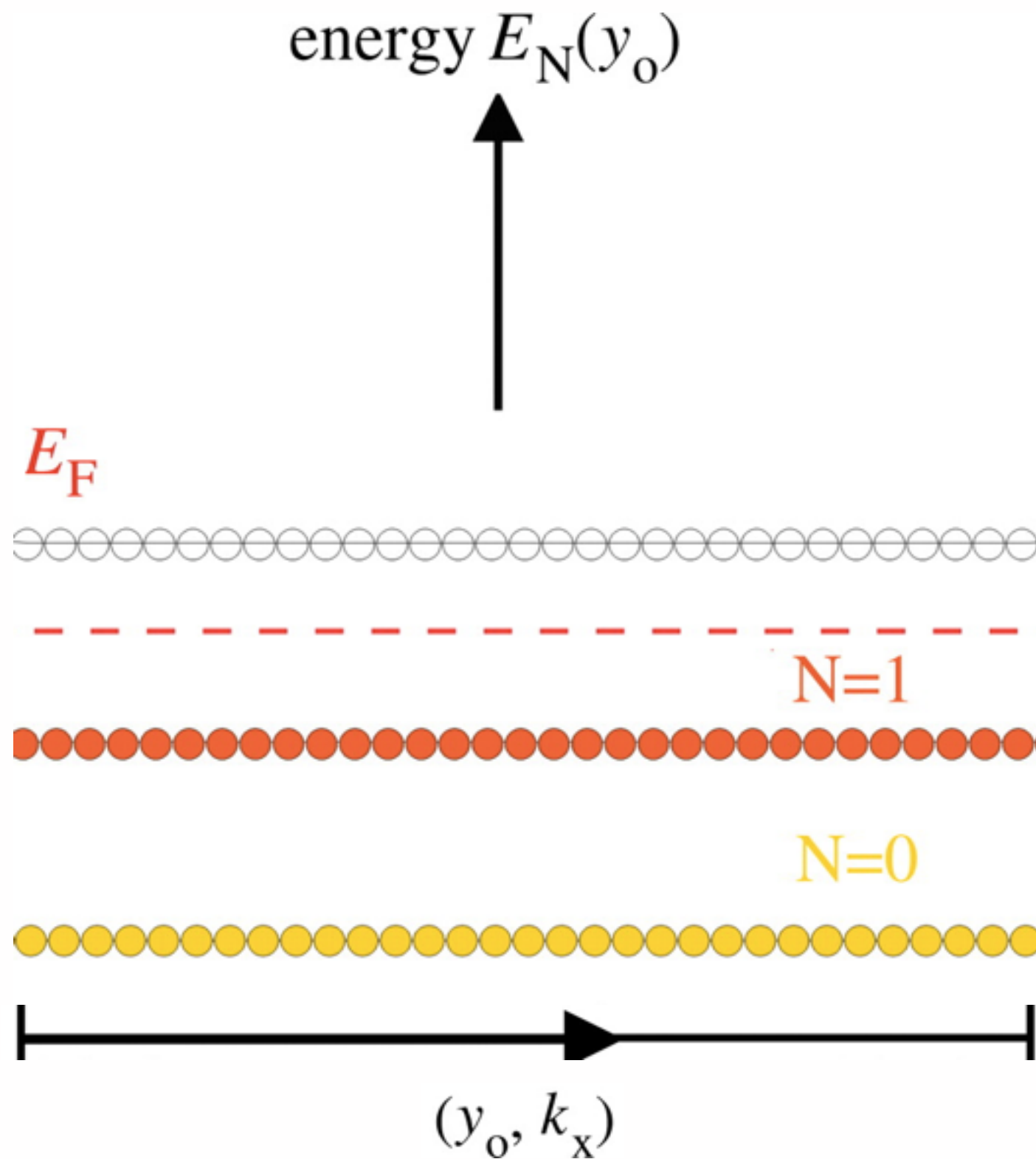
Quantum Hall effect

$$\mathbb{H} = -\frac{1}{2m} \left[\partial_2^2 + (\partial_1 + ieBx_2)^2 \right]$$

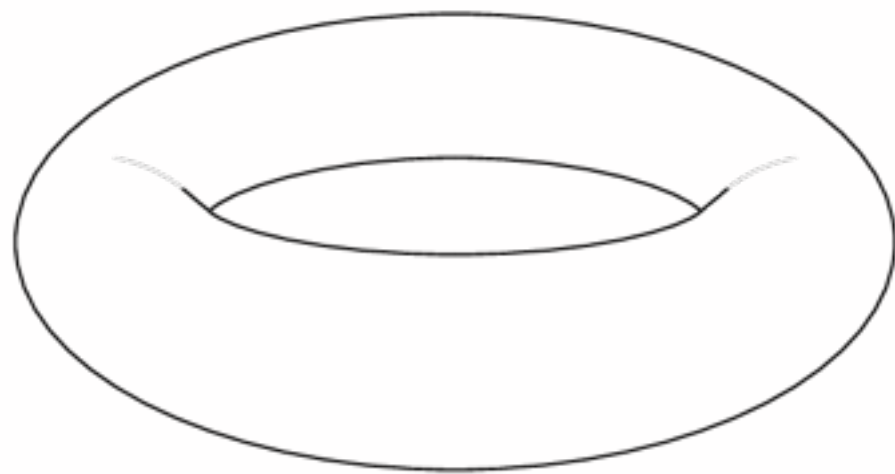
$$E_n = \frac{eB}{2m} \left(n + \frac{1}{2} \right)$$

$$\psi_{n,k_1}(x) = e^{ik_1x_1} H_n(eBx_2) e^{-eBx_2^2/2}$$

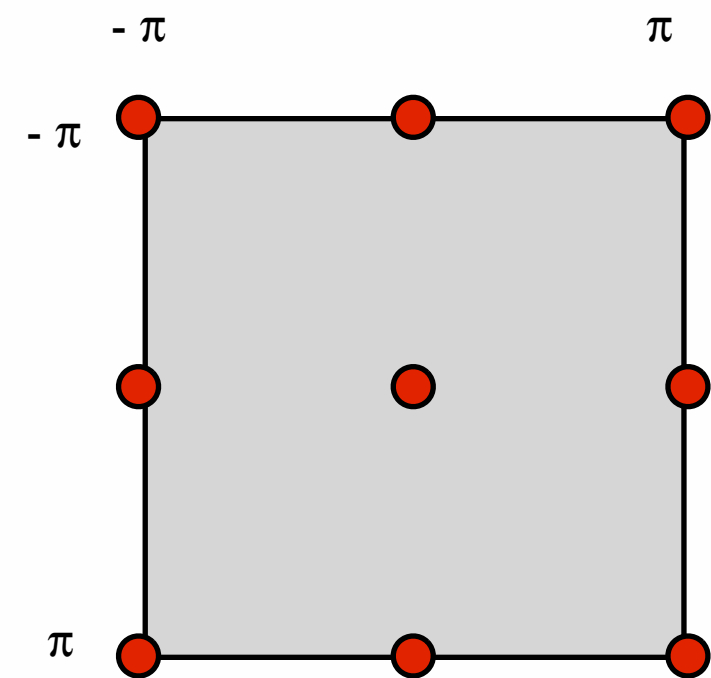
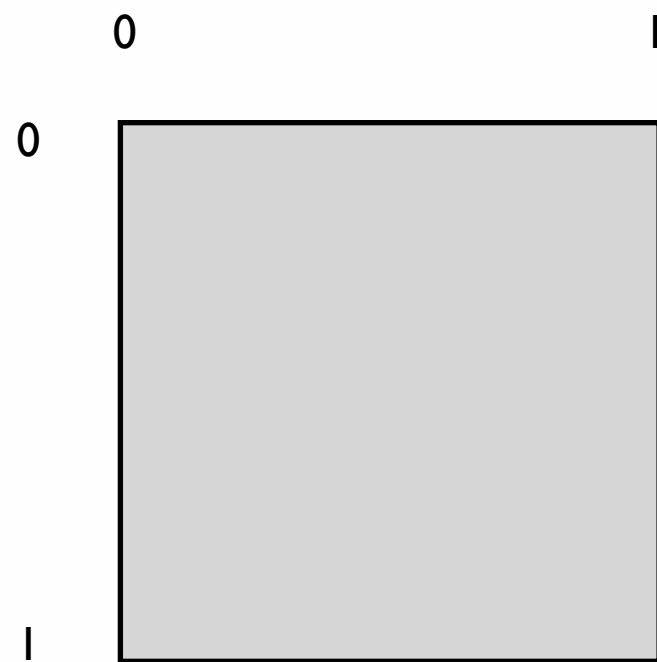
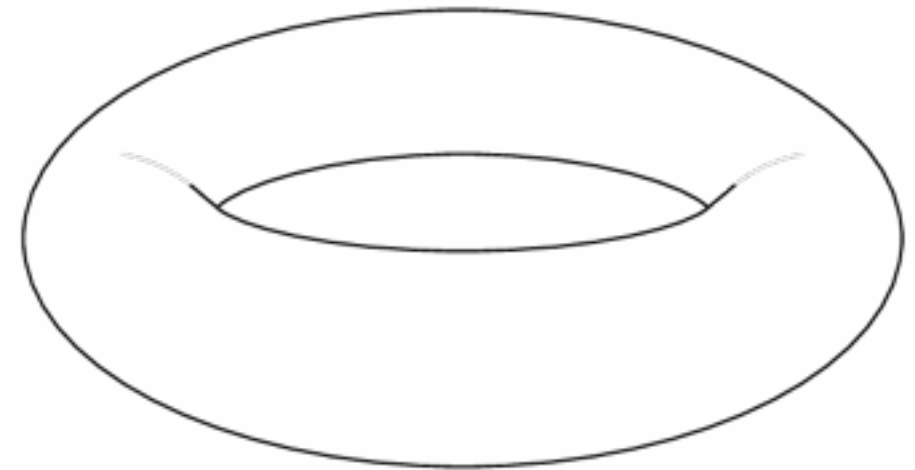
Integer Quantum Hall effect



Real Space

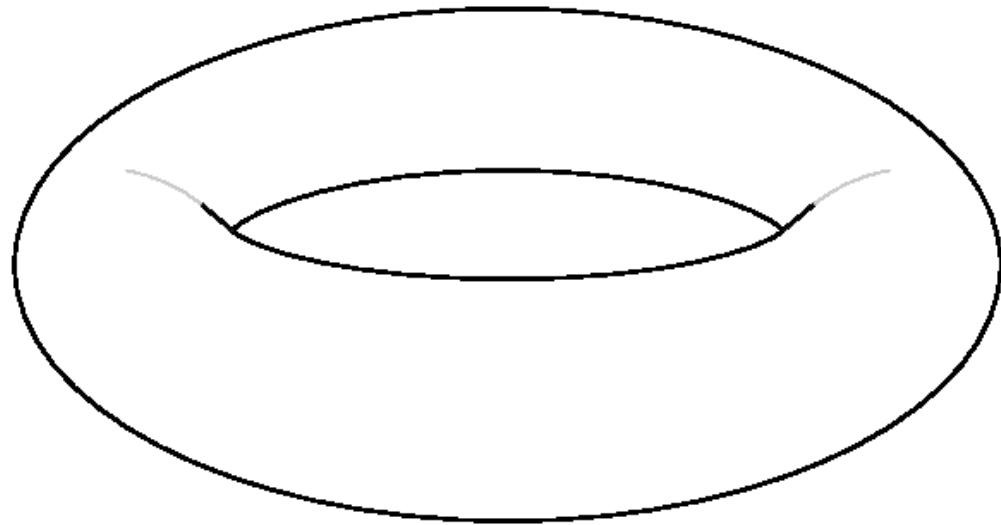


Brillouin Zone



Kramers points

Hall Effect in 2D Torus \mathbb{T}



$$\frac{e}{2\pi} \int_T \mathbf{F} = k \in \mathbb{Z} \quad k = eB/2\pi$$

$$\psi(\phi_1 + 2\pi, \phi_2) = e^{i\frac{k}{2}\phi_2} \psi(\phi_1, \phi_2)$$

In complex coordinates:

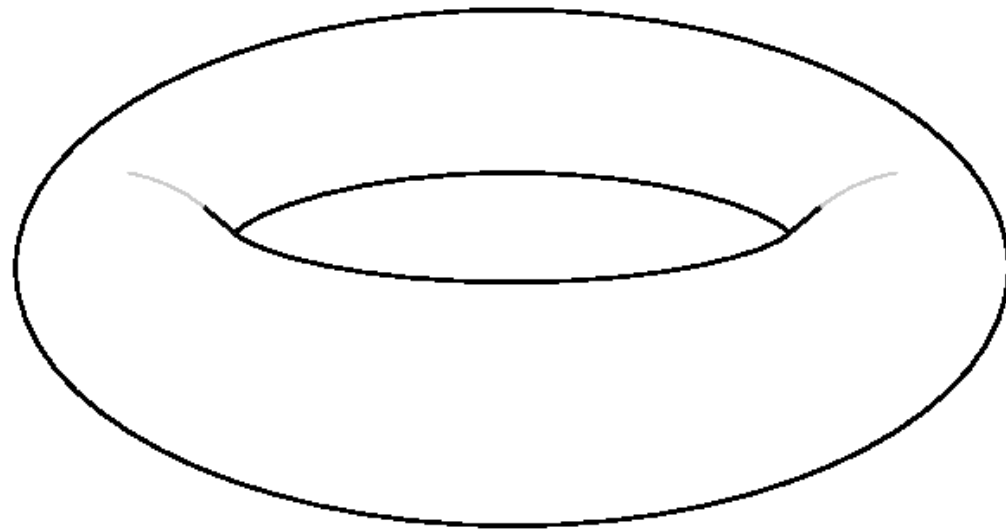
$$\psi(\phi_1, \phi_2 + 2\pi) = e^{-i\frac{k}{2}\phi_1} \psi(\phi_1, \phi_2)$$

$$\mathbb{H} = \frac{1}{2m} \left[\left(\partial_1 + i\frac{B}{2}(\phi_2 + \epsilon_2) \right)^2 + \left(\partial_2 + i\frac{B}{2}(-\phi_1 - \epsilon_1) \right)^2 \right]$$

Energy levels (degeneracy: $|k|$) [Landau]

$$E_n = \frac{2\pi|k|}{m} \left(n + \frac{1}{2} \right)$$

Hall Effect in 2D Torus \mathbb{T}



$$\frac{e}{2\pi} \int_T \mathbf{F} = k \in \mathbb{Z} \quad k = eB/2\pi$$

Ground State Eigenfunctions (degeneracy: $|k|$) :
Holomorphic sections of $E(T^2, \mathbb{C})$

$$\psi_0^l(\epsilon, \phi) = \frac{e^{i \frac{k}{4\pi} (\phi_1 + 2\epsilon_1) \phi_2}}{(8\pi^4 k)^{\frac{1}{4}}} \sum_{m=-\infty}^{\infty} e^{im \left(\phi_1 + \epsilon_1 + 2\pi \frac{l}{k} \right) - \frac{1}{4\pi k} (2\pi m + k\phi_2 + k\epsilon_2)^2}$$

$$l = 0, 1, 2, \dots, |k| - 1.$$

Quantum Hall effect and Fiber bundles

Floquet-Bloch

$$L^2(\mathbb{R}^2) = \bigoplus_{\lambda \in \hat{\mathbb{T}}^2} L^2(\mathbb{T}^2)$$

The space of states acquires a bundle structure

$$L^2(\mathbb{R}^2) \left(\hat{\mathbb{T}}^2, L^2(\mathbb{T}^2) \right)$$

Spectral Floquet-Bloch theorem

$$\mathbb{H}_{\mathbb{R}^2} = \bigoplus_{\lambda \in \hat{\mathbb{T}}^2} \mathbb{H}_{\mathbb{T}^2}^{\lambda}$$

TKKN and the Hidden topology

The states with energies below the Fermi level define a vector bundle over the Brillouin zone torus.

$$E \left(\hat{\mathbb{T}}^2, \mathbb{C}^N \right)$$

In this bundle there are gauge fields defined by the Berry phases of the different states

$$\mathcal{A}_{jn}^{l,l'}(\epsilon) = -i \int_{\mathbb{T}^2} \psi_n^{l*} \partial_{\epsilon_j} \psi_n^{l'}$$

$$\mathcal{F}_n^{l,l'}(\epsilon) = \partial_{\epsilon_1} \mathcal{A}_{2n}^{l,l'} - \partial_{\epsilon_2} \mathcal{A}_{1n}^{l,l'}$$

TKKN and the Bloch bundle

First Chern class of Bloch bundle

$$C_1 = -\frac{i}{4\pi} \sum_{n=0}^{\nu} \sum_{l=0}^{|k|-1} \int_{\hat{\mathbb{T}}^2} \mathcal{F}_n^{l,l} = \nu$$

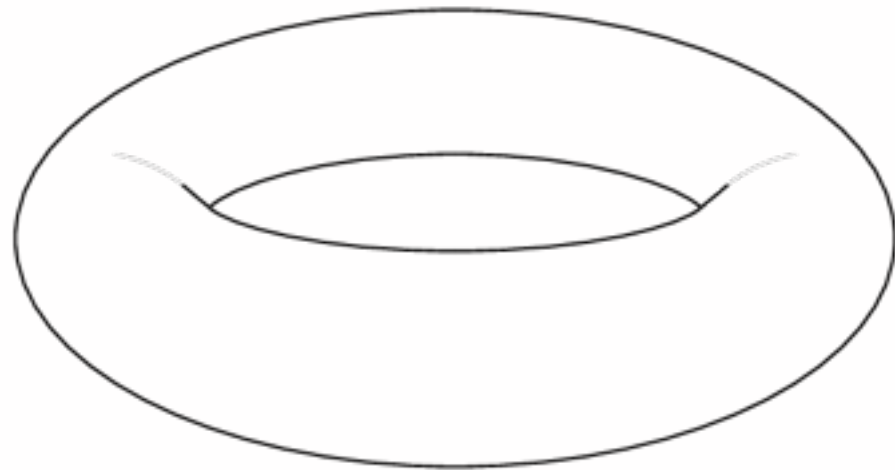
TKKN formula:

$$\sigma_{xy} = \frac{e^2}{2\pi} \nu$$

Quantization of Hall conductivity

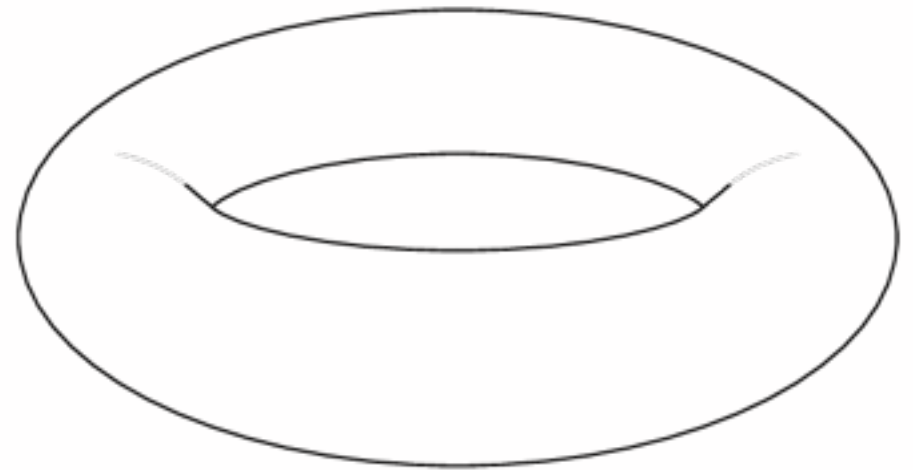
Fourier-Mukai transform

Real Space



$U(N)$ gauge field A_μ
with $c_1(A)=k$

Brillouin Zone



$U(k)$ gauge field A_μ
with $c_1(A)=N$

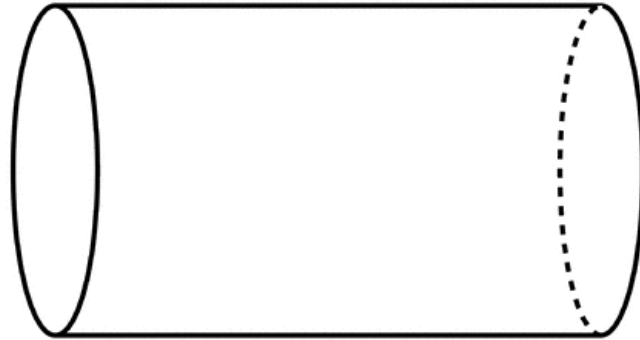
Nahm transform

[Asorey, Nature Phys. 2016]

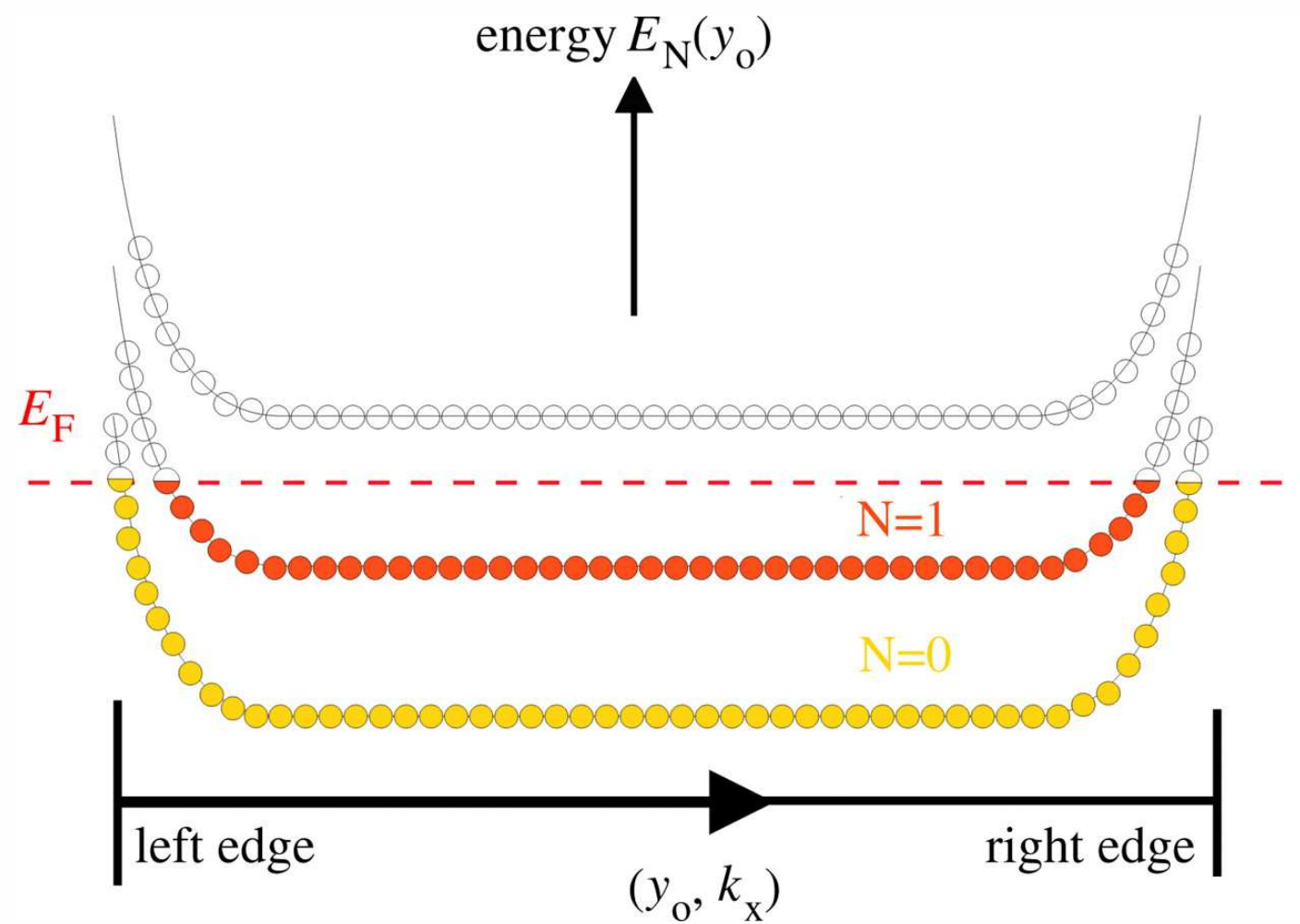


God created the volumes, the Devil the boundaries

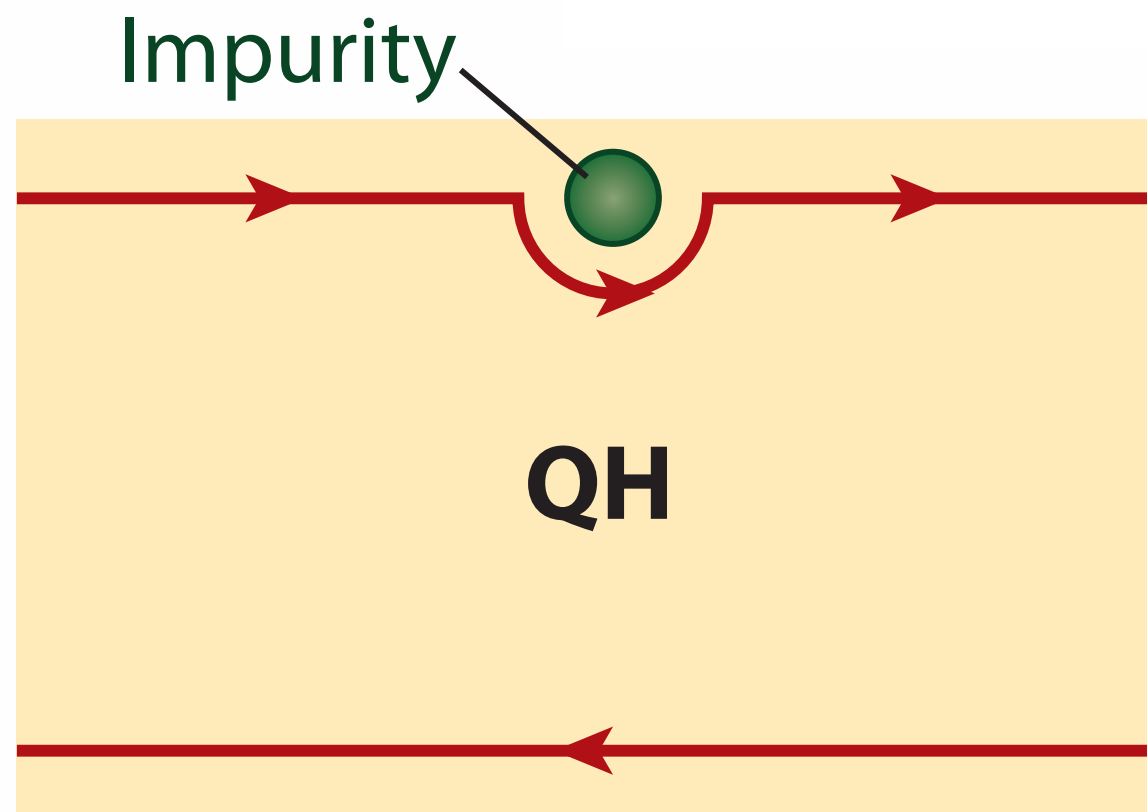
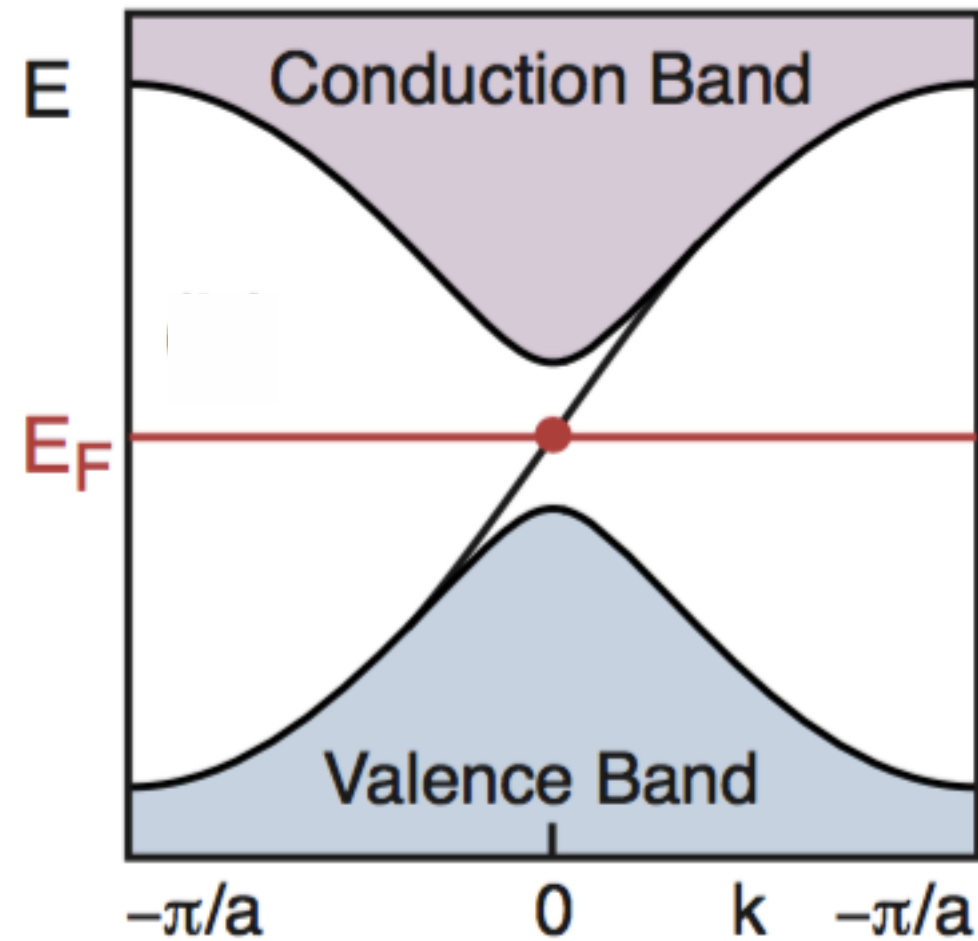
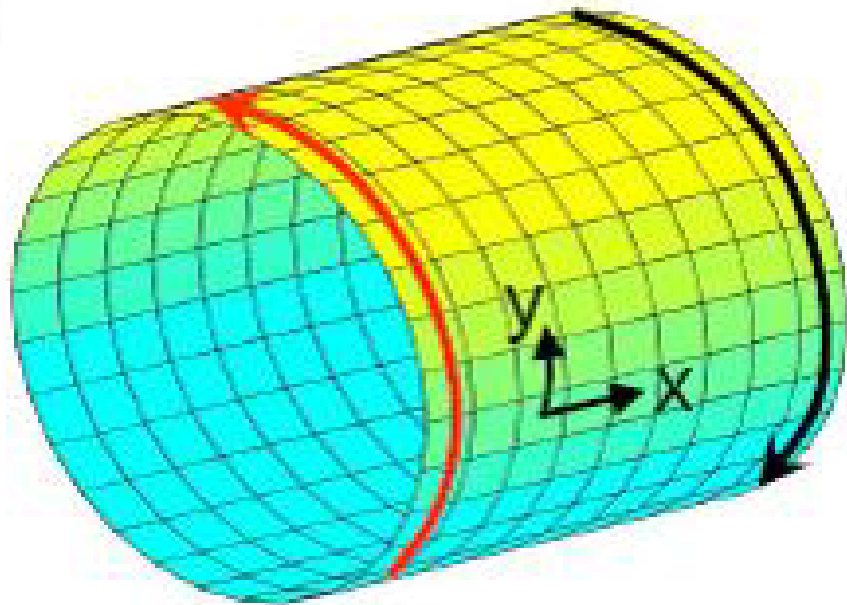
Hall effect with boundaries



Finite size effects



Edge states and bands structure

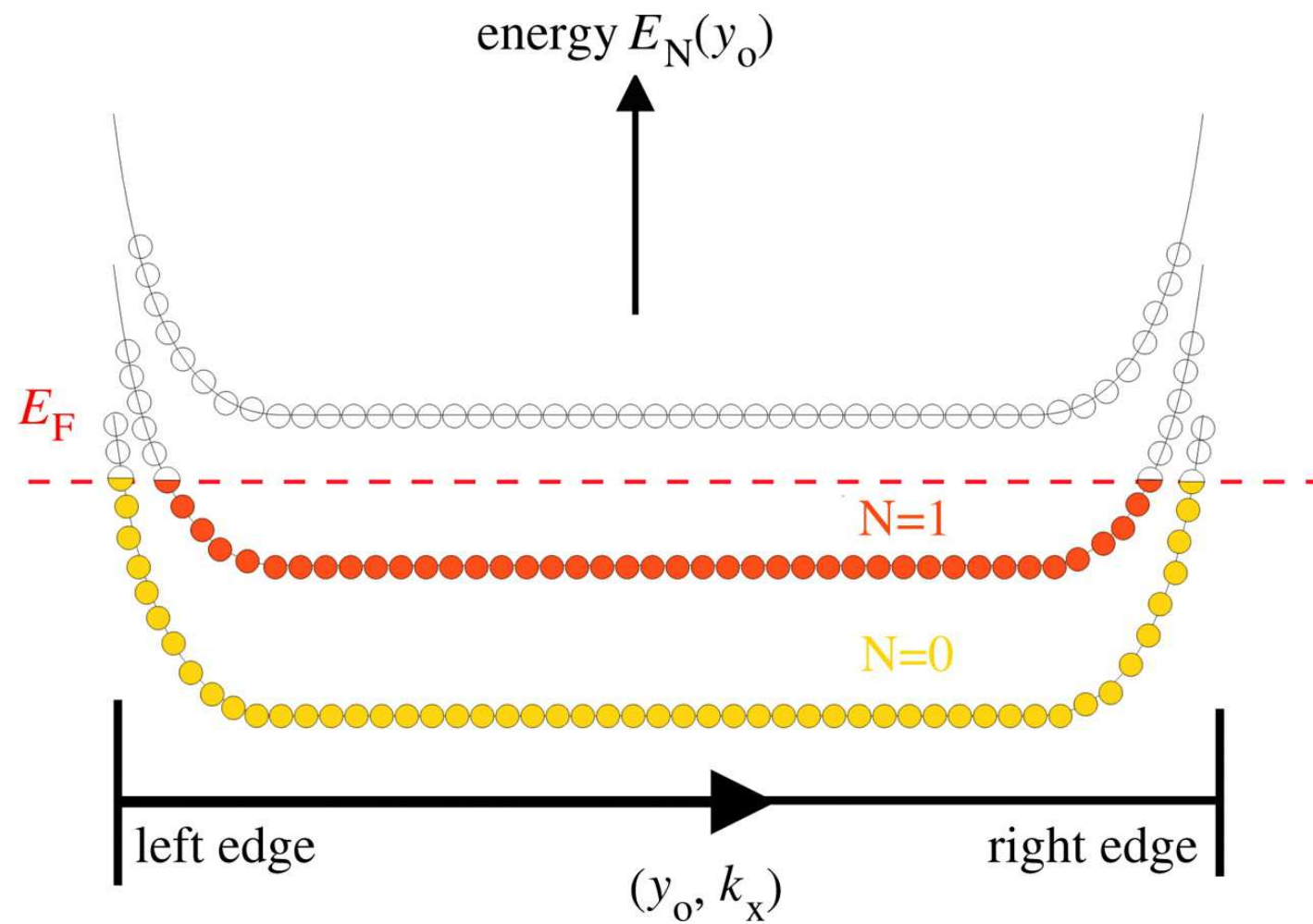


Boundary Insulators

Boundary interactions \Rightarrow Anderson localization



Finite size effects



$$\sigma_{xy} = \frac{e^2}{2\pi} \nu$$

[Halperin, O'Laughlin]

Edge states and Bulk-Edge correspondence

Chern-class on the cylinder C_1 is not any more an integer but

$$C_1 = -\frac{i}{4\pi} \sum_{n=0}^{\nu} \sum_{l=0}^{|k|-1} \left[\int_C \mathcal{F}_n^{l,l} - \oint_{\partial C} \mathcal{A}_n^{ll} \right] = \nu$$
$$C = S^1 \times [0, 1]$$

is an integer quantum number

Edge states are chiral, due to the TR violation introduced by the magnetic field

Edge states and Bulk-Edge correspondence

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Can edge states survive without magnetic field?

Edge states and Bulk-Edge correspondence

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$$C = S^1 \times [0, 1]$$

is an integer quantum number

Edge states are chiral, due to the TR violation introduced by the magnetic field

Can edge states survive without magnetic field?

Yes adding SPIN and having spin-orbit couplings

Time Reversal and Kramers degeneracy

$s = \frac{1}{2}$ spin systems

$$\Theta\psi = e^{i\pi S_y} \psi^*$$

$$\Theta^2 = -I$$

Kramers theorem:

For a time reversal invariant Hamiltonian all energy levels are double degenerated **at CP Kramers points**

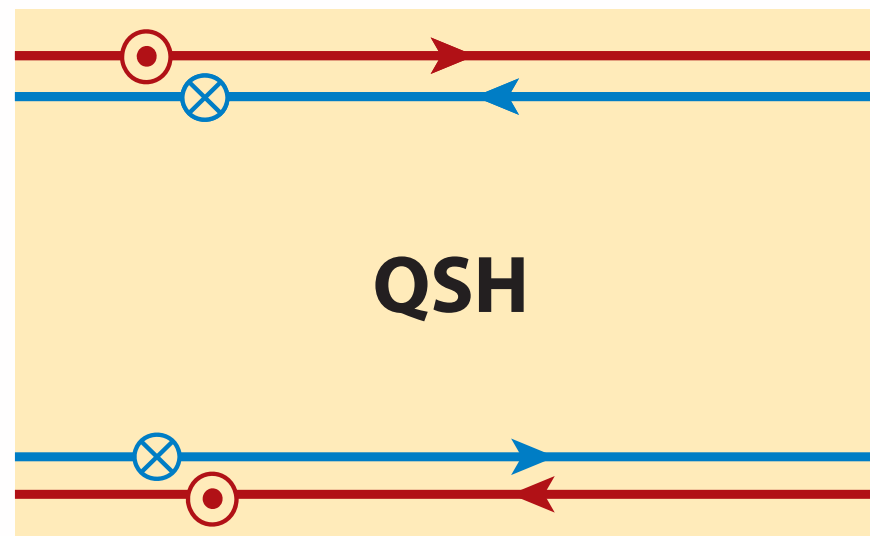
$$\Theta\psi = \lambda\psi, \quad \Theta^2\psi = |\lambda|^2\psi = -\psi$$

For a non-degenerate energy level ψ

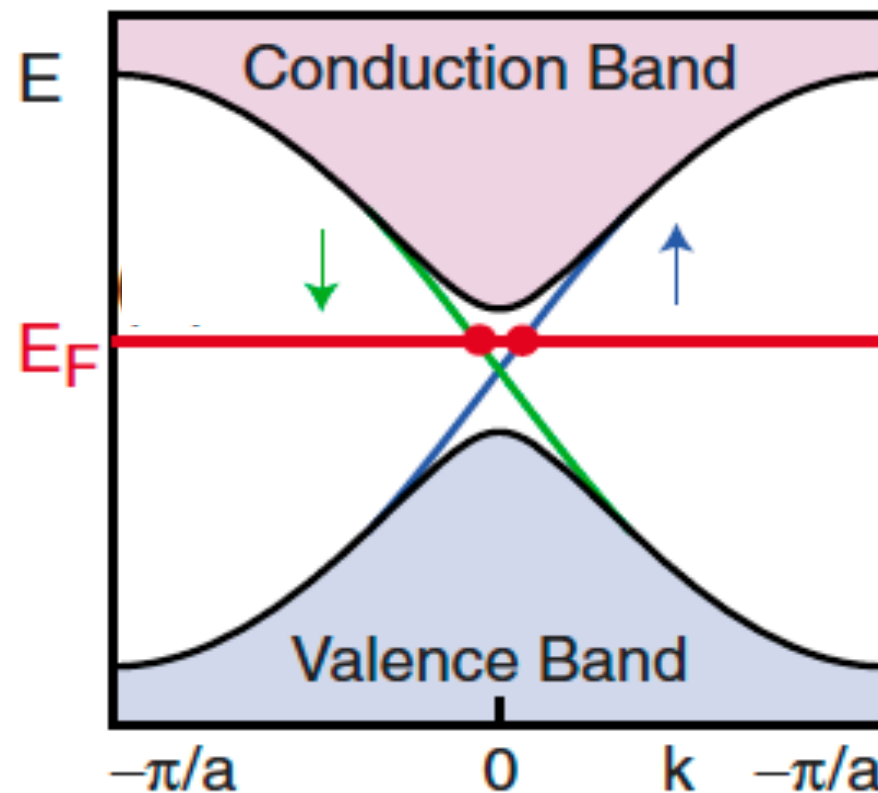
Nielsen-Ninomiya theorem: Lattice fermion doubling

Quantum Spin Hall

Two copies of Haldane model



[Topological Insulators]



[Kane-Mele]

[Bernevig-Zhang]

Hall
(1879)

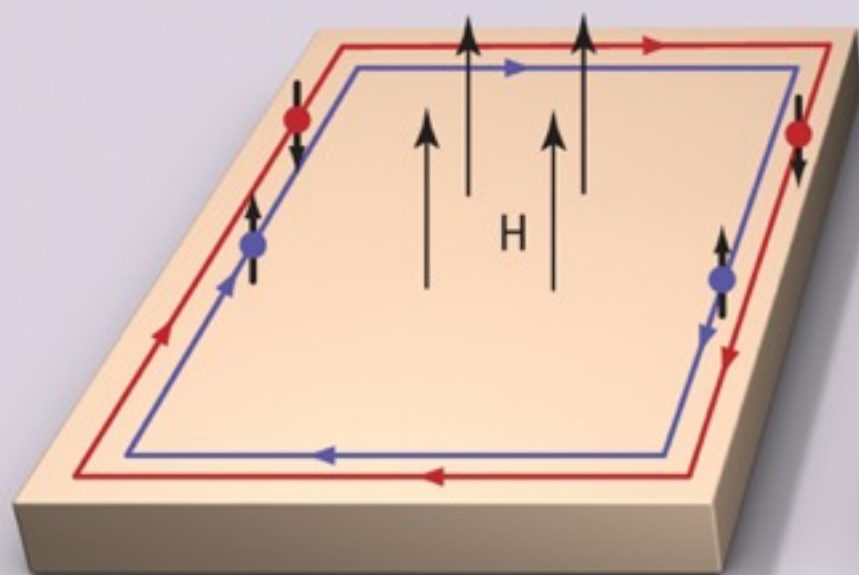
Spin Hall
(2004)

Anomalous Hall
(1881)

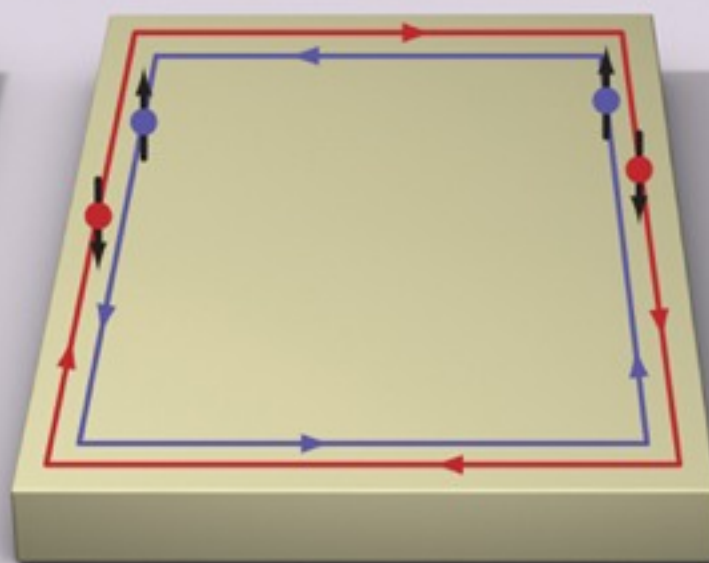
Quantum Hall
(1980)

Quantum spin Hall
(2007)

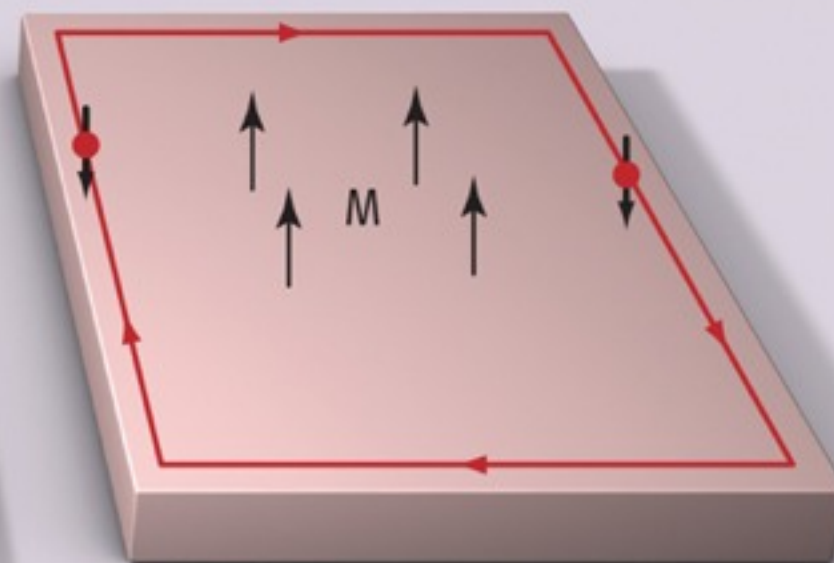
Quantum anomalous Hall
(2013)



Quantum Hall

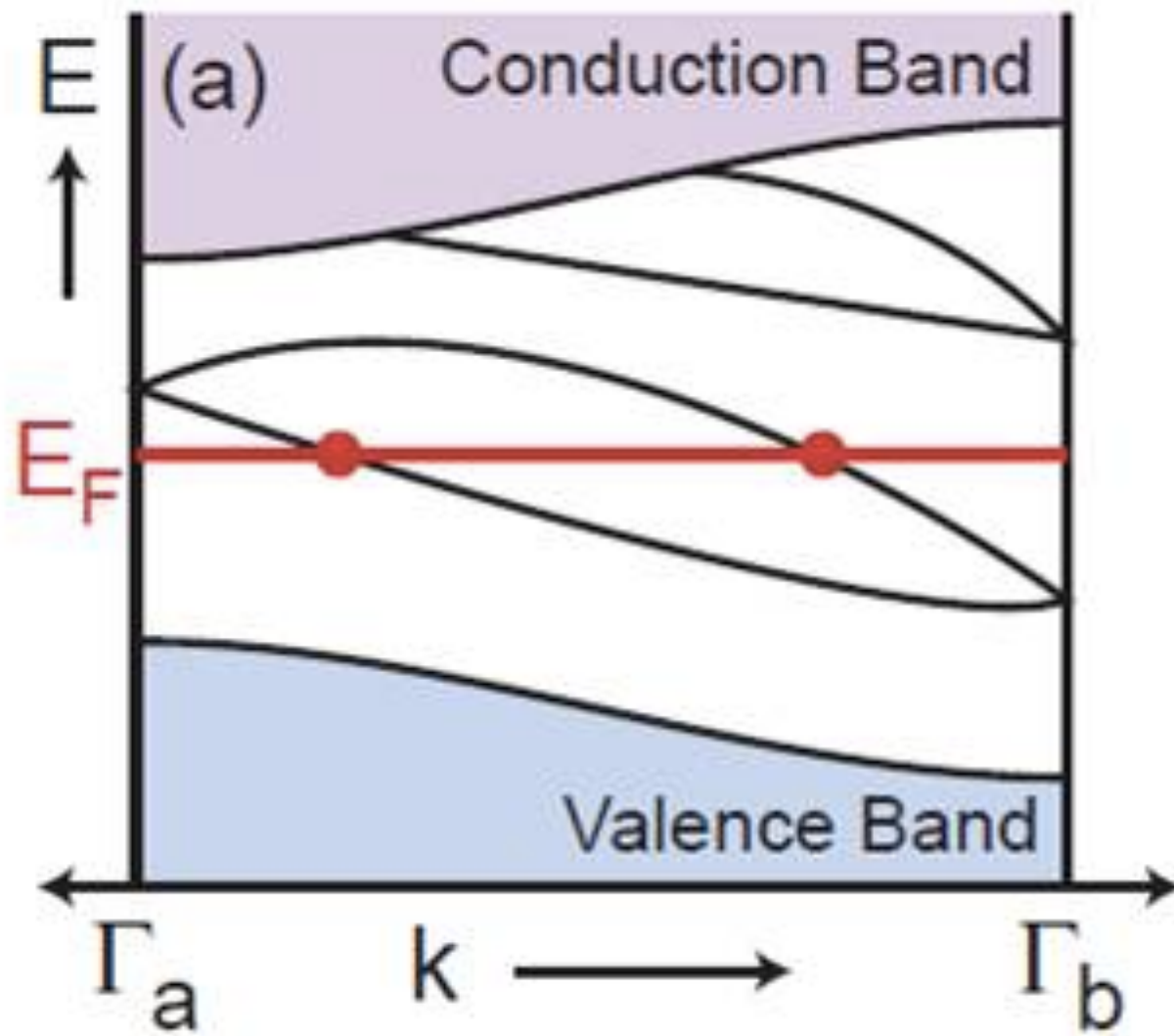


Quantum spin Hall

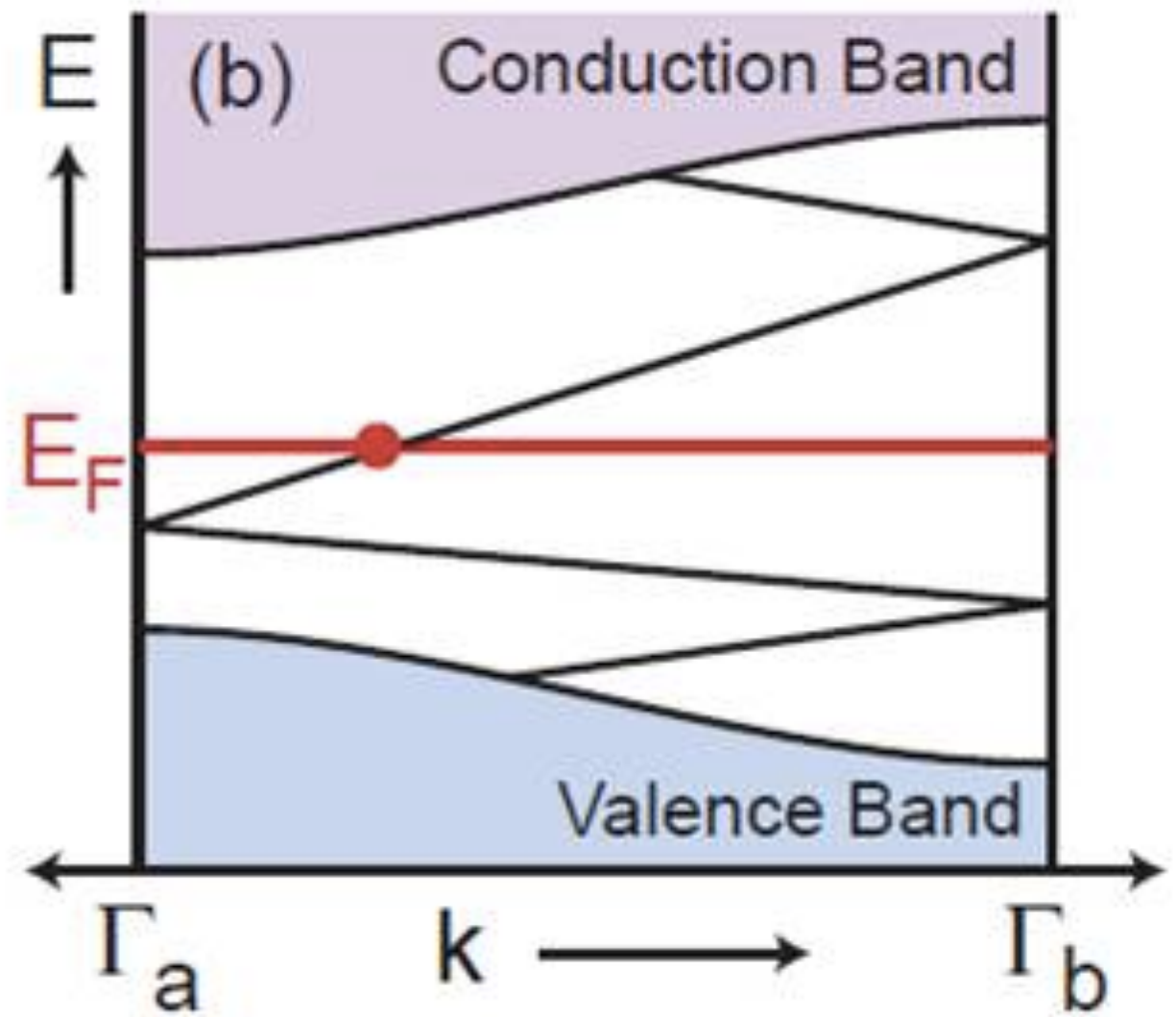


Quantum anomalous Hall

Topological Insulators

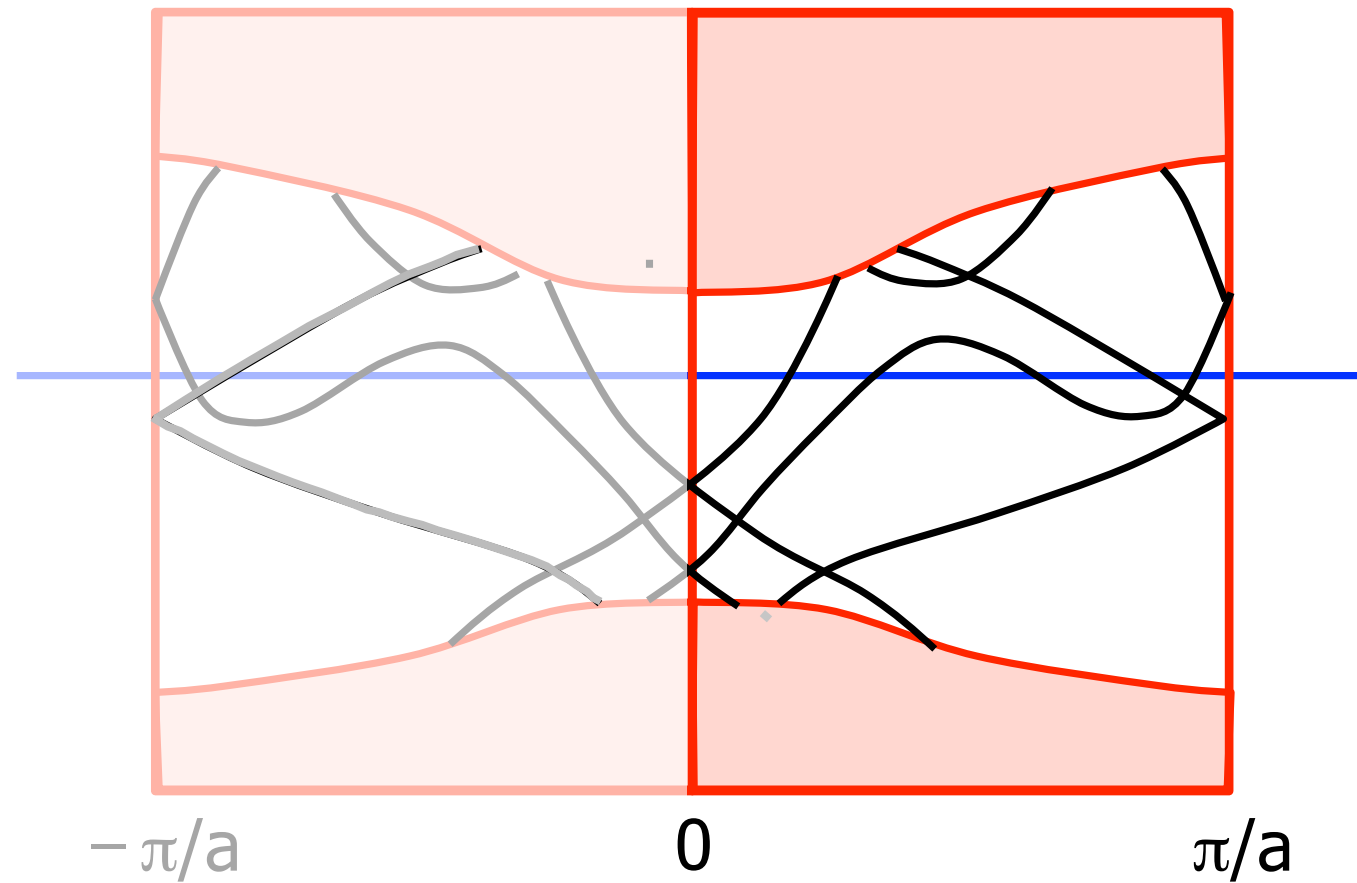


Normal Insulators



Topological Insulators

Kane-Mele Z_2 index



$$Z_2 = N_{\text{cross}} \pmod{2} = \text{Invariant}$$

[Fu-Kane]

\mathbb{Z}_2 Index

Time reversal matrix

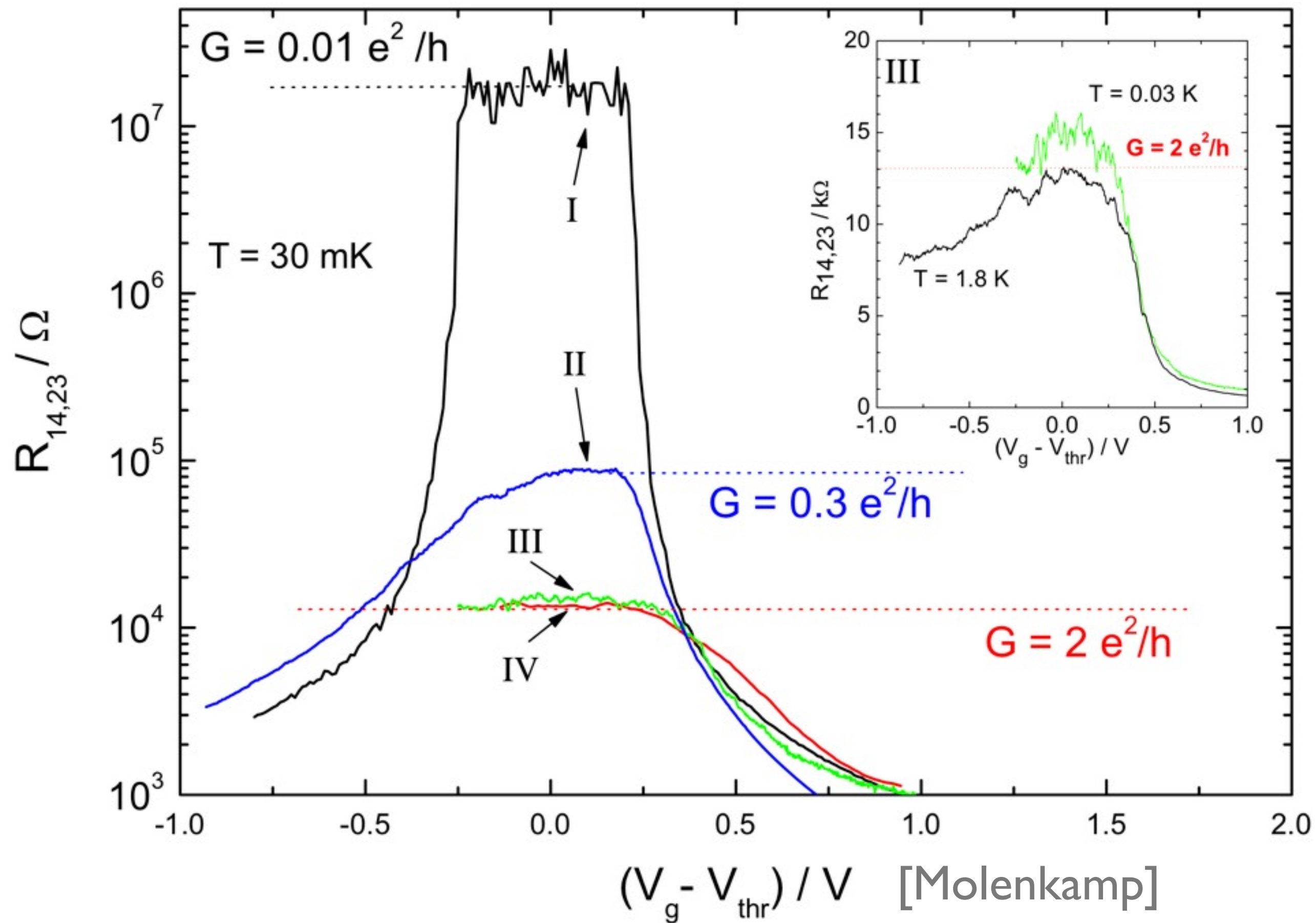
$$w_{mn}(k) = \langle u_m(k) | \Theta | u_n(-k) \rangle \quad |u_n(k)\rangle \text{ filled states}$$

$$w_{mn}(k) = -w_{nm}(-k)$$

For TR invariant k_a the matrix $w(k_a)$ is antisymmetric
 \mathbb{Z}_2 invariant ν is defined by

$$(-1)^\nu = \prod_a \frac{\text{Pf}(w(k_a))}{\det w(k_a)} = \pm 1$$

[Fu-Kane]



SUMMARY

- Zoo of new topological materials with amazing properties
- Essential ingredients: topology, discrete symmetries and boundaries
- Spectral band structures engineering
- Beyond Solid state physics systems: optical lattices, topological fluids, classical systems



Thanks

3D Topological Insulators

Four \mathbb{Z}_2 indices

$$\nu_0 \ \nu_1 \ \nu_2 \ \nu_3$$

$$\nu_0 = \frac{1}{4\pi} \int \epsilon^{ijk} \left(\mathcal{A}_i^a \partial_j \mathcal{A}_k^a + \frac{2}{3} f_{abc} \mathcal{A}_i^a \mathcal{A}_j^b \mathcal{A}_k^c \right)$$

Weak topological insulators $\nu_0 = 2n$

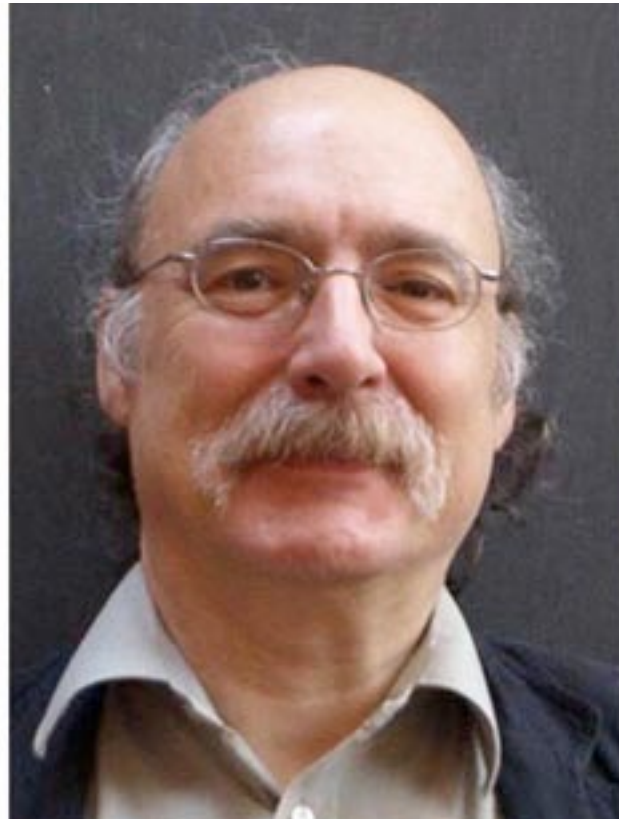
Strong topological insulators $\nu_0 = 2n + 1$

Non-trivial TR Bloch bundle

Topological Insulators



[Zhang]



[Haldane]



[Kane]

Weyl semimetals



**One shouldn't work on semiconductors,
that is a filthy mess; who knows whether
any semiconductors exist.**

Weyl semimetals



Hermann Weyl
1929

Weyl semimetals



Hermann Weyl
1929

basis vectors for a real representation of the space group of the crystal, and that the normal modes belonging to a representation which is irreducible in the field of real numbers, even though reducible in the complex field, must all have the same frequency.⁷ Thus mathematically the theory of normal modes and their frequencies

is just like the theory of electronic wave functions and their energies: frequency can be plotted as a function of wave vector, and sticking together of two or more of these frequency bands will occur at wave vectors \mathbf{k} where G^k has multidimensional representations or where case (b) or case (c), as defined above, occurs.

It is a pleasure for me to express my thanks to Professor E. Wigner, who suggested this problem.

⁷ Cf. E. Wigner, Gött. Nachr. (1930), p. 133.

Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING

Princeton University, Princeton, New Jersey

(Received June 16, 1937)

The circumstances are investigated under which two wave functions occurring in the Hartree or Fock solution for a crystal can have the same reduced wave vector and the same energy. It is found that coincidence of the energies of wave functions with the same symmetry properties, as well as those with different symmetries, is often to be expected. Some qualitative features are derived of the way in which energy varies with wave vector near wave vectors for which degeneracy occurs. All these results, like those of the preceding paper, should be applicable also to the frequency spectrum of the normal modes of vibration of a crystal.

Weyl semimetals



Hermann Weyl
1929

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Herring

Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

Hongming Weng,^{1,2,*} Chen Fang,³ Zhong Fang,^{1,2} B. Andrei Bernevig,⁴ and Xi Dai^{1,2}¹*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*²*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*³*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*⁴*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

(Received 12 January 2015; published 17 March 2015)

Based on first-principle calculations, we show that a family of nonmagnetic materials including TaAs, TaP, NbAs, and NbP are Weyl semimetals (WSM) without inversion centers. We find twelve pairs of Weyl points in the whole Brillouin zone (BZ) for each of them. In the absence of spin-orbit coupling (SOC), band inversions in mirror-invariant planes lead to gapless nodal rings in the energy-momentum dispersion. The strong SOC in these materials then opens full gaps in the mirror planes, generating nonzero mirror Chern numbers and Weyl points off the mirror planes. The resulting surface-state Fermi arc structures on both (001) and (100) surfaces are also obtained, and they show interesting shapes, pointing to fascinating flavorounds for future experimental studies.

tantalum arsenide (TaAs). Using the combination of the vacuum ultraviolet (low-photon-energy) and soft x-ray (SX) angle-resolved photoemission spectroscopy (ARPES), we systematically and differentially study the surface and bulk electronic structure of TaAs. Our ultraviolet (low-photon-energy) ARPES measurements, which are highly surface sensitive, demonstrate the existence of the Fermi arc surface states, consistent with our band calculations presented here. Moreover, our SX-ARPES measurements, which are reasonably bulk sensitive, reveal the 3D linearly dispersive bulk Weyl cones and Weyl nodes. Furthermore, by combining the low-photon-energy and SX-ARPES data, we show that the locations of the projected bulk Weyl nodes correspond to the terminations of the Fermi arcs within our experimental resolution. These systematic measurements demonstrate TaAs as a Weyl semimetal.

The material system and theoretical considerations

Tantalum arsenide is a semimetallic material that crystallizes in a body-centered tetragonal

2015

TOPOLOGICAL MATTER

Discovery of a Weyl fermion semimetal and topological Fermi arcs

Su-Yang Xu,^{1,2,*} Ilya Belopolski,^{1,*} Nasser Alidoust,^{1,2,*} Madhab Neupane,^{1,3,*} Guang Bian,¹ Chenglong Zhang,⁴ Raman Sankar,⁵ Guoqing Chang,^{6,7} Zhujun Yuan,⁴ Chi-Cheng Lee,^{6,7} Shin-Ming Huang,^{6,7} Hao Zheng,¹ Jie Ma,⁸ Daniel S. Sanchez,¹ BaoKai Wang,^{6,7,9} Arun Bansil,⁹ Fangcheng Chou,⁵ Pavel P. Shibayev,^{1,10} Hsin Lin,^{6,7} Shuang Jia,^{4,11} M. Zahid Hasan^{1,2,†}

A Weyl semimetal is a new state of matter that hosts Weyl fermions as emergent quasiparticles and admits a topological classification that protects Fermi arc surface states on the boundary of a bulk sample. This unusual electronic structure has deep analogies with particle physics and leads to unique topological properties. We report the experimental discovery of a Weyl semimetal, tantalum arsenide (TaAs). Using photoemission spectroscopy, we directly observe Fermi arcs on the surface, as well as the Weyl fermion cones and Weyl nodes in the bulk of TaAs single crystals. We find that Fermi arcs terminate on the Weyl fermion nodes, consistent with their topological character. Our work opens the field for the experimental study of Weyl fermions in physics and materials science.

ARTICLES

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nature
photonics

Weyl points and line nodes in gyroid photonic crystals

Ling Lu*, Liang Fu, John D. Joannopoulos and Marin Soljačić

Weyl points and line nodes are three-dimensional linear point and line degeneracies between two bands. In contrast to two-dimensional Dirac points, which are their lower-dimensional analogues, Weyl points are stable in momentum space and the associated surface states are predicted to be topologically non-trivial. However, Weyl points are yet to be discovered in nature. Here, we report photonic crystals based on double-gyroid structures, exhibiting frequency-isolated Weyl points with complete phase diagrams by breaking the parity and time-reversal symmetries. Gapless surface dispersions associated with non-zero Chern numbers are demonstrated. Line nodes are also found in similar geometries, the associated surface states forming flat dispersion bands. Our results are based on realistic *ab initio* calculations with true predictive power and should be readily realizable experimentally from microwave to optical frequencies.

Nielsen-Ninomiya theorem II

Chiral fermions cannot be regularized on a lattice

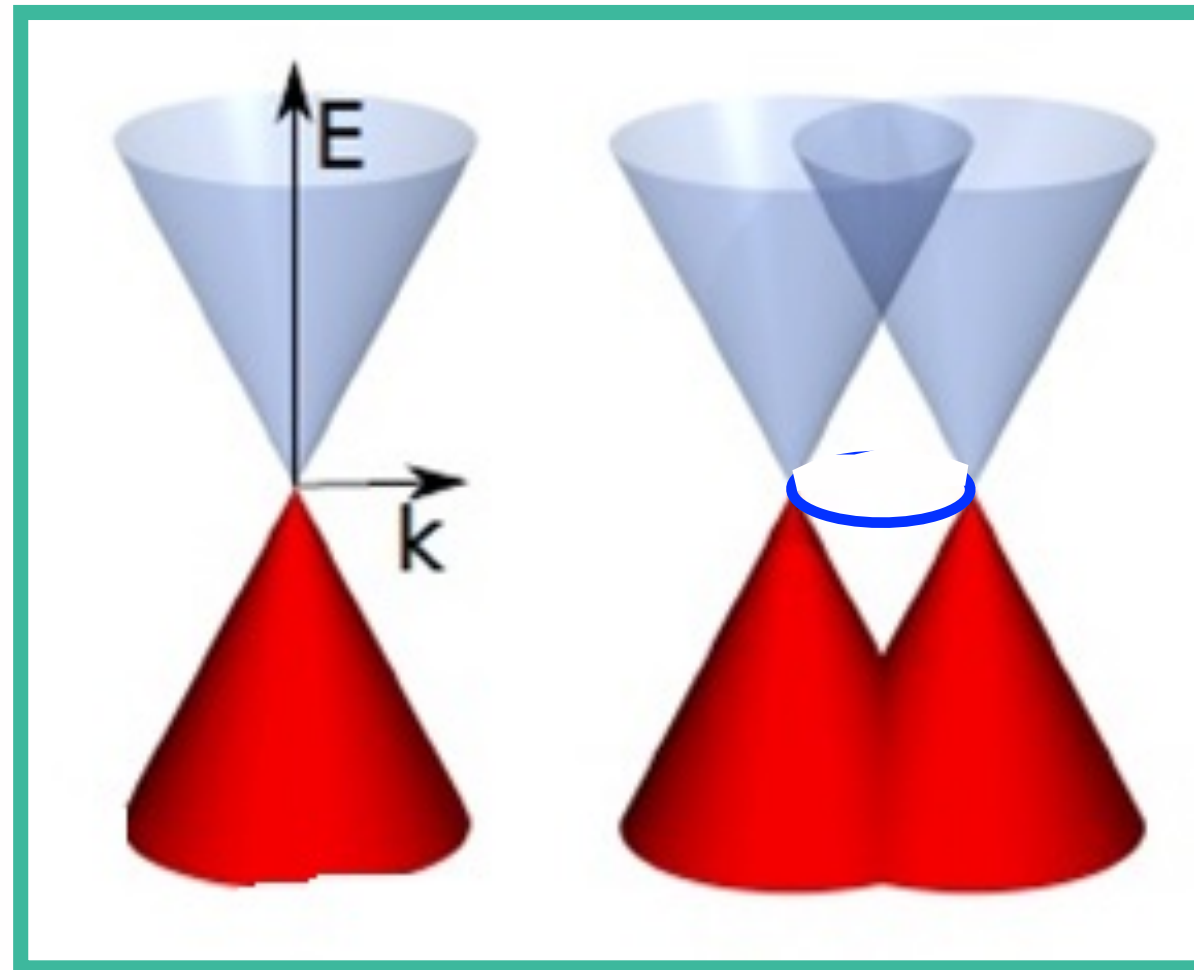
Axial anomaly:

flow of charge from left to right Weyl points

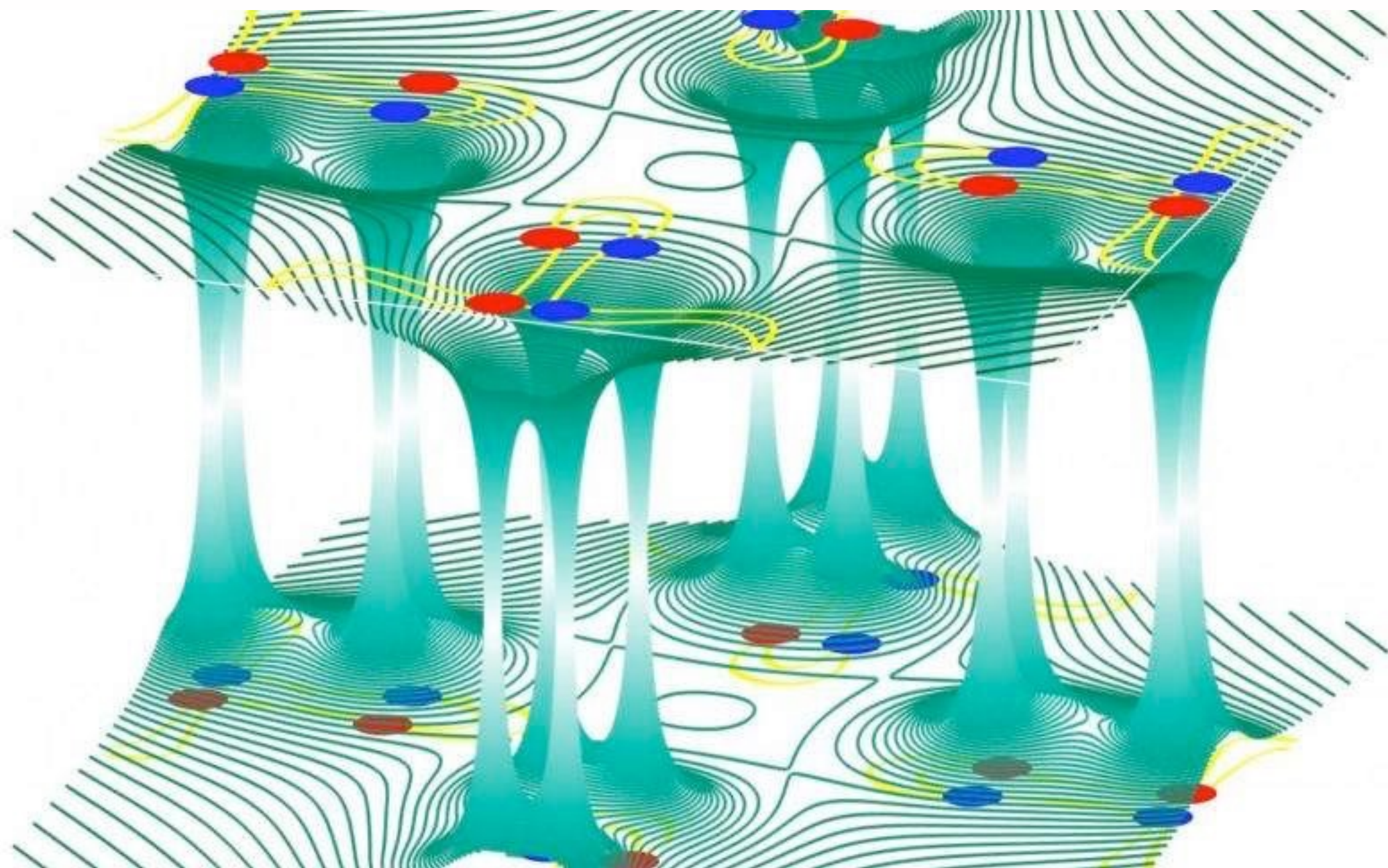
$$H = \alpha \cdot \nabla + m\gamma_0 + \gamma_5 b \cdot \alpha + \mu\gamma_5$$

TR breaking + Parity breaking symmetries

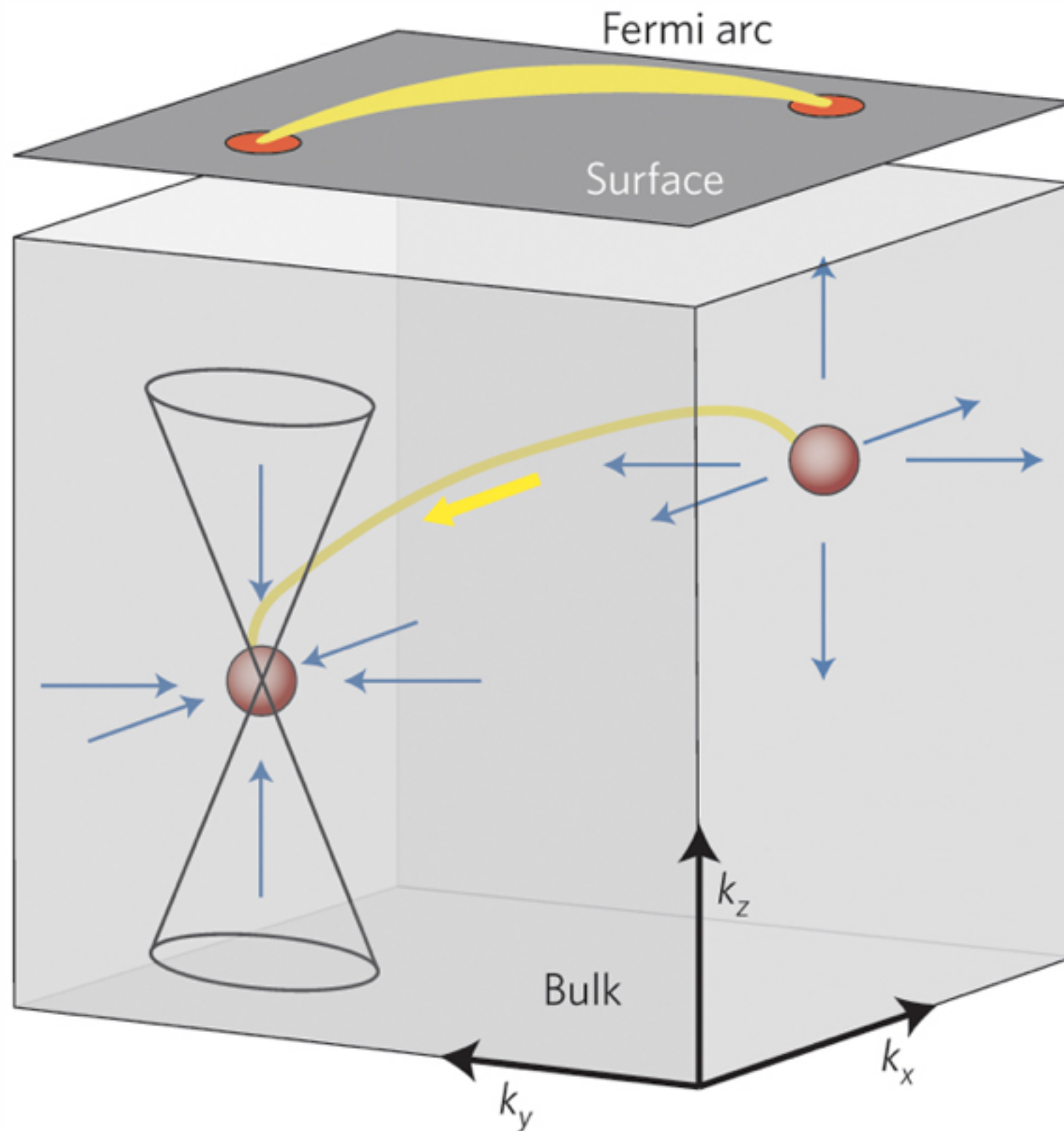
Dirac points split into two Weyl points with opposite chiralities



Fermi Arc

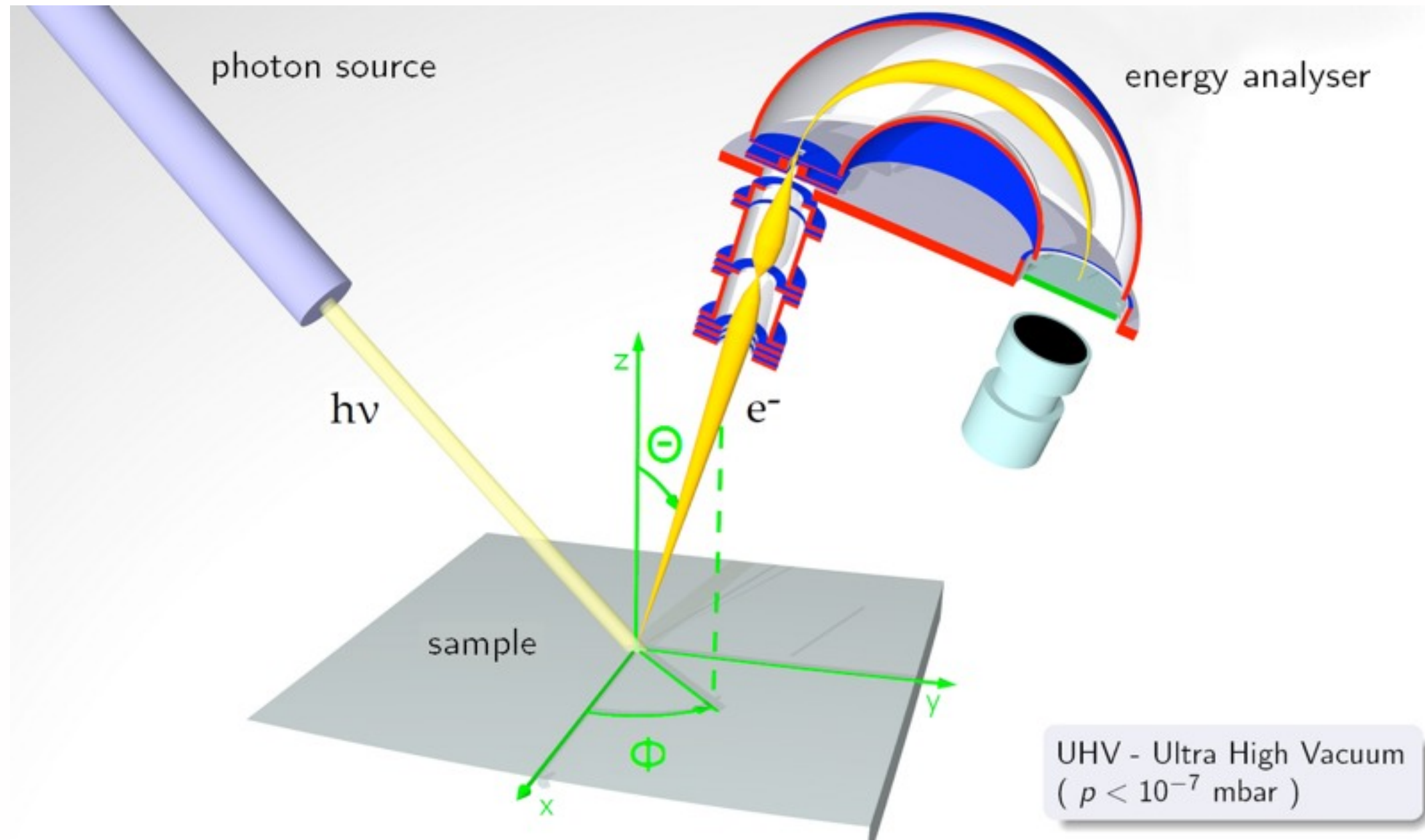


Weyl semimetals (2015)

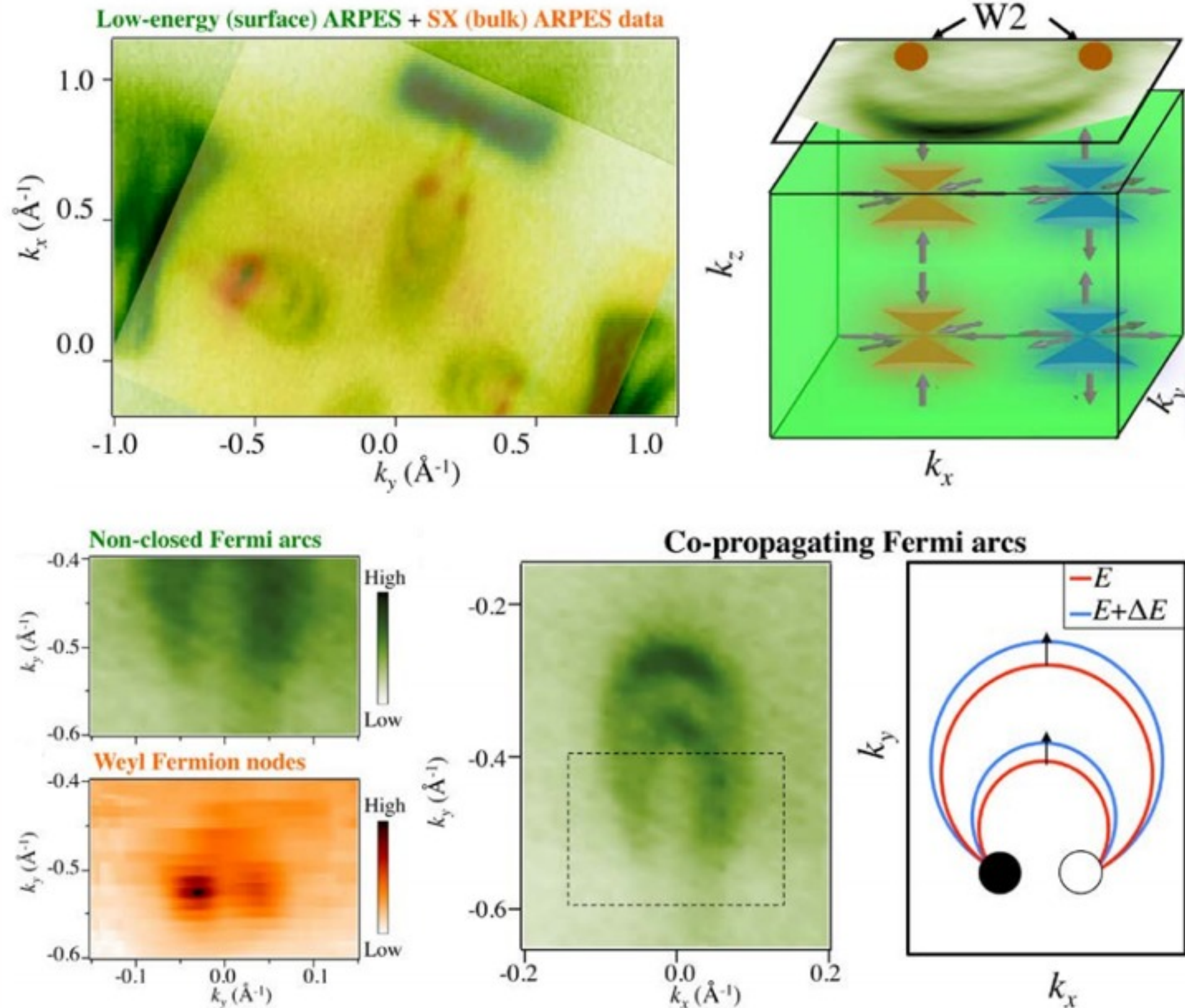


ARPES

Angle-resolved photoemission spectroscopy



Weyl Fermion nodes and Topological Fermi arcs



[Hassan group]

SUMMARY

- Topological matter is a brand new area of CM developing very fast
- Tools of HEP are fundamental in the theory
- Topological insulators do have applications for spintronics and quantum computation
- Weyl semimetals have interesting conducting properties which are being explored for apps.

BACKUP

TOPOLOGICAL MATTER

- New conducting effects in topological materials
- New band analysis unveils a hidden topological structure
- Topological insulators with edge currents
- Dirac semimetal on edges of TPI
- Topological superconductors. Majorana Fermions
- Topological Semimetals. Weyl Fermions. Fermi Arcs
- Semimetals with nodal points

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- Stability provided by topological robustness

TOPOLOGICAL MATTER

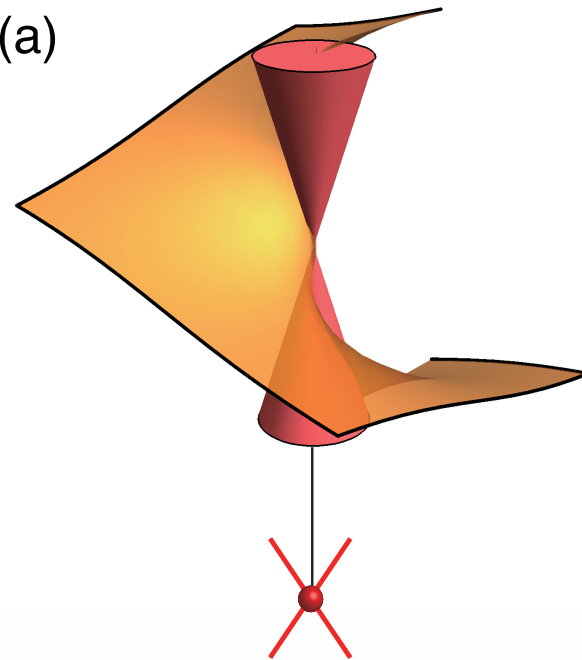
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- Applications to spintronic and quantum computation

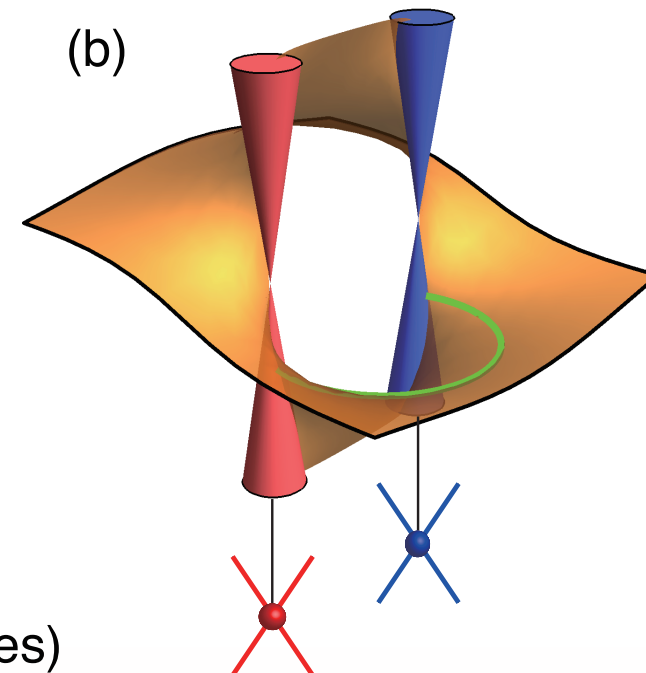
Helicoid Riemann surface state

(a)



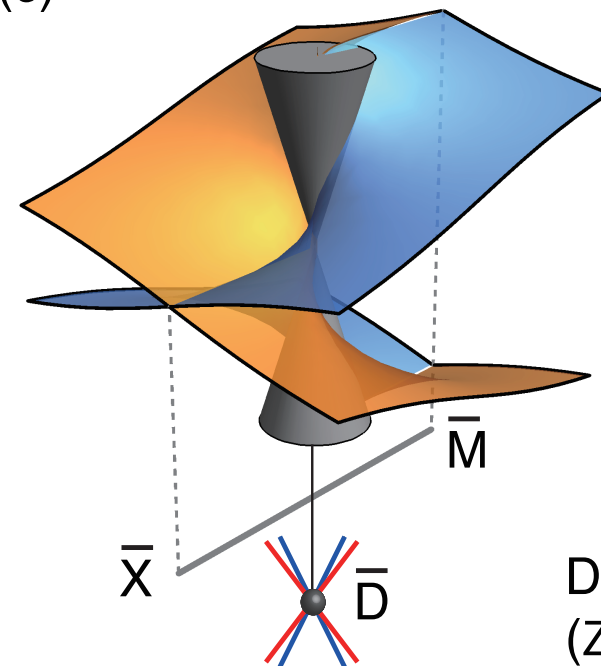
Weyl points
(Berry charges)

(b)



Double-helicoid Riemann surface state

(c)



Dirac points
(Z_2 monopoles)

(d)

