Topological Insulators in 2D and 3D

I. Introduction

- Graphene
- Time reversal symmetry and Kramers' theorem

II. 2D quantum spin Hall insulator

- Z_2 topological invariant
- Edge states
- HgCdTe quantum wells, expts

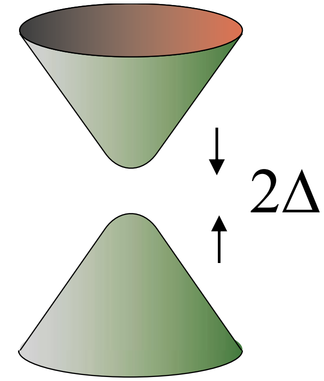
III. Topological Insulators in 3D

- Weak vs strong
- Topological invariants from band structure

IV. The surface of a topological insulator

- Dirac Fermions
- Absence of backscattering and localization
- Quantum Hall effect
- θ term and topological magnetoelectric effect

Energy gaps in graphene:



σ_z ~ sublattice

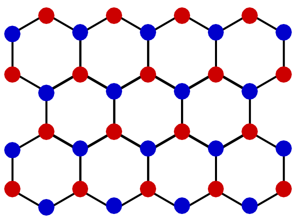
τ_z ~ valley

s_z ~ spin

$$H = \mathrm{v}_F \sigma \cdot p + V$$

$$E(p) = \pm\sqrt{\mathrm{v}_\mathrm{F}^2 p^2 + \Delta^2}$$

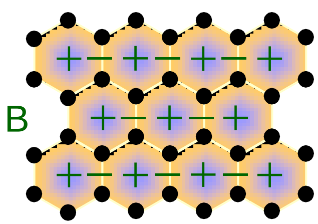
1. Staggered Sublattice Potential (e.g. BN)



$$V = \Delta_{CDW} \sigma^z$$

Broken Inversion Symmetry

2. Periodic Magnetic Field with no net flux (Haldane PRL '88)



$$V = \Delta_{\mathrm{Haldane}} \sigma^z \tau^z$$

Broken Time Reversal Symmetry

Quantized Hall Effect $\sigma_{xy} = \mathrm{sgn}\,\Delta \frac{e^2}{h}$

3. Intrinsic Spin Orbit Potential

$$V = \Delta_{SO} \sigma^z \tau^z s^z$$

Respects ALL symmetries

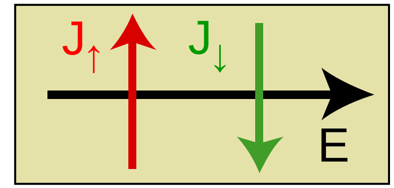
Quantum Spin-Hall Effect

Quantum Spin Hall Effect in Graphene

The intrinsic spin orbit interaction leads to a small (~10mK-1K) energy gap

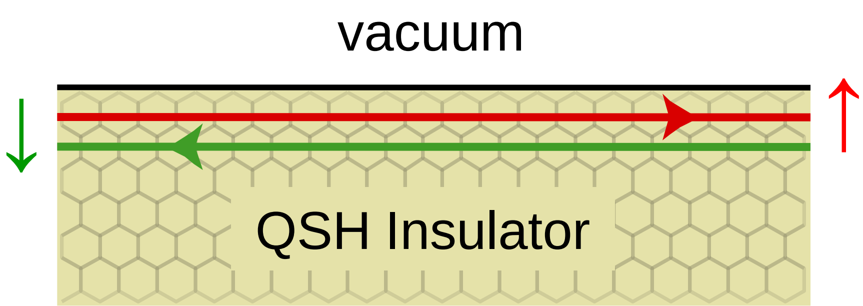
Simplest model:
|Haldane|^2
(conserves S_z)

$$H = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{\text{Haldane}} & 0 \\ 0 & H^*_{\text{Haldane}} \end{pmatrix}$$

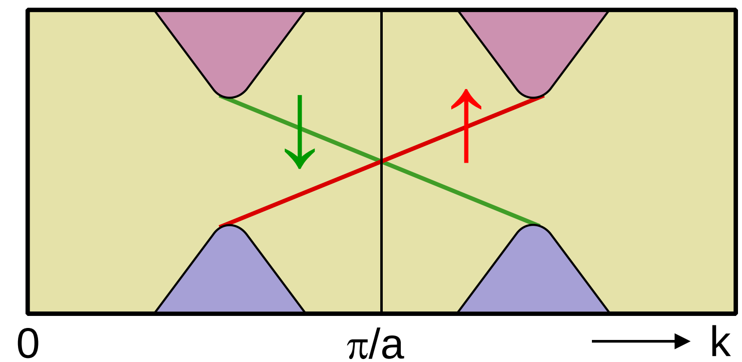


Bulk energy gap, but gapless edge states

"Spin Filtered" or "helical" edge states



Edge band structure



Edge states form a unique 1D electronic conductor

- HALF an ordinary 1D electron gas
- Protected by Time Reversal Symmetry

Time Reversal Symmetry : $[H,\Theta]=0$

Anti Unitary time reversal operator : $\Theta\psi = e^{i\pi S^y/\hbar}\psi^*$

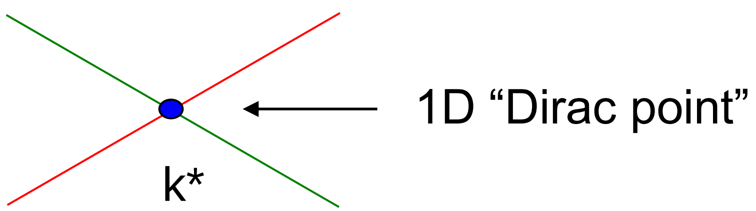
Spin ½ : $\Theta\begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix} = \begin{pmatrix}\psi^*_\downarrow \\ -\psi^*_\uparrow\end{pmatrix}$ $\qquad \Theta^2 = -1$

Kramers' Theorem: for spin ½ all eigenstates are at least 2 fold degenerate

Proof : for a non degenerate eigenstate $\begin{array}{l}\Theta|\chi\rangle = c|\chi\rangle \\ \Theta^2|\chi\rangle = |c|^2|\chi\rangle\end{array}$ $\qquad \Theta^2 = |c|^2 \neq -1$

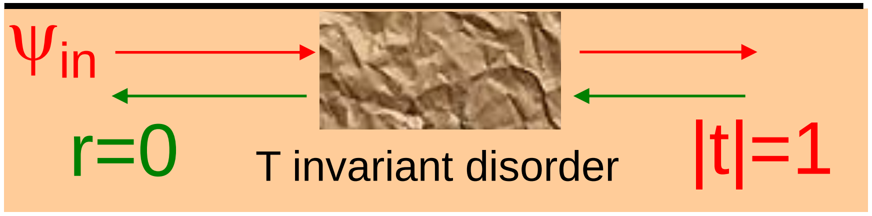
Consequences for edge states :

States at "time reversal invariant momenta" k*=0 and k*=π/a (=-π/a) are degenerate.



The crossing of the edge states is protected, even if spin conservation is volated.

Absence of backscattering, even for strong disorder. No Anderson localization



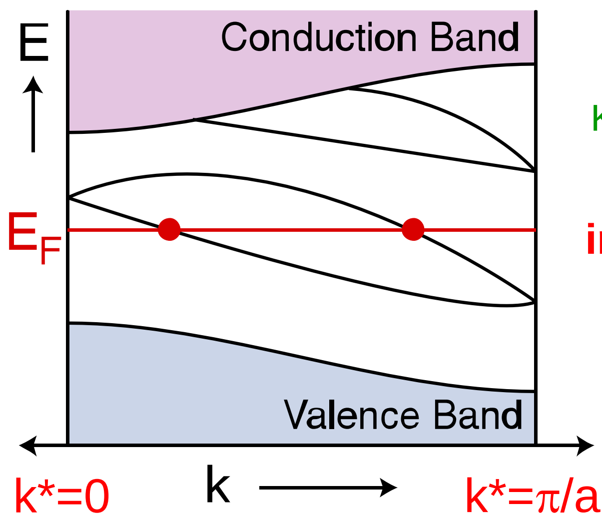
Time Reversal Invariant $\mathbb{Z}_2$ Topological Insulator

2D Bloch Hamiltonians subject to the T constraint $\Theta H(\mathbf{k})\Theta^{-1} = H(-\mathbf{k})$

with $\Theta^2 = -1$ are classified by a $\mathbb{Z}_2$ topological invariant (ν = 0,1)

Understand via Bulk-Boundary correspondence : Edge States for $0<k<\pi/a$

ν=0 : Conventional Insulator



Even number of bands
crossing Fermi energy

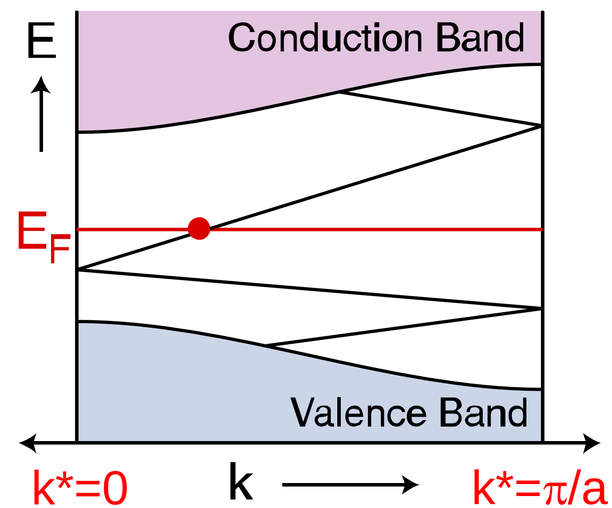
Kramers degenerate at

time reversal

invariant momenta

$k^* = -k^* + G$

ν=1 : Topological Insulator

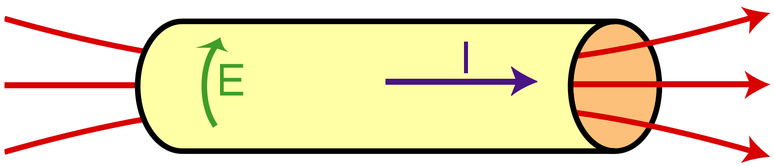


Odd number of bands
crossing Fermi energy

Physical Meaning of $\mathbb{Z}_2$ Invariant

Sensitivity to boundary conditions in a multiply connected geometry

ν=N IQHE on cylinder: Laughlin Argument

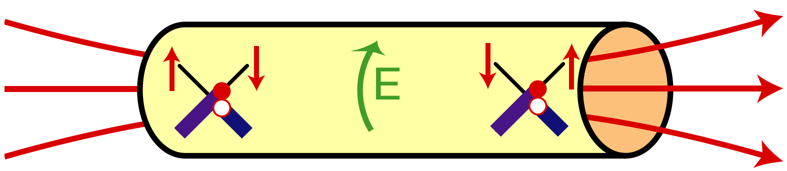


$\Delta\Phi = \phi_0 = h/e$

$\Delta Q = N e$

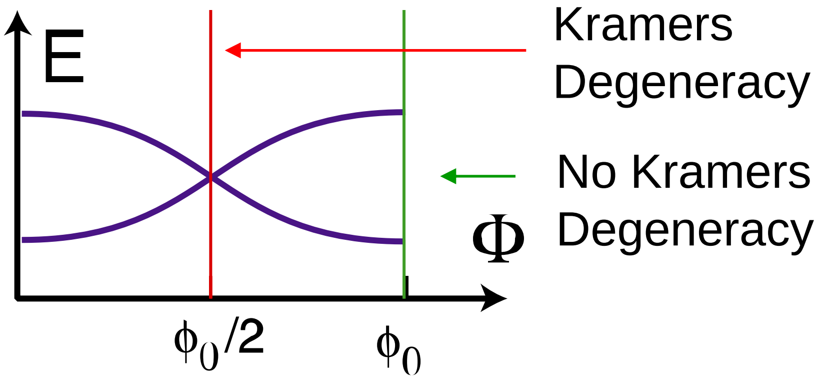
Flux $\phi_0 \Rightarrow$ Quantized change in Electron Number at the end.

Quantum Spin Hall Effect on cylinder



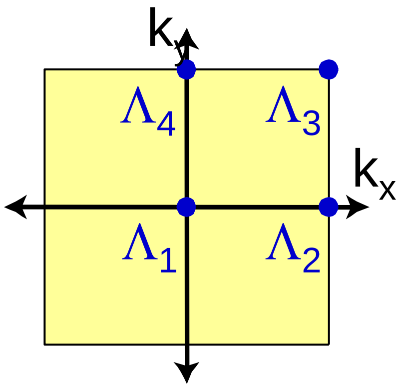
$\Delta\Phi = \phi_0 / 2$

Flux $\phi_0 /2 \Rightarrow$ Change in Electron Number Parity at the end, signaling change in Kramers degeneracy.



Formula for the $\mathbb{Z}_2$ invariant

- Bloch wavefunctions : $|u_n(\mathbf{k})\rangle$ (N occupied bands)
- T - Reversal Matrix : $w_{mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|\Theta|u_n(-\mathbf{k})\rangle \in U(\mathrm{N})$
- Antisymmetry property : $\Theta^2 = -1 \Rightarrow w(\mathbf{k}) = -w^T(-\mathbf{k})$
- T - invariant momenta : $\mathbf{k} = \Lambda_a = -\Lambda_a \Rightarrow w(\Lambda_a) = -w^T(\Lambda_a)$



Bulk 2D Brillouin Zone

- Pfaffian : $\det[w(\Lambda_a)] = \left(\mathrm{Pf}[w(\Lambda_a)]\right)^2$ e.g. $\det\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z^2$
- Fixed point parity : $\delta(\Lambda_a) = \dfrac{\mathrm{Pf}[w(\Lambda_a)]}{\sqrt{\det[w(\Lambda_a)]}} = \pm 1$
- Gauge dependent product : $\delta(\Lambda_a)\delta(\Lambda_b)$

  "time reversal polarization" analogous to $\frac{e}{2\pi}\oint A(k)dk$

- Z_2 invariant : $(-1)^\nu = \prod_{a=1}^{4} \delta(\Lambda_a) = \pm 1$

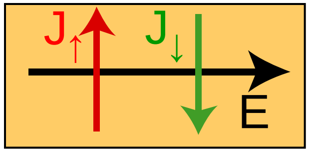
  Gauge invariant, but requires continuous gauge

ν is easier to determine if there is extra symmetry:

1. S_z conserved : independent spin Chern integers :

$$n_\uparrow = -\, n_\downarrow \quad \text{(due to time reversal)}$$

Quantum spin Hall Effect :



$$\boxed{\nu = n_{\uparrow,\downarrow} \ \mathrm{mod}\ 2}$$

2. Inversion (P) Symmetry : determined by Parity of occupied 2D Bloch states

$$P\left|\psi_n(\Lambda_a)\right\rangle = \xi_n(\Lambda_a)\left|\psi_n(\Lambda_a)\right\rangle$$

$$\xi_n(\Lambda_a) = \pm 1$$

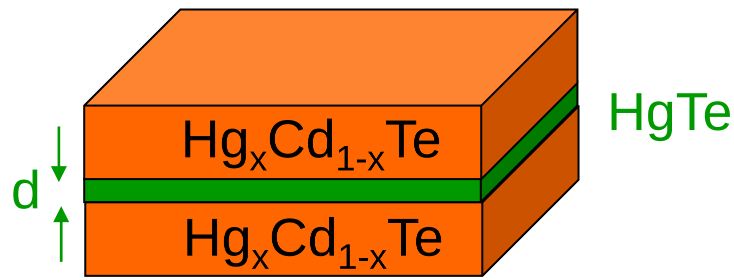
In a special gauge: $\delta(\Lambda_a) = \prod_n \xi_n(\Lambda_a)$

$$\boxed{(-1)^{\upsilon} = \prod_{a=1}^{4} \prod_n \xi_{2n}(\Lambda_a)}$$

Allows a straightforward determination of ν from band structure calculations.

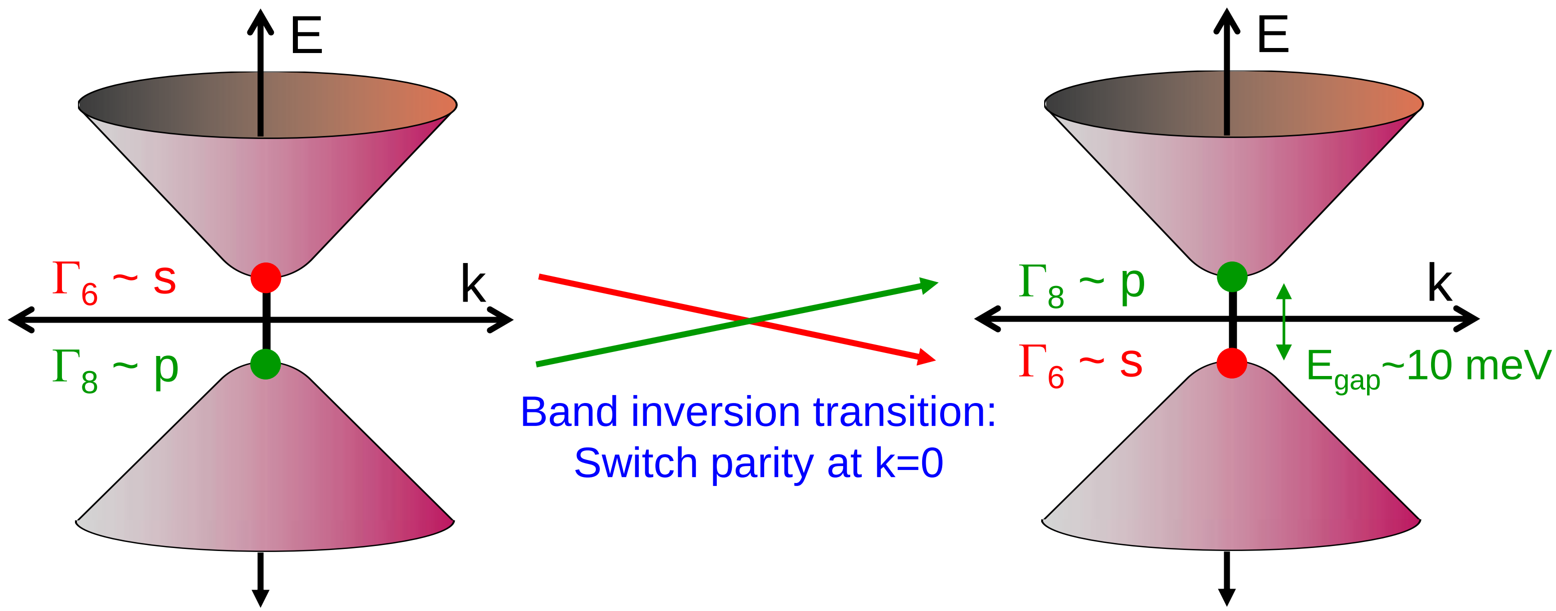
Quantum Spin Hall Effect in HgTe quantum wells

Theory: Bernevig, Hughes and Zhang, Science ‘06



d < 6.3 nm : Normal band order

d > 6.3 nm : Inverted band order



Conventional Insulator

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

Quantum spin Hall Insulator with topological edge states

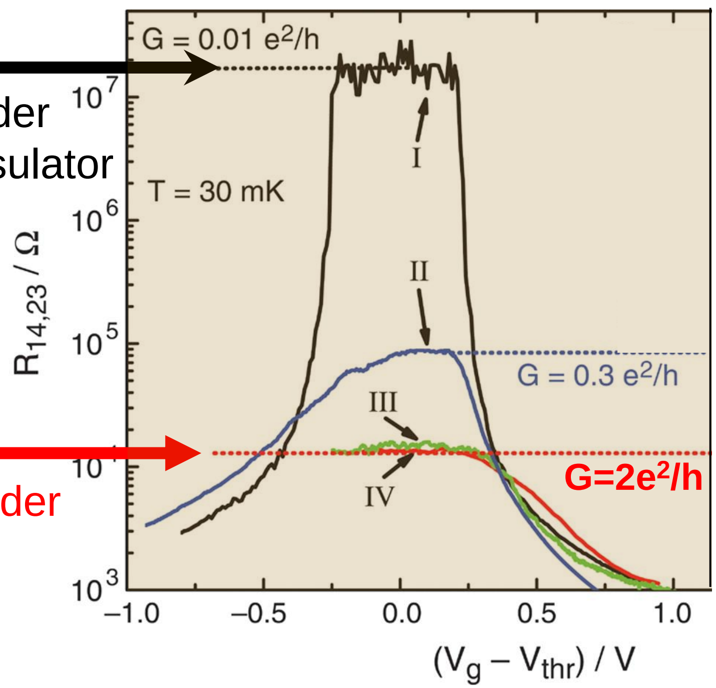
$$\prod \xi_{2n}(\Lambda_a) = -1$$

Experiments on HgCdTe quantum wells

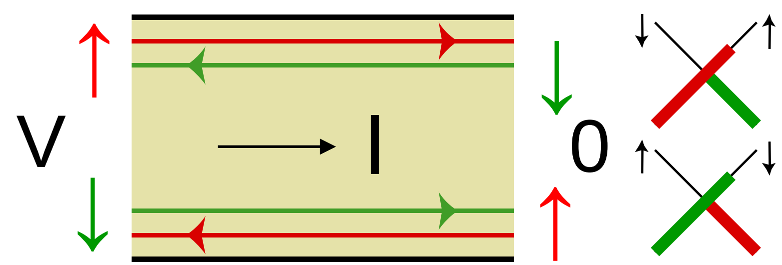
Expt: Konig, Wiedmann, Brune, Roth, Buhmann, Molenkamp, Qi, Zhang Science 2007

d< 6.3 nm
normal band order
conventional insulator

d> 6.3nm
inverted band order
QSH insulator



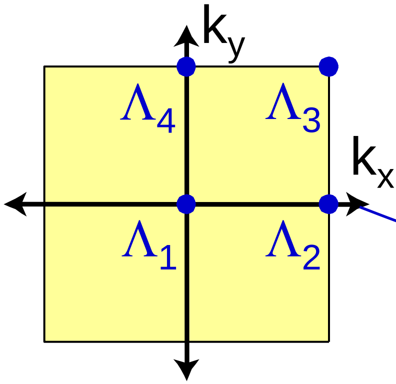
Landauer Conductance $G=2e^2/h$



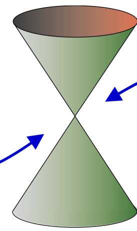
Measured conductance $2e^2/h$ independent of W for short samples ($L<L_{in}$)

3D Topological Insulators

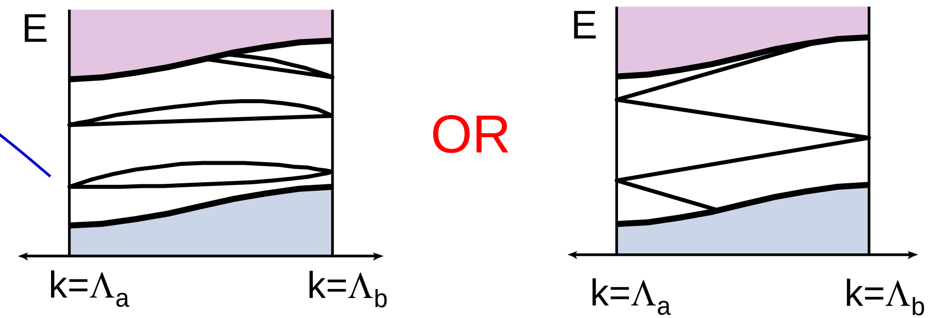
There are 4 surface Dirac Points due to Kramers degeneracy



Surface Brillouin Zone



2D Dirac Point

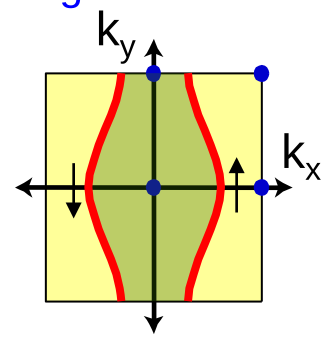


How do the Dirac points connect? Determined by 4 bulk Z_2 topological invariants ν_0 ; $(\nu_1\nu_2\nu_3)$

$\nu_0 = 0$: Weak Topological Insulator

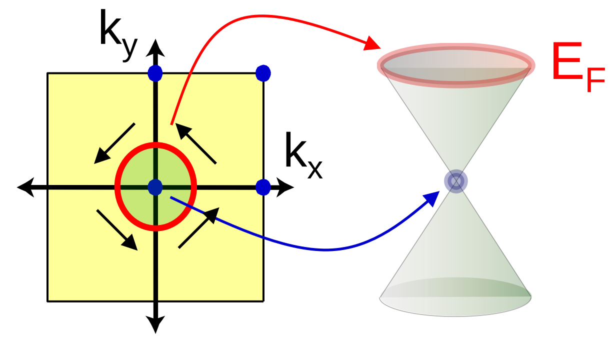
Related to layered 2D QSHI ; $(\nu_1\nu_2\nu_3)$ ~ Miller indices

Fermi surface encloses even number of Dirac points



$\nu_0 = 1$: Strong Topological Insulator

Fermi circle encloses odd number of Dirac points



Topological Metal :

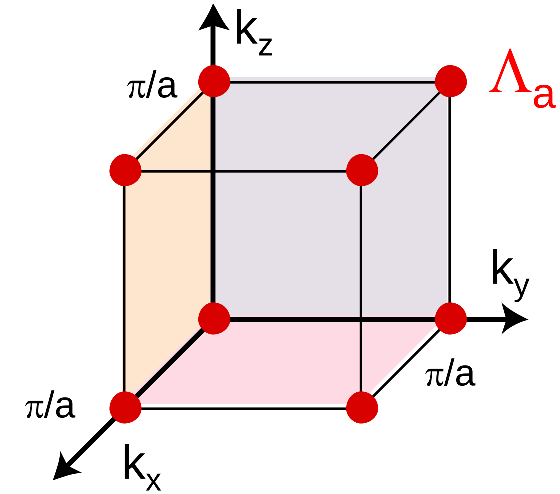
- 1/4 graphene
- Berry's phase π
- Robust to disorder: impossible to localize

Topological Invariants in 3D

1. 2D → 3D : Time reversal invariant planes

The 2D invariant

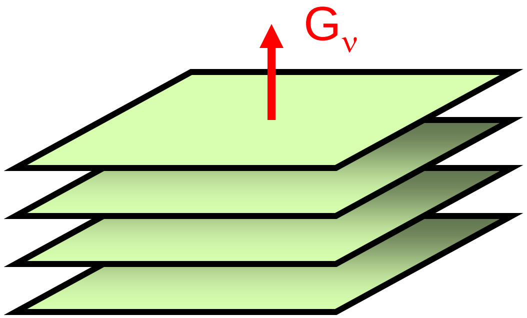
$$(-1)^{\nu} = \prod_{a=1}^{4} \delta(\Lambda_a) \qquad \delta(\Lambda_a) = \frac{\mathrm{Pf}[w(\Lambda_a)]}{\sqrt{\det[w(\Lambda_a)]}}$$



Each of the time reversal invariant planes in the 3D Brillouin zone is characterized by a 2D invariant.

Weak Topological Invariants (vector):

$$(-1)^{\nu_i} = \prod_{a=1}^{4} \delta(\Lambda_a) \Big|_{k_i=0 \text{ plane}} \qquad \mathbf{G}_{\nu} = \frac{2\pi}{a}(\nu_1, \nu_2, \nu_3)$$



"mod 2" reciprocal lattice vector indexes lattice planes for layered 2D QSHI

Strong Topological Invariant (scalar)

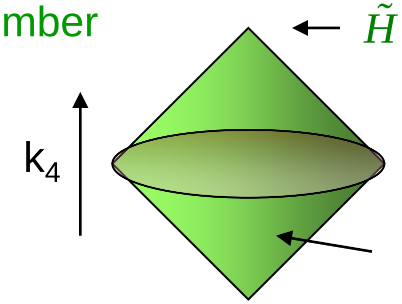
$$(-1)^{\nu_o} = \prod_{a=1}^{8} \delta(\Lambda_a)$$

Topological Invariants in 3D

2. 4D $\rightarrow$ 3D : Dimensional Reduction

Add an extra parameter, k_4, that smoothly connects the topological insulator to a trivial insulator (while breaking time reversal symmetry)

H($\mathbf{k}$,k_4) is characterized by its second Chern number



$$n = \frac{1}{8\pi^2}\int d^4k \,\mathrm{Tr}[\mathbf{F}\wedge\mathbf{F}]$$

n depends on how H($\mathbf{k}$) is connected to H_0, but due to time reversal, the difference must be even.

$$\nu_0 = n \bmod 2$$

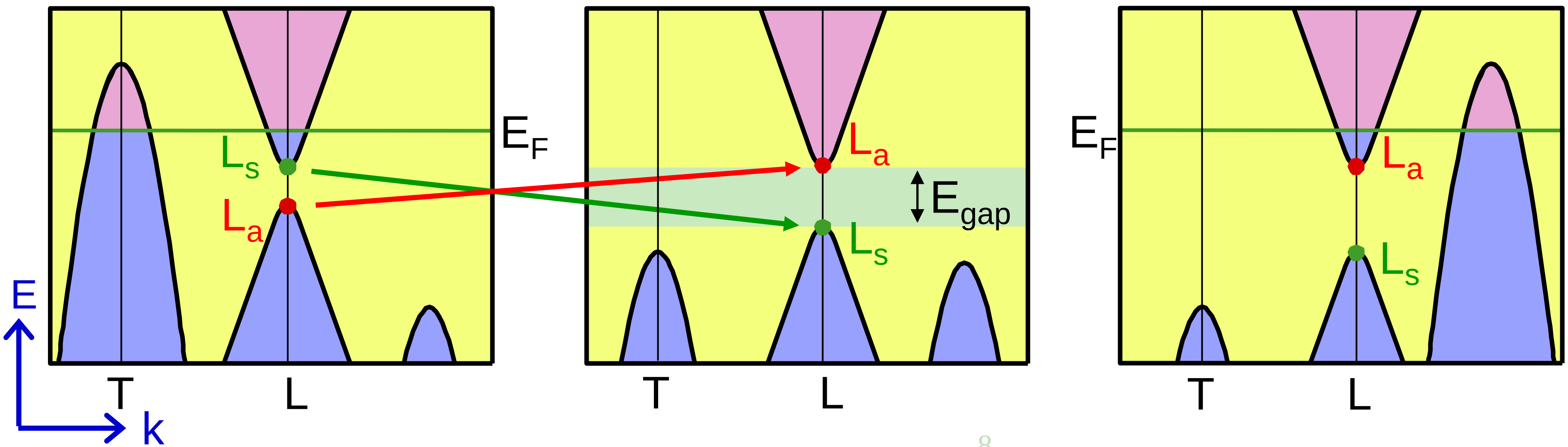
Express in terms of Chern Simons 3-form : $\mathrm{Tr}[\mathbf{F}\wedge\mathbf{F}] = dQ_3$

$$\nu_0 = \frac{1}{4\pi^2}\int \mathrm{d}^3k\, Q_3(\mathbf{k}) \bmod 2 \qquad Q_3(\mathbf{k}) = \mathrm{Tr}[\mathbf{A}\wedge d\mathbf{A} + \frac{2}{3}\mathbf{A}\wedge\mathbf{A}\wedge\mathbf{A}]$$

Gauge invariant up to an even integer.

$Bi_{1-x}Sb_x$

Pure Bismuth	Alloy : .09<x<.18	Pure Antimony
semimetal	semiconductor E_{gap} ~ 30 meV	semimetal



Inversion symmetry $\Rightarrow$ $(-1)^{\nu_0} = \prod_{i=1}^{8} \prod_n \xi_{2n}(\Gamma_i)$

Bismuth

1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	$-$
$3L$	L_s	L_a	L_s	L_a	L_a	$-$
$3X$	X_a	X_s	X_s	X_a	X_a	$-$
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	$-$
	Z_2 class					$(0;000)$

Antimony

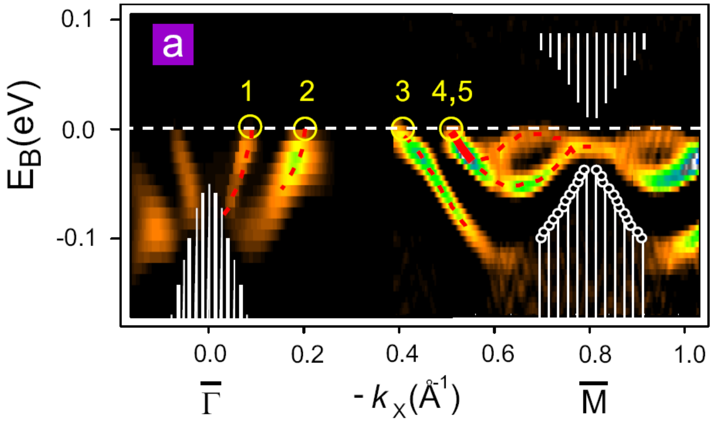
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	$-$
$3L$	L_s	L_a	L_s	L_a	L_s	$+$
$3X$	X_a	X_s	X_s	X_a	X_a	$-$
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	$-$
	Z_2 class					$(1;111)$

Predict $Bi_{1-x}Sb_x$ is a strong topological insulator: (1 ; 111).

$Bi_{1-x}Sb_x$

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

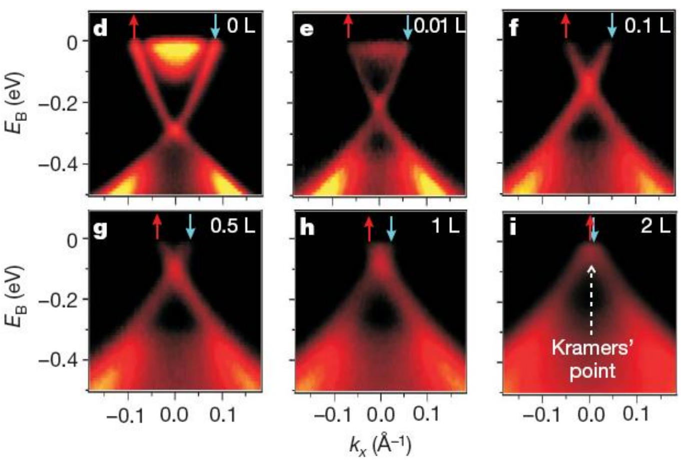
Experiment: ARPES (Hsieh et al. Nature '08)



- $Bi_{1-x}Sb_x$ 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

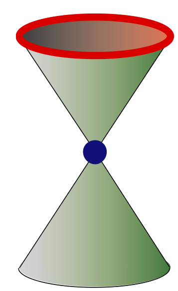
Bi_2Se_3

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

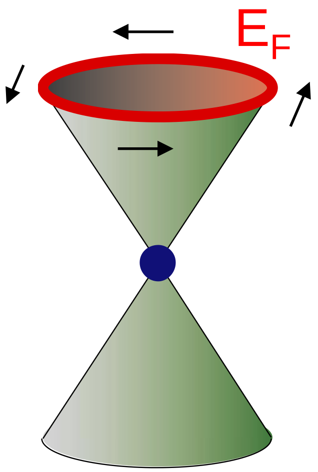
- $\nu_0;(\nu_1,\nu_2,\nu_3) = 1;(000)$: Band inversion at Γ
- Energy gap: $\Delta \sim .3$ eV : A room temperature topological insulator
- Simple surface state structure : Similar to graphene, except only a single Dirac point



E_F

Unique Properties of Topological Insulator Surface States

"Half" an ordinary 2DEG ; ¼ Graphene



Spin polarized Fermi surface

- Charge Current ~ Spin Density
- Spin Current ~ Charge Density

π Berry's phase

- Robust to disorder
- Weak Antilocalization
- Impossible to localize, Klein paradox

Exotic States when broken symmetry leads to surface energy gap:

- Quantum Hall state, topological magnetoelectric effect

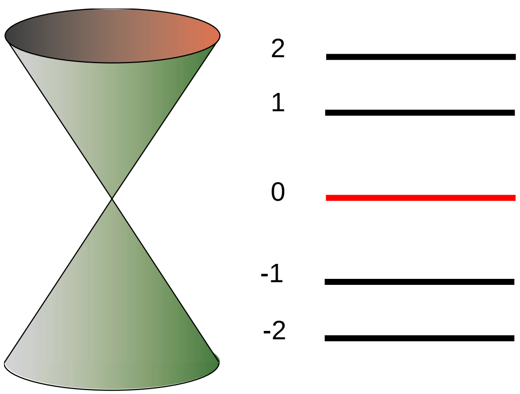
  Fu, Kane '07; Qi, Hughes, Zhang '08, Essin, Moore, Vanderbilt '09

- Superconducting state

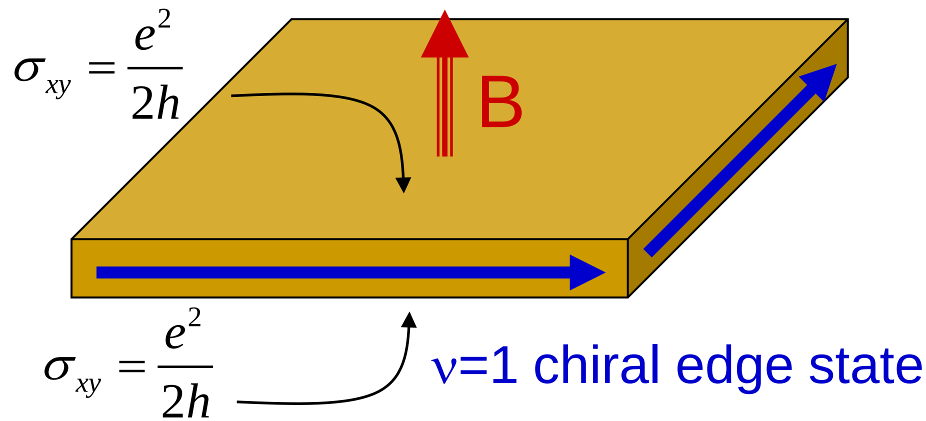
  Fu, Kane '08

Surface Quantum Hall Effect

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



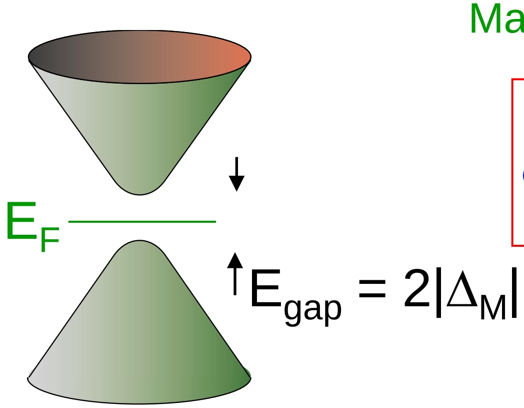
$$\sigma_{xy} = \frac{e^2}{h}\left(n + \frac{1}{2}\right)$$



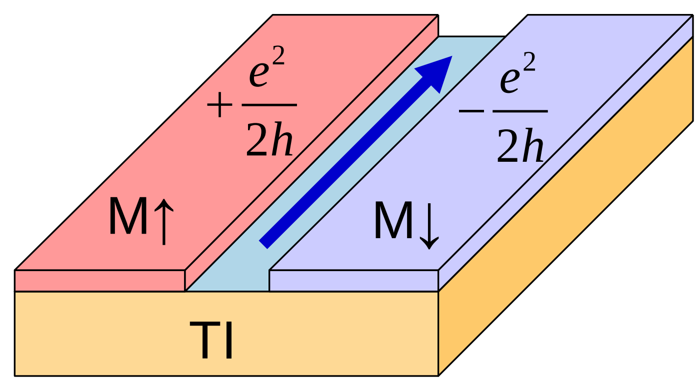
Anomalous QHE :   Induce a surface gap by depositing magnetic material

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

Mass due to Exchange field



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

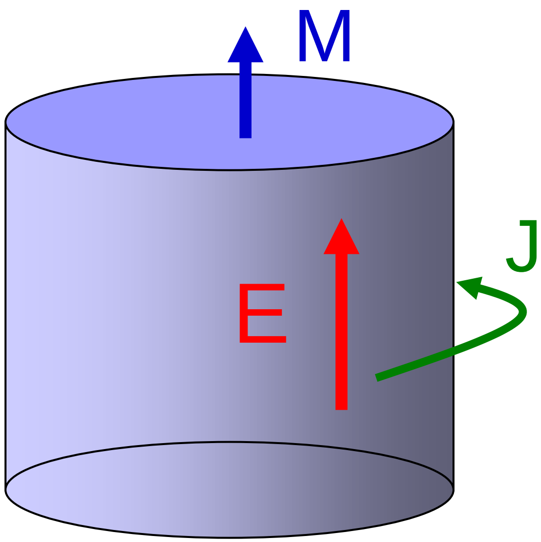


Chiral Edge State at Domain Wall : $\Delta_M \leftrightarrow -\Delta_M$

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)