Topological Insulators and Superconductors

Charles L. Kane, University of Pennsylvania

I. Topological Insulators and Band Theory

Unifying theme: bulk – boundary correspondence

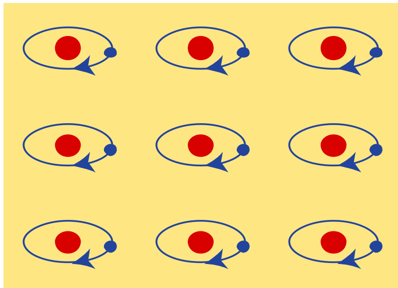
- Integer Quantum Hall Effect
- 2D Quantum Spin Hall Insulator
- 3D Topological Insulator
- Topological Superconductivity, Majorana fermions

II. Summary and Outlook

- What we have accomplished
- Challenges for the Future

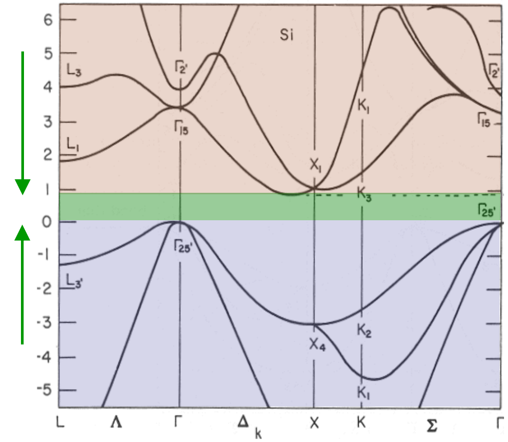
Thanks to Gene Mele, Liang Fu, Jeffrey Teo

The Insulating State

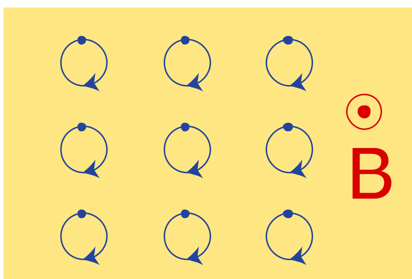


e.g. Silicon

$E_g \sim 1$ eV

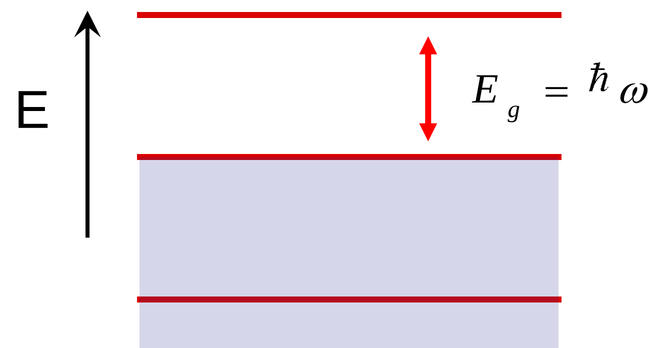


The Integer Quantum Hall State



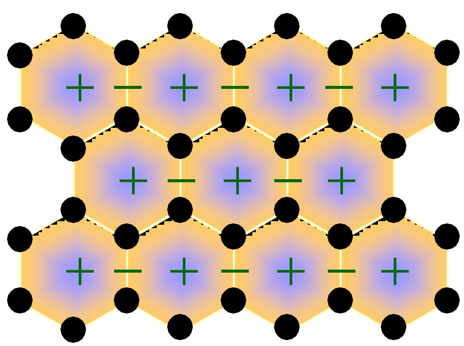
2D Cyclotron Motion,
Landau Levels

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



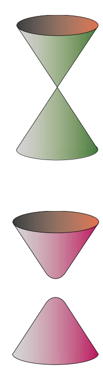
IQHE with zero net magnetic field

Graphene with a periodic magnetic field B(r) (Haldane PRL 1988)

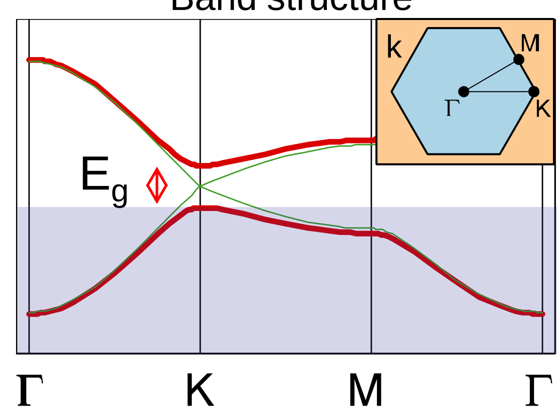


B(r) = 0
Zero gap,
Dirac point

B(r) ≠ 0
Energy gap
$\sigma_{xy} = e^2/h$



Band structure



Topological Band Theory

The distinction between a conventional insulator and the quantum Hall state is a **topological** property of the band structure

$H(\mathbf{k})$: Brillouin zone (= torus T^2) $\mapsto$ Bloch Hamiltonans with energy gap

The set of N occupied Bloch wavefunctions $\{|u_i(\mathbf{k})\rangle\}_{i=1}^{N}$ defines a *U(N)* vector bundle over the Brillouin zone torus.

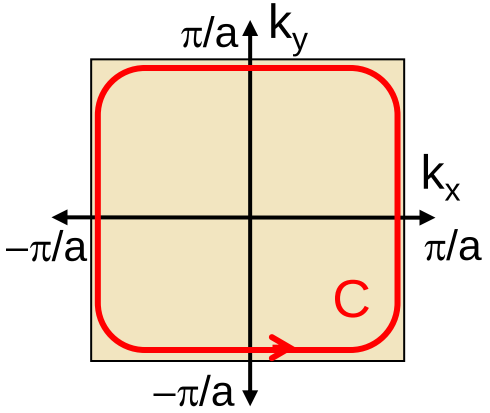
Classified by the first Chern number (or TKNN invariant) (Thouless et al, 1984)

Closely related to theory of electric polarization

Berry connection $\mathbf{A}(\mathbf{k}) = -i\sum_{i=1}^{N}\langle u_i(\mathbf{k})|\nabla_{\mathbf{k}}|u_i(\mathbf{k})\rangle$

Berry curvature $\mathbf{F}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}(\mathbf{k})$

1st Chern number $n = \frac{1}{2\pi}\oint_C \mathbf{A}\cdot d\mathbf{k} = \frac{1}{2\pi}\int_{T^2} \mathbf{F}\, d^2\mathbf{k} \in \mathbb{Z}$



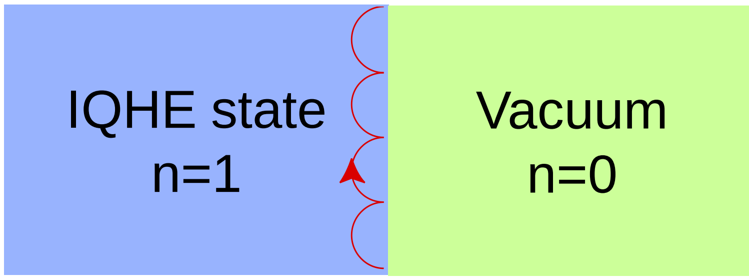
Insulator : $n = 0$

IQHE state : $\sigma_{xy} = n\, e^2/h$

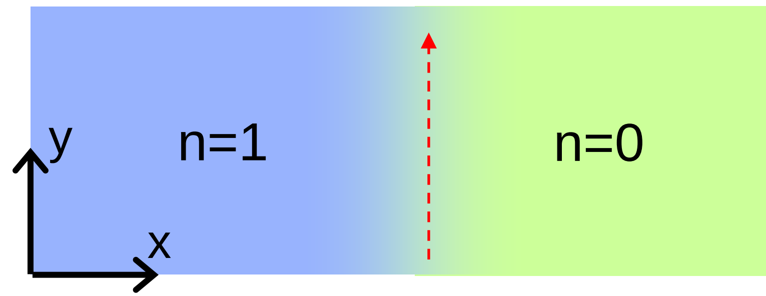
The TKNN invariant can only change at a phase transition where the energy gap goes to zero

Edge States

Gapless states must exist at the interface between different topological phases

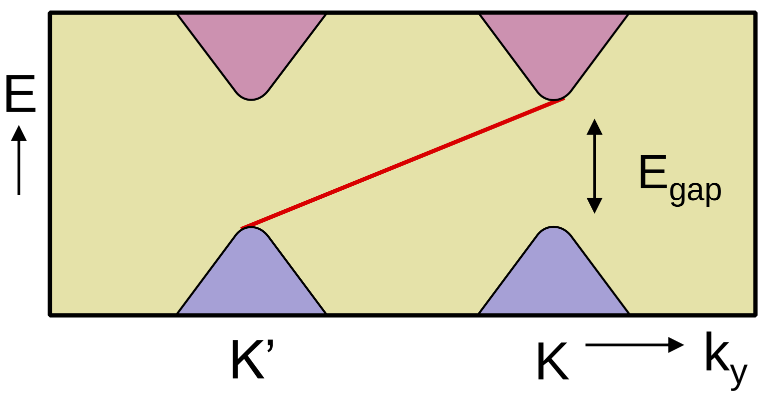


Edge states ~ skipping orbits



Smooth transition : band inversion

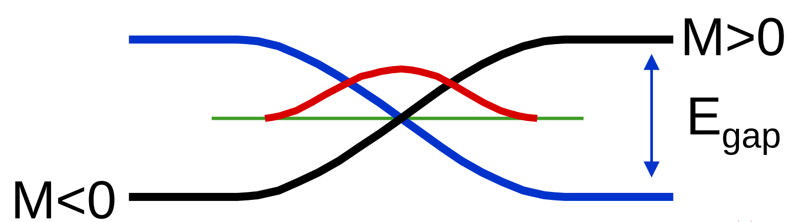
Gapless Chiral Fermions : E = v k



Haldane Model

Dirac Equation :

$$H = -iv\left(\sigma_x \partial_x + \sigma_y \partial_y\right) + M(x)\sigma_z$$



Domain wall bound state $\psi_0 \sim e^{ik_y y} e^{-\int^{|x|} M(x')dx'/v}$

Jackiw, Rebbi (1976)
Su, Schrieffer, Heeger (1980)

Bulk – Boundary Correspondence : Δn = # Chiral Edge Modes

Time Reversal Invariant Z_2 Topological Insulator

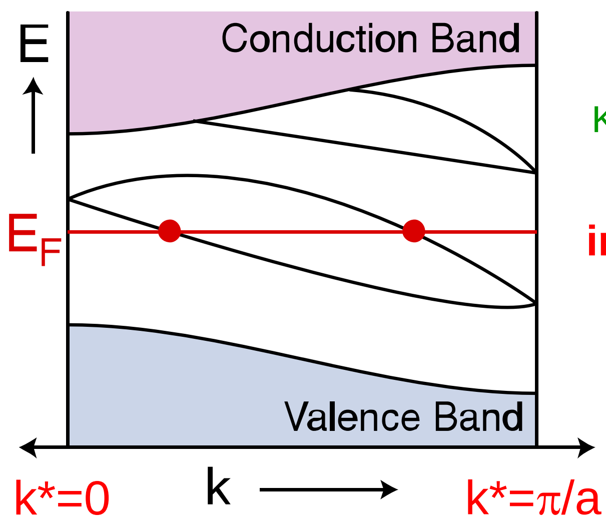
Time Reversal Symmetry : $\Theta H(\mathbf{k})\Theta^{-1} = H(-\mathbf{k})$ $\Theta\psi = i\sigma^y\psi^*$

Kramers' Theorem : $\Theta^2 = -1$ $\Rightarrow$ All states doubly degenerate

Z_2 topological invariant (ν = 0,1) for 2D T-invariant band structures

Understand via Bulk-Boundary correspondence : Edge States for 0<k<π/a

ν=0 : Conventional Insulator



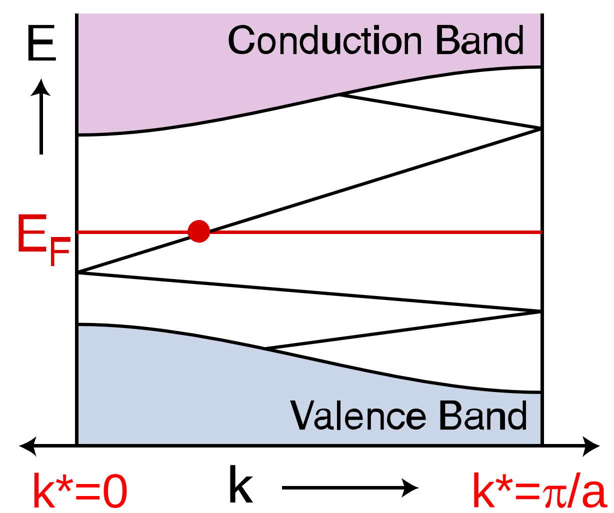
Even number of bands crossing Fermi energy

Kramers degenerate at

time reversal invariant momenta

k* = –k* + G

ν=1 : Topological Insulator



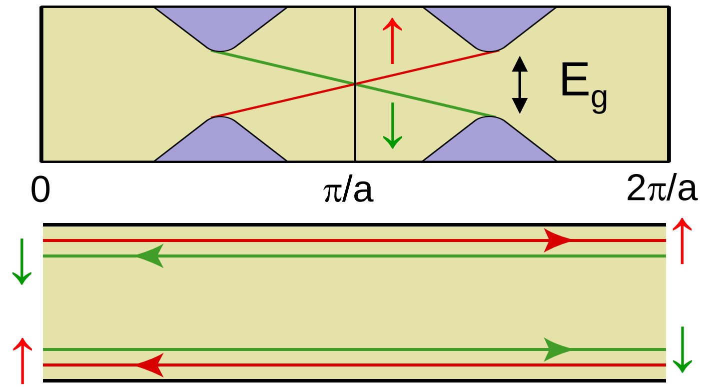
Odd number of bands crossing Fermi energy

2D Quantum Spin Hall Insulator

I. Graphene

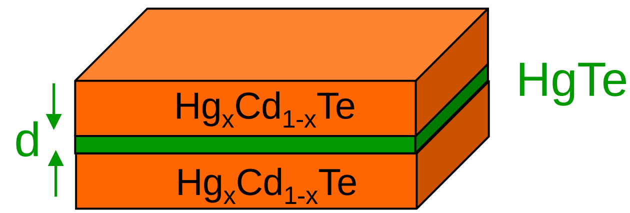
Kane, Mele PRL '05

- Intrinsic spin orbit interaction
  $\Rightarrow$ small (~10mK-1K) band gap
- S_z conserved : "| Haldane model $|^2$"
- Edge states : $G = 2\ e^2/h$

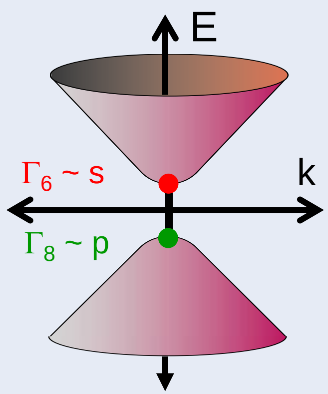


II. HgCdTe quantum wells

Theory: Bernevig, Hughes and Zhang, Science '06
Experiement: Konig et al. Science '07

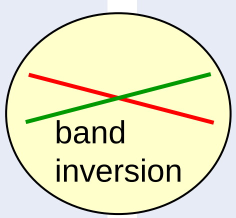


d < 6.3 nm : Normal band order

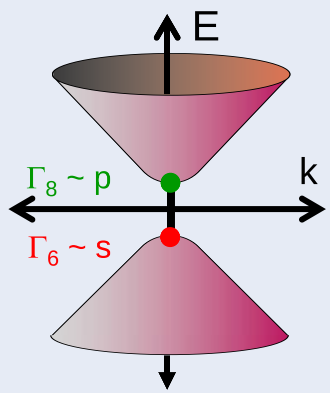


Conventional Insulator

$$\prod \xi_{2n}(\Lambda_a) = +1$$



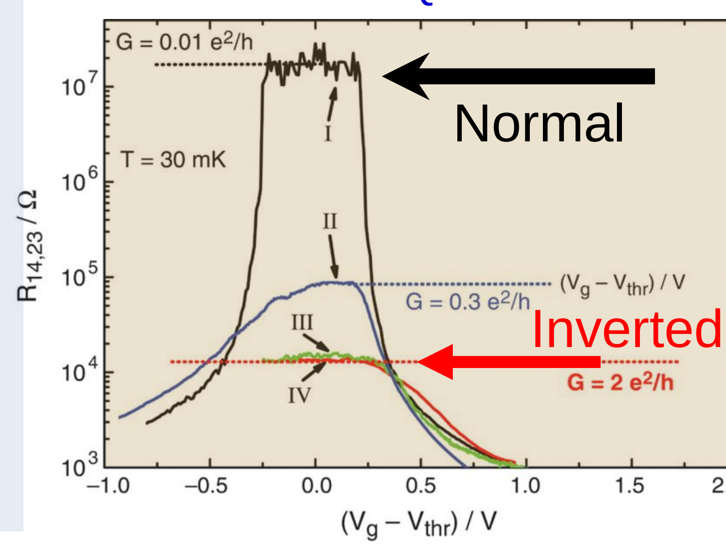
d > 6.3 nm : Inverted band order



QSH Insulator

$$\prod \xi_{2n}(\Lambda_a) = -1$$

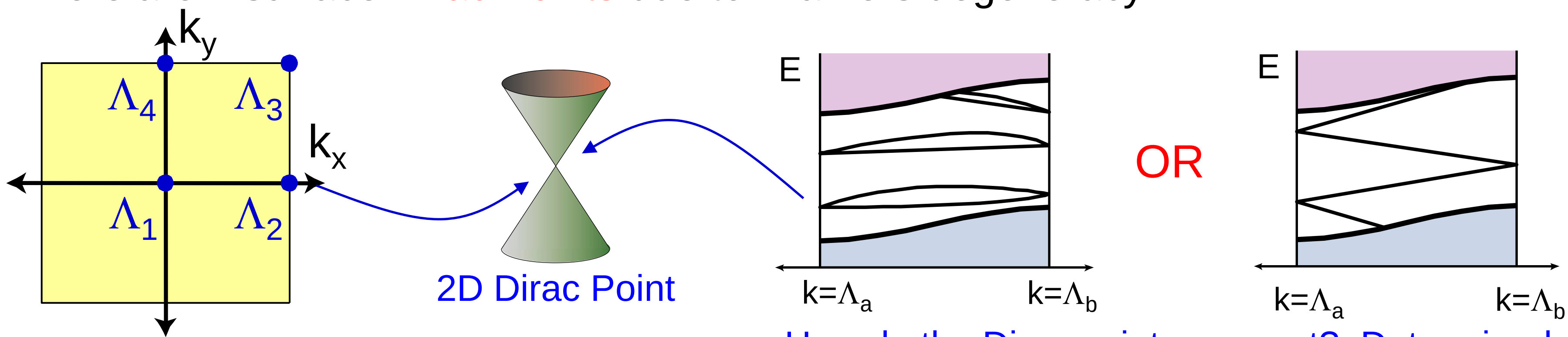
G ~ $2e^2/h$ in QSHI



3D Topological Insulators

Moore & Balents PRB 07
Roy, cond-mat 06
Fu, Kane & Mele PRL 07

There are 4 surface Dirac Points due to Kramers degeneracy



Surface Brillouin Zone

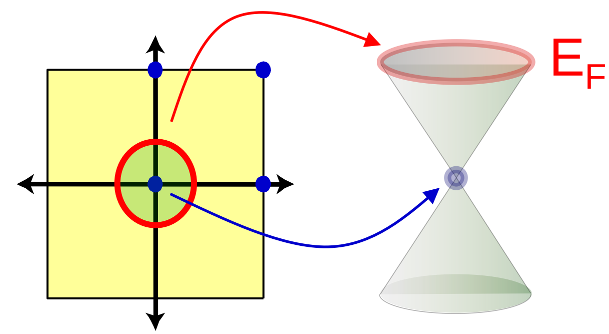
How do the Dirac points connect? Determined by 4 bulk Z_2 topological invariants $\nu_0 ; (\nu_1\nu_2\nu_3)$

ν_0 = 1 : Strong Topological Insulator

Fermi circle encloses odd number of Dirac points

Topological Metal :

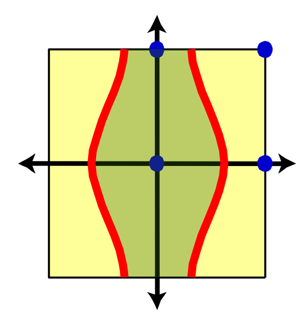
- 1/4 graphene
- Robust to disorder: impossible to localize



ν_0 = 0 : Weak Topological Insulator

Fermi circle encloses even number of Dirac points

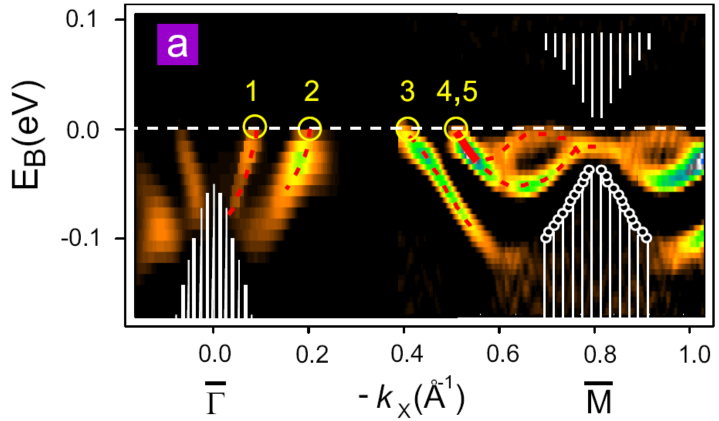
Related to layered 2D QSHI



$Bi_{1-x}Sb_x$

Theory: Predict $Bi_{1-x}Sb_x$ is a topological insulator by exploiting inversion symmetry of pure Bi, Sb (Fu,Kane PRL'07)

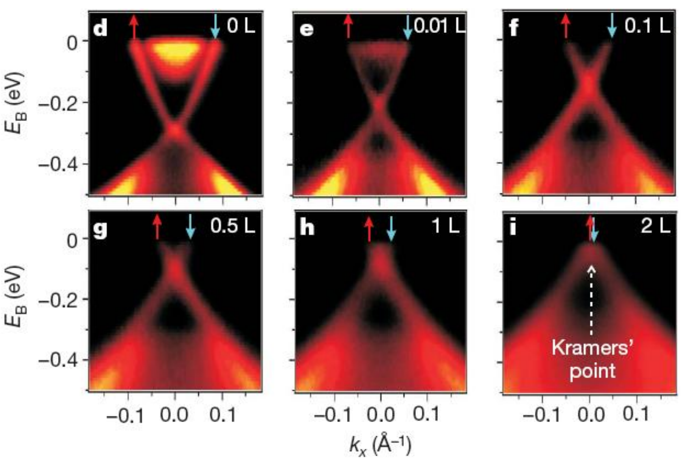
Experiment: ARPES (Hsieh et al. Nature '08)



- $Bi_{1-x}Sb_x$ is a Strong Topological Insulator $\nu_0;(\nu_1,\nu_2,\nu_3) = 1;(111)$
- 5 surface state bands cross E_F between Γ and M

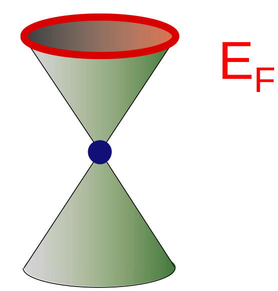
Bi_2Se_3

ARPES Experiment : Y. Xia et al., Nature Phys. (2009).
Band Theory : H. Zhang et. al, Nature Phys. (2009).



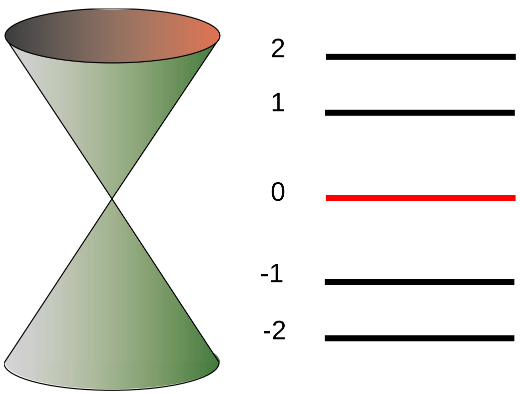
Control E_F on surface by exposing to NO_2

- $\nu_0;(\nu_1,\nu_2,\nu_3) = 1;(000)$: Band inversion at Γ
- Energy gap: $\Delta \sim .3$ eV : A room temperature topological insulator
- Simple surface state structure : Similar to graphene, except only a single Dirac point

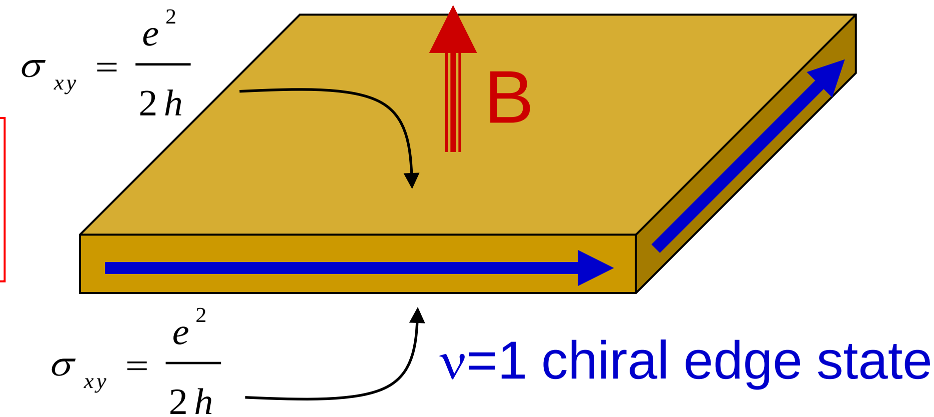


Surface Quantum Hall Effect

Orbital QHE : E=0 Landau Level for Dirac fermions. "Fractional" IQHE



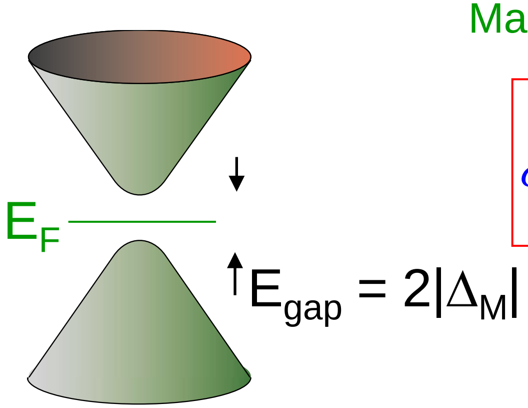
$$\sigma_{xy} = \frac{e^2}{h}\left(n + \frac{1}{2}\right)$$



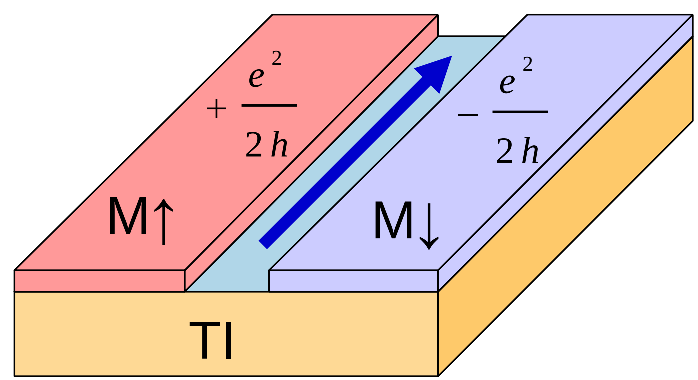
Anomalous QHE : Induce a surface gap by depositing magnetic material

$$H_0 = \psi^\dagger(-iv\vec{\sigma}\cdot\vec{\nabla} - \mu + \Delta_M \sigma_z)\psi$$

Mass due to Exchange field



$$\sigma_{xy} = \mathrm{sgn}(\Delta_M)\frac{e^2}{2h}$$

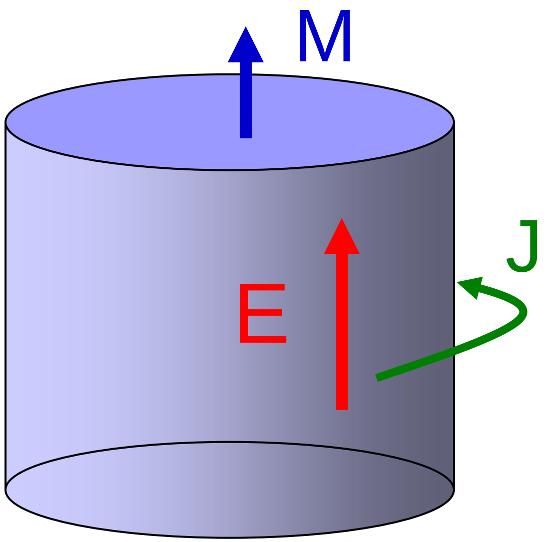


Chiral Edge State at Domain Wall : $\Delta_M \leftrightarrow -\Delta_M$

Topological Magnetoelectric Effect

Qi, Hughes, Zhang ’08; Essin, Moore, Vanderbilt ‘09

Consider a solid cylinder of TI with a magnetically gapped surface



$$J = \sigma_{xy} E = \frac{e^2}{h}\left(n + \frac{1}{2}\right) E = M$$

Magnetoelectric Polarizability

$$M = \alpha E \qquad \alpha = \frac{e^2}{h}\left(n + \frac{1}{2}\right)$$

topological “θ term”

$$\Delta L = \alpha \mathbf{E} \cdot \mathbf{B}$$

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

TR sym.: $\theta = 0$ or π mod 2π

The fractional part of the magnetoelectric polarizability is determined by the bulk, and independent of the surface (provided there is a gap)
Analogous to the electric polarization, P, in 1D.

	ΔL	formula	“uncertainty quantum”	
d=1 : Polarization P	$P \cdot \mathbf{E}$	$\frac{e}{2\pi}\int_{BZ} \mathrm{Tr}[\mathbf{A}]$	e	(extra end electron)
d=3 : Magnetoelectric poliarizability α	$\alpha \mathbf{E} \cdot \mathbf{B}$	$\frac{e^2}{4\pi^2 h}\int_{BZ} \mathrm{Tr}[\mathbf{A} \wedge d\mathbf{A} + \frac{2}{3}\mathbf{A} \wedge \mathbf{A} \wedge \mathbf{A}]$	e^2/h	(extra surface quantum Hall layer)

Topological Superconductivity

BCS mean field theory : $\Psi^\dagger \Psi \Psi^\dagger \Psi \quad \Rightarrow \quad \langle \Psi^\dagger \Psi^\dagger \rangle \Psi \Psi = \Delta^* \Psi \Psi$

$$H = \frac{1}{2} \sum_{\mathbf{k}} \begin{pmatrix} \Psi^\dagger & \Psi \end{pmatrix} H_{BdG} \begin{pmatrix} \Psi \\ \Psi^\dagger \end{pmatrix}$$

Bogoliubov de Gennes Hamiltonian

$$H_{BdG} = \begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0 \end{pmatrix}$$

Intrinsic anti-unitary particle – hole symmetry

$$\Xi H_{BdG} \Xi^{-1} = -H_{BdG}$$

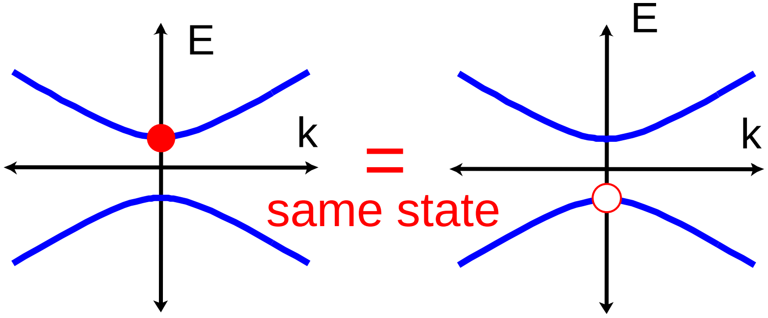
$$\Xi \varphi = \tau_x \varphi^*$$

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\Xi^2 = +1$$

Particle – hole redundancy

$$\varphi_{-E} = \Xi \varphi_E \quad \Rightarrow \quad \gamma_E^\dagger = \gamma_{-E}$$

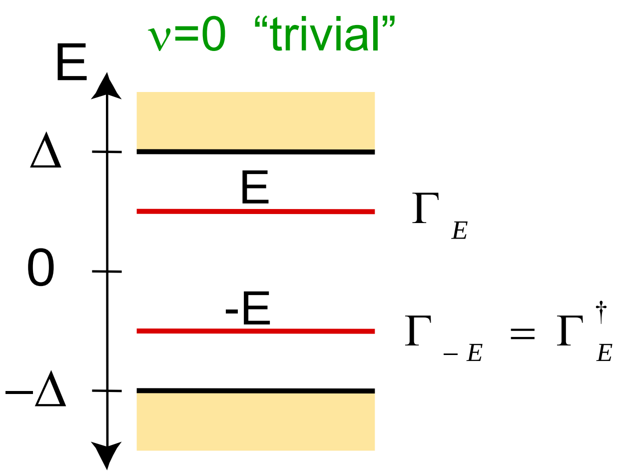


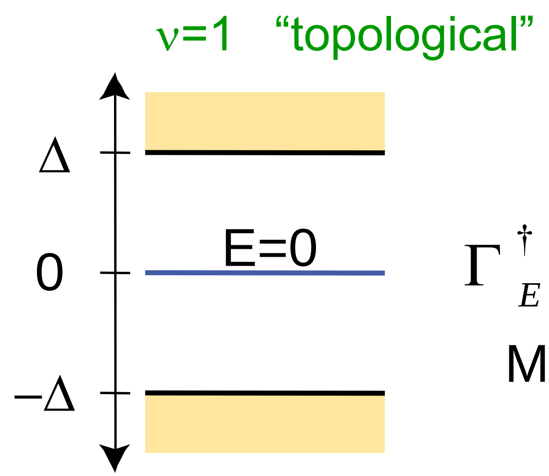
Bloch - BdG Hamiltonians satisfy $\Xi H_{BdG}(\mathbf{k}) \Xi^{-1} = -H_{BdG}(-\mathbf{k})$

Topological classification problem similar to time reversal symmetry

1D Z_2 Topological Superconductor : ν = 0,1 (Kitaev, 2000)

Bulk-Boundary correspondence : Discrete end state spectrum





Zero mode

$$\Gamma_{E=0}^\dagger = \Gamma_{E=0} \equiv \gamma$$

Majorana fermion bound state

Majorana Fermion : Particle = Antiparticle $\gamma = \gamma^\dagger$

Real part of a Dirac fermion :

$$\begin{cases} \gamma_1 = \Psi + \Psi^\dagger & ; \quad \Psi = \gamma_1 + i\gamma_2 \\ \gamma_2 = -i(\Psi - \Psi^\dagger) & ; \quad \Psi^\dagger = \gamma_1 - i\gamma_2 \end{cases}$$

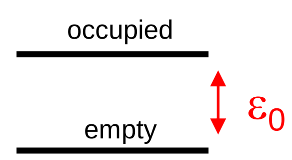
$$\gamma_i^2 = 1$$

$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}$$

“Half a state”

Two Majorana fermions define a single two level system

$$H = 2i\varepsilon_0\gamma_1\gamma_2 = \varepsilon_0\Psi^\dagger\Psi$$



Periodic Table of Topological Insulators and Superconductors

Schnyder, Ryu, Furusaki, Ludwig 2008
Kitaev, 2008

Anti-Unitary Symmetries :

- Time Reversal : $\Theta H(\mathbf{k})\Theta^{-1} = +H(-\mathbf{k})$; $\Theta^2 = \pm 1$
- Particle - Hole : $\Xi H(\mathbf{k})\Xi^{-1} = -H(-\mathbf{k})$; $\Xi^2 = \pm 1$

Unitary (chiral) symmetry : $\Pi H(\mathbf{k})\Pi^{-1} = -H(\mathbf{k})$; $\Pi = \Theta\Xi$

	Θ^2	Ξ^2	Π^2	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	$d=7$	$d=0$
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

Complex K-theory (A, AIII)

Real K-theory (AI through CI)

Altland-Zirnbauer Random Matrix Classes

Bott Periodicity

Further Reading:

Hasan and Kane, Rev Mod Phys **82**, 3045 (2010).

Moore, Nature **464**, 194 (2010).

Qi and Zhang, Phys. Today **63**, 33 (2010).

Ryu, Schnyder, Furusaki and Ludwig, New J. Phys. **12**, 065010 (2010).

Qi and Zhang, Rev Mod Phys, to appear, arXiv:1008.2026.

Moore and Hasan, Annual Review of Condensed Matter, 2, 44 (2010).

Major accomplishments :

Topological band theory of insulators and superconductors is well understood:

- Topological Invariants and bulk-boundary correspondence
- Robustness to disorder and weak interactions
- Electromagnetic and/or gravitational response

Rapid materials progress:

- Several materials have been identified and characterized experimentally.

- Even more materials have been predicted, based on band structure calculations.

- Detailed characterization of topological insulators via transport, optics and spectroscopy is developing.

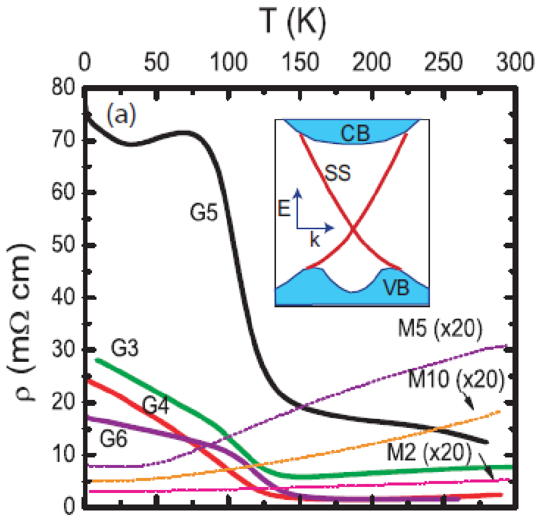
Grand Challenges

- Perfect existing and new materials
- Design and implement heterostructure devices
- Find Majorana
- Classify and characterize many body topological phases
- Find applications for technology

Perfect New and Existing Materials

Real 3D topological insulator materials are not such great insulators. Electrical conductance is dominated by the bulk.

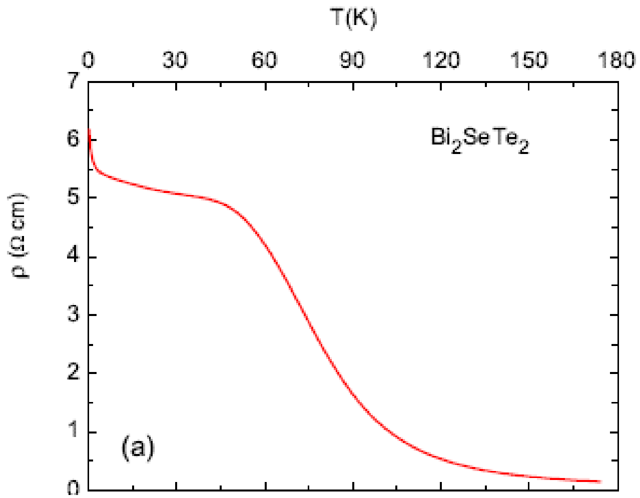
Challenge for materials theory in conjunction with experiments.

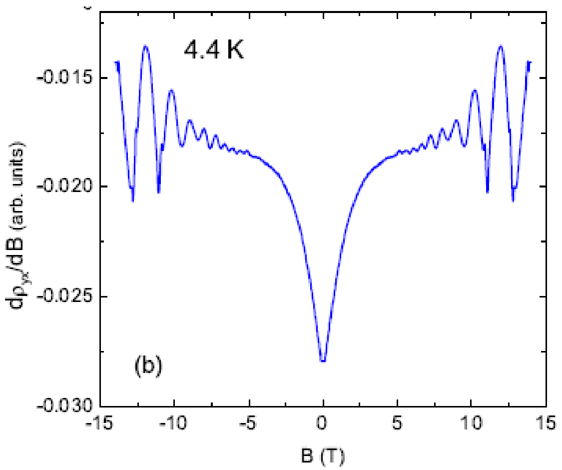


Electrical resistivity in Bi_2Se_3 (Checkelsky et al '09)

Success Story : Bi_2Te_2Se

Xiong, et al (Princeton) '11

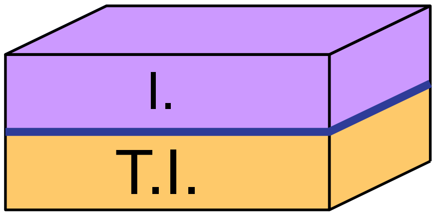




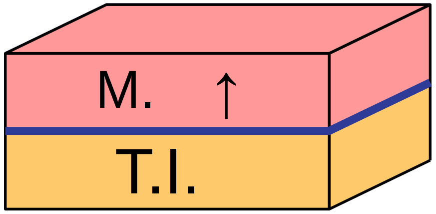
Topological insulator devices

Requires control interfaces between materials.
Challenge for materials theory and experiment

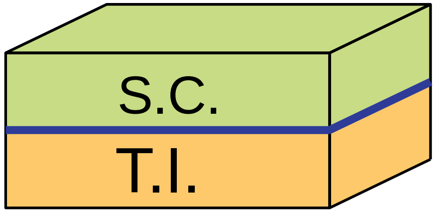
- Topological Insulator – Trivial Insulator
  - protect the surface states
  - control the surface state Fermi energy (modulation doping)



- Topological Insulator – Magnetic Insulator
  - achieve magnetically gapped surface states
  - anomalous quantum Hall effect
  - topological magnetoelectric effect



- Topological Insulator – Superconductor
  - achieve proximity induced superconductivity in the surface states.

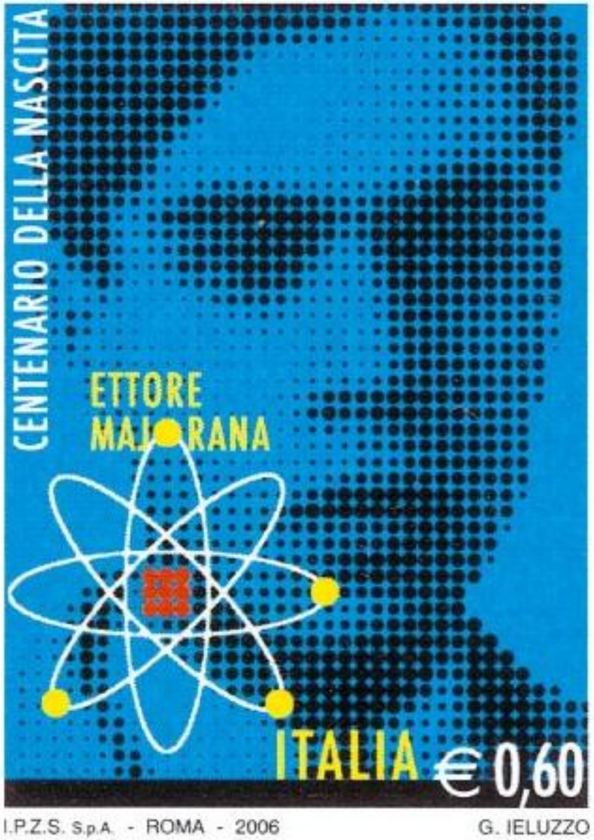


Find Majorana

1937 : Majorana publishes his modification of the Dirac equation that allowes spin ½ particles to be their own antiparticle.

1938 : Majorana mysteriously disappears at sea

Observation of a Majorana fermion is among the great challenges of physics today

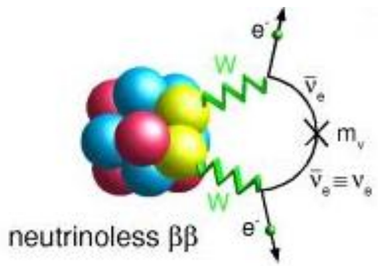


Ettore Majorana 1906 – 1938?

Potential Hosts :

Particle Physics : Neutrino (maybe)

- Allows neutrinoless double β-decay.



Condensed matter physics : Possible due to pair condensation $\langle \Psi^\dagger \Psi^\dagger \rangle \neq 0$

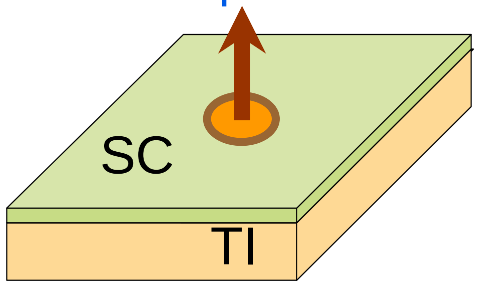
- ν=5/2 Fractional quantum Hall effect
- Topological superconductivity

Topological Quantum Computation

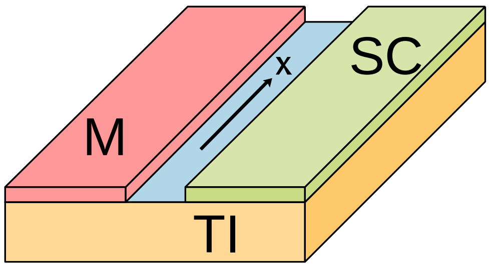
What is the best way to achieve topological superconductivity?

- Exotic superconductors (superfluids)
  - Surface of ^{4}He
  - p+ip superconductor (eg Sr_2RuO_4)
  - $Cu_xBi_2Se_3$?

- Ordinary superconductor heterostructures
  - superconductor – topological insulator

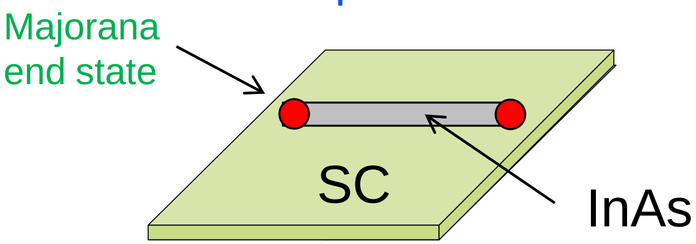


Majorana bound state at a vortex (0D)



1D Chiral Majorana mode at a interface with a magnetic material

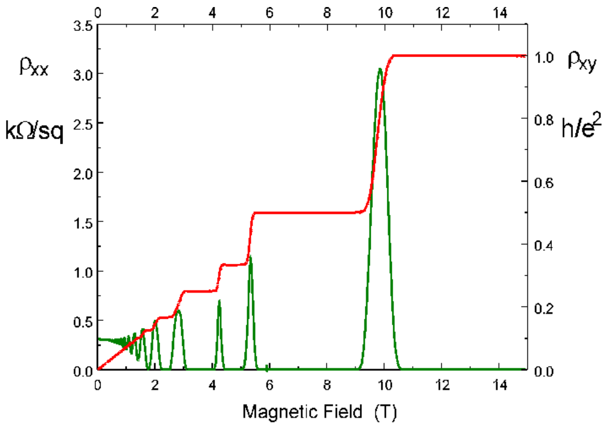
  - superconductor – semiconductor (eg InAs wire)



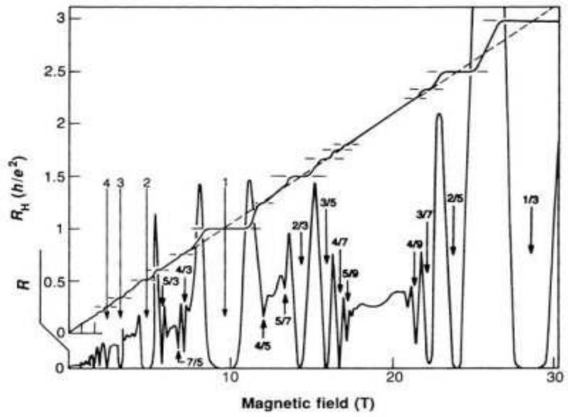
What are the most feasible experimental signatures of Majorana modes ?

Classify and Characterize Interacting Topological States

Topological Insulators are like the Integer Quantum Hall effect. The single particle energy gap is correctly described by non interacting band theory.



Interacting systems exhibit a much richer collection of fractional quantum Hall states. Understanding these was one of the greatest triumphs of many body physics.



What is a fractional topological insulator ?

Classify possible states
Characterize quasiparticle excitations and surface states.

Need to develop new techniques:

- Parton construction?
- B-F theory?
- Entanglement spectrum?

What is the generalization of the bulk – boundary correspondence for interacting systems ?