Topological Insulators in 2D and 3D

0. Electric polarization, Chern Number, Integer Quantum Hall Effect

I. Graphene
  - Haldane model
  - Time reversal symmetry and Kramers' theorem

II. 2D quantum spin Hall insulator
  - Z_2 topological invariant
  - Edge states
  - HgCdTe quantum wells, expts

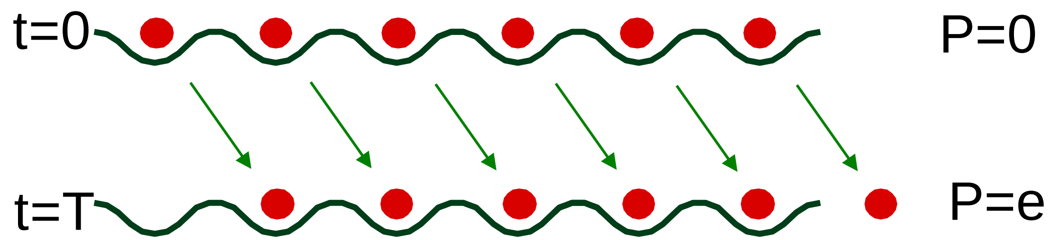
III. Topological Insulators in 3D
  - Weak vs strong
  - Topological invariants from band structure

IV. The surface of a topological insulator
  - Dirac Fermions
  - Absence of backscattering and localization
  - Quantum Hall effect
  - θ term and topological magnetoelectric effect

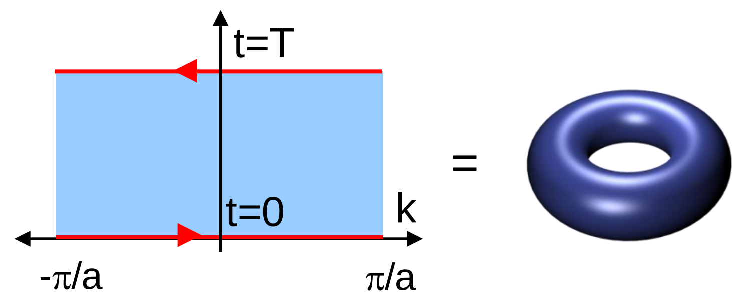
Thouless Charge Pump

The integer charge pumped across a 1D insulator in one period of an adiabatic cycle is a topological invariant that characterizes the cycle.

$$H(k,t+T)=H(k,t)$$



$$\Delta P=\frac{e}{2\pi}\left(\oint A(k,T)dk-\oint A(k,0)dk\right)=ne$$

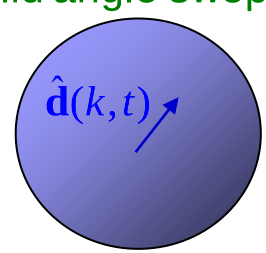


$$n=\frac{1}{2\pi}\int_{T^2}\mathbf{F}dkdt$$

The integral of the Berry curvature defines the first Chern number, n, an integer topological invariant characterizing the occupied Bloch states, $|u(k,t)\rangle$

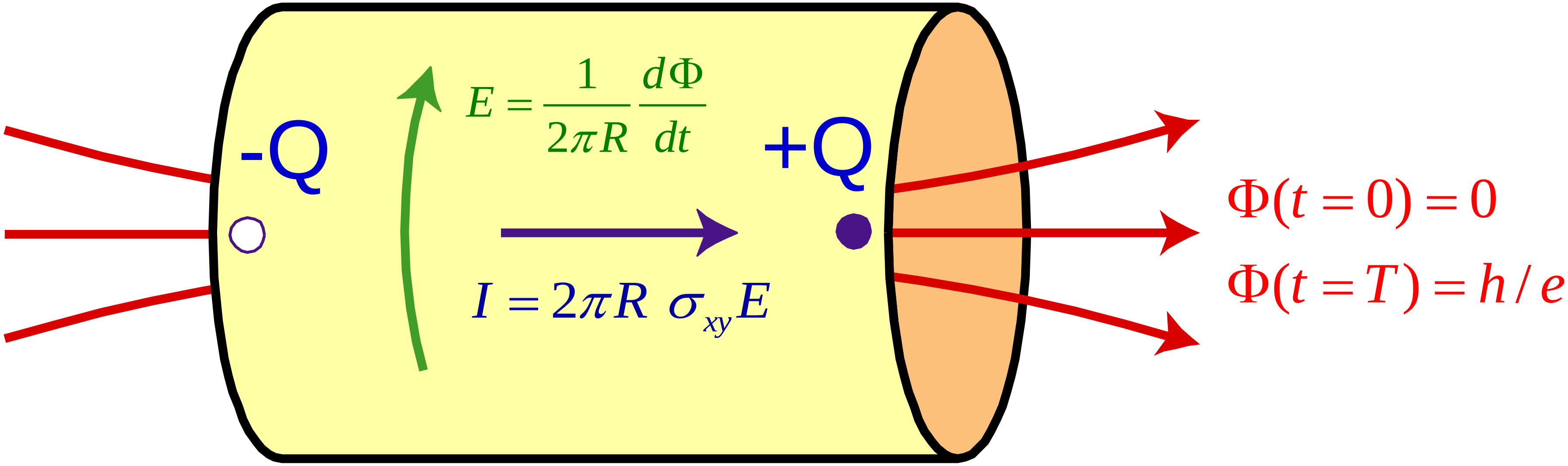
In the 2 band model, the Chern number is related to the solid angle swept out by $\hat{\mathbf{d}}(k,t)$, which must wrap around the sphere an integer n times.

$$n=\frac{1}{4\pi}\int_{T^2}dkdt\ \hat{\mathbf{d}}\cdot(\partial_k\hat{\mathbf{d}}\times\partial_t\hat{\mathbf{d}})$$



Integer Quantum Hall Effect : Laughlin Argument

Adiabatically thread a quantum of magnetic flux through cylinder.



$$\Delta Q = \int_0^T \sigma_{xy}\frac{d\Phi}{dt}dt = \sigma_{xy}\frac{h}{e}$$

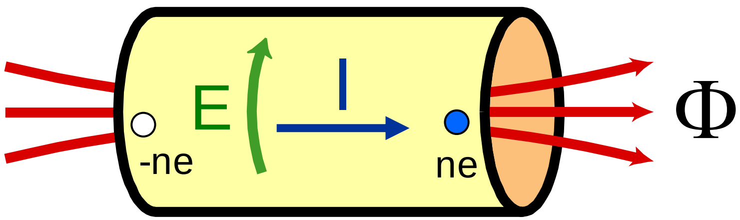
Just like a Thouless pump : $H(T) = U^\dagger H(0) U$

$$\Delta Q = ne \quad \rightarrow \quad \sigma_{xy} = n\frac{e^2}{h}$$

TKNN Invariant

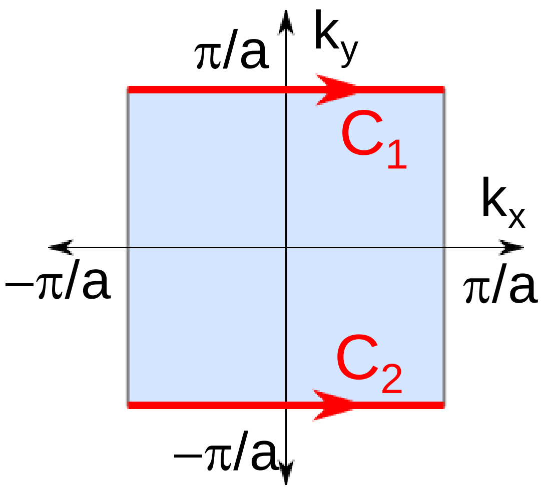
Thouless, Kohmoto, Nightingale and den Nijs 82

Consider cylinder with circumference 1 lattice constant :
Flux Φ plays role of momentum k_y : $\Phi = h/e \quad \Rightarrow \quad k_y = 2\pi/a$



$$\Delta P = ne$$

For 2D band structure, define $\mathbf{A}(\mathbf{k}) = -i\langle u(\mathbf{k})|\nabla_{\mathbf{k}}|u(\mathbf{k})\rangle$



$$n = \frac{1}{2\pi}\oint_{C_1} \mathbf{A}\cdot d\mathbf{k} - \frac{1}{2\pi}\oint_{C_2} \mathbf{A}\cdot d\mathbf{k} \in \mathbb{Z}$$

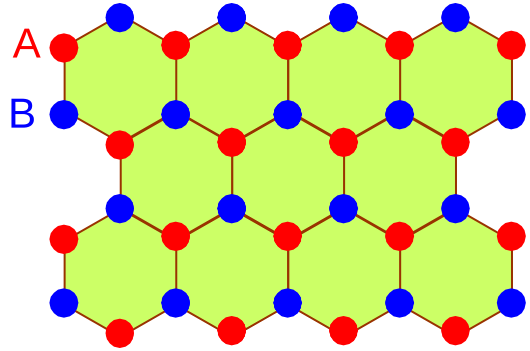
$$= \frac{1}{2\pi}\int_{BZ} d^2k\,\mathbf{F}(\mathbf{k})$$

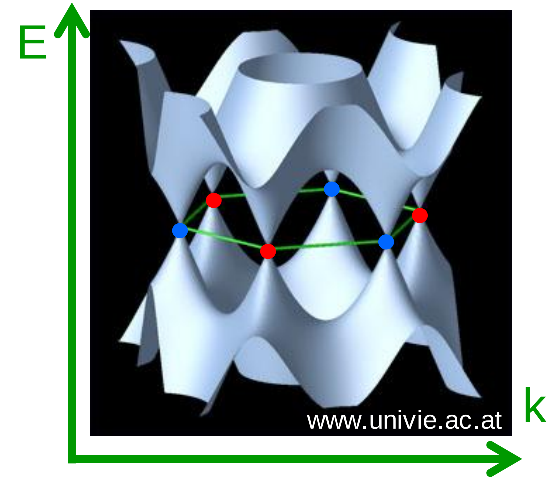
Physical meaning: Hall conductivity $\sigma_{xy} = n\frac{e^2}{h}$

Alternative caluculation: compute σ_{xy} via Kubo formula

Graphene

Novoselov et al. '05



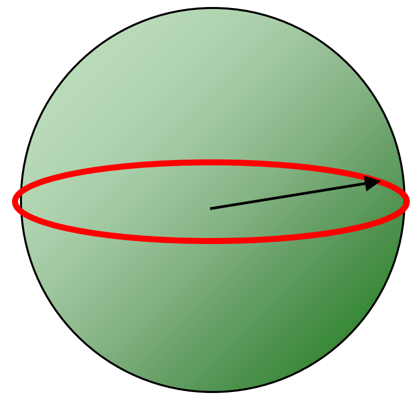


Two band model $H = -t \sum_{<ij>} c_{Ai}^{\dagger} c_{Bj}$

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma}$$

$$E(\mathbf{k}) = \pm |\mathbf{d}(\mathbf{k})|$$

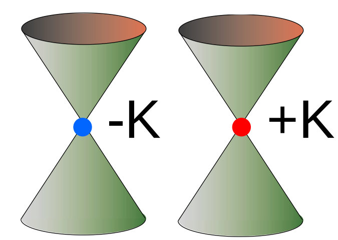
$$\mathbf{d}(\mathbf{k}) = \sum_{j=1}^{3} -t\left(\hat{x}\cos\mathbf{k}\cdot\mathbf{r}_j + \hat{y}\sin\mathbf{k}\cdot\mathbf{r}_j\right)$$



$\hat{\mathbf{d}}(k_x, k_y)$

Inversion and Time reversal symmetry require $d_z(\mathbf{k}) = 0$

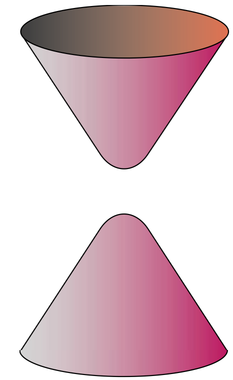
2D Dirac points at $\mathbf{k} = \pm\mathbf{K}$ point vortices in (d_x, d_y)



$$H(\pm\mathbf{K} + \mathbf{q}) = v\vec{\sigma}\cdot\mathbf{q}$$ Massless Dirac Hamiltonian

Berry's phase π around Dirac point

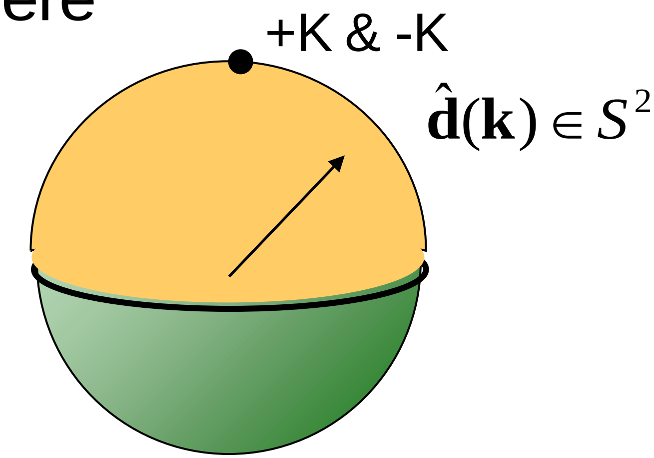
Topological gapped phases in Graphene



Break P or T symmetry : $H(\pm\mathbf{K}+\mathbf{q}) = \mathrm{v}\,\mathbf{q}\bullet\sigma + m_{\pm}\sigma_z$

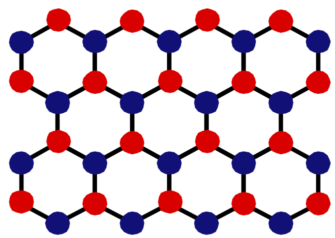
$$E(\mathbf{q}) = \pm\sqrt{\mathrm{v}^2\,|\,\mathbf{q}\,|^2 + m_{\pm}^2}$$

$n = \#$times $\hat{\mathbf{d}}(\mathbf{k})$ wraps around sphere



1. Broken P : eg Boron Nitride

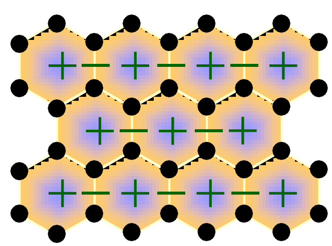
$m_+ = m_-$

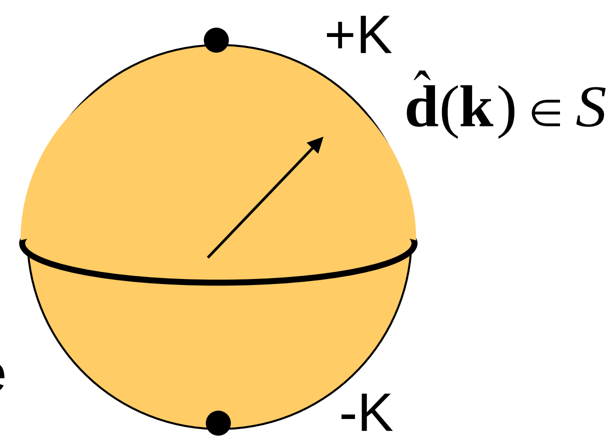


Chern number n=0 : Trivial Insulator

2. Broken T : Haldane Model '88

$m_+ = -m_-$

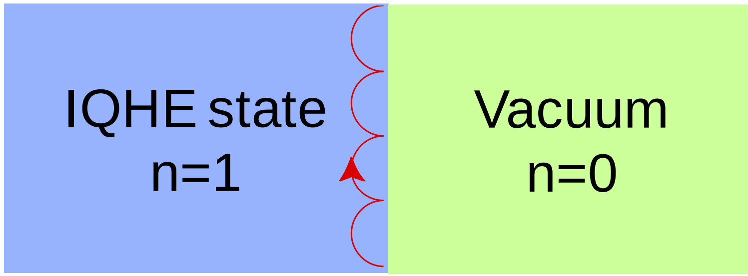




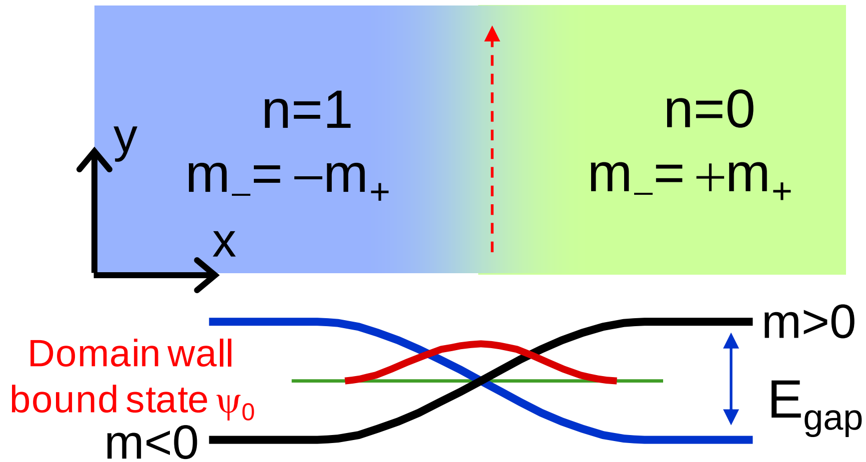
Chern number n=1 : Quantum Hall state

Edge States

Gapless states at the interface between topologically distinct phases



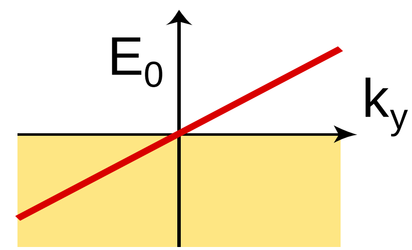
Edge states ~ skipping orbits
Lead to quantized transport



Band inversion transition : Dirac Equation

$$H = \mathrm{v_F}(-i\sigma_x\partial_x + \sigma_y k_y) + m(x)\sigma_z$$

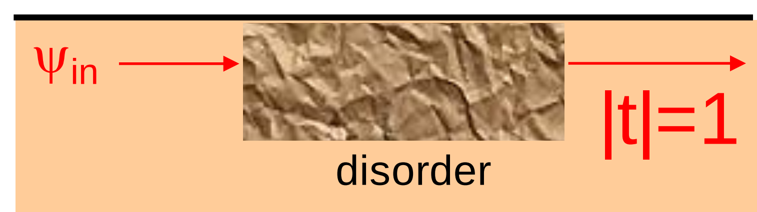
$$\psi_0(x) \sim e^{ik_y y} e^{-\int_0^x m(x')dx'/\mathrm{v_F}} \qquad E_0(k_y) = \mathrm{v_F} k_y$$



Chiral Dirac Fermions

Chiral Dirac fermions are unique 1D states :

"One way" ballistic transport, responsible for quantized conductance. Insensitive to disorder, impossible to localize



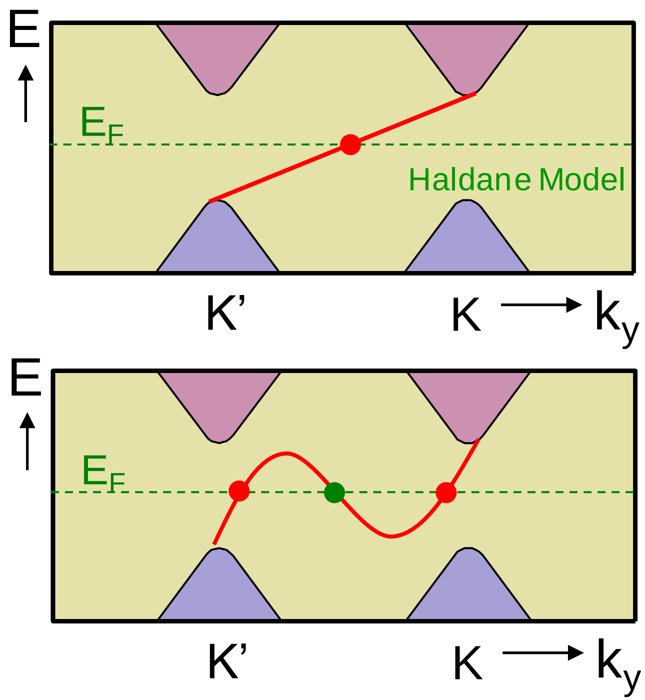
Fermion Doubling Theorem :

Chiral Dirac Fermions can not exist in a purely 1D system.

Bulk - Boundary Correspondence

$\Delta N = N_R - N_L$ is a topological invariant characterizing the boundary.

N_R (N_L) = # Right (Left) moving chiral fermion branches intersecting E_F



$\Delta N = 1 – 0 = 1$

$\Delta N = 2 – 1 = 1$

Bulk – Boundary Correspondence :

The boundary topological invariant ΔN characterizing the gapless modes = Difference in the topological invariants Δn characterizing the bulk on either side

Energy gaps in graphene:

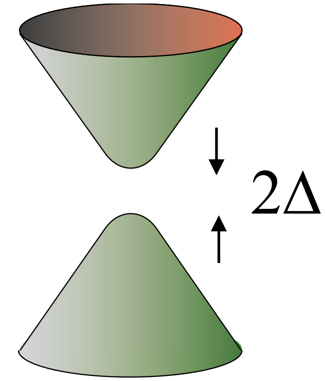
$\sigma_z \sim$ sublattice

$\tau_z \sim$ valley

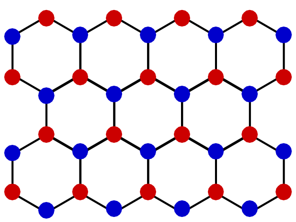
$s_z \sim$ spin

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

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



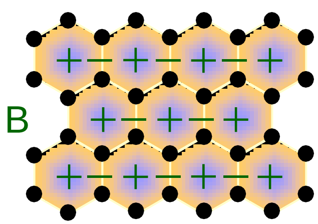
1. Staggered Sublattice Potential (e.g. BN)



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

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

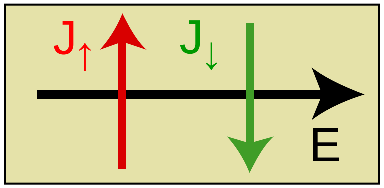
Quantum Spin-Hall Effect

Quantum Spin Hall Effect in Graphene

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

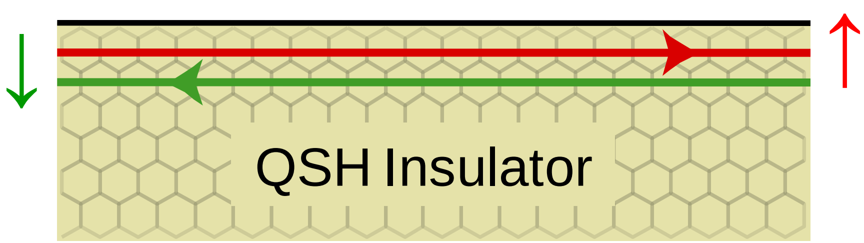
Simplest model:
|Haldane|²
(conserves S_z)

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

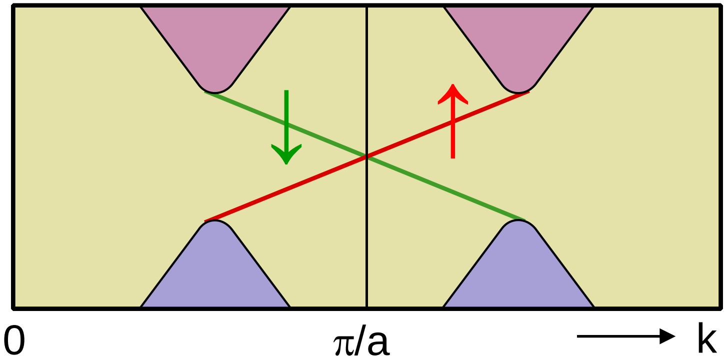


Bulk energy gap, but gapless edge states

"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 : $\Theta\psi = e^{i\pi S^y/\hbar}\psi^*$

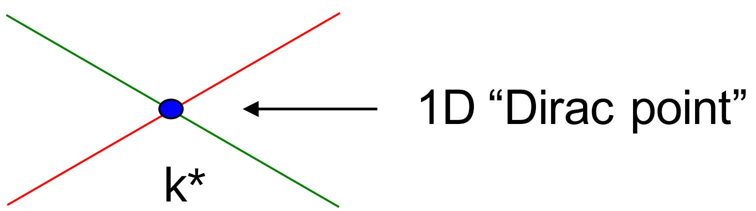
Spin ½ : $\Theta\begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix} = \begin{pmatrix}\psi^*_\downarrow \\ -\psi^*_\uparrow\end{pmatrix}$ $\qquad \Theta^2 = -1$

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

Proof : for a non degenerate eigenstate $\Theta|\chi\rangle = c|\chi\rangle$, $\Theta^2|\chi\rangle = |c|^2|\chi\rangle$ $\qquad \Theta^2 = |c|^2 \neq -1$

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.

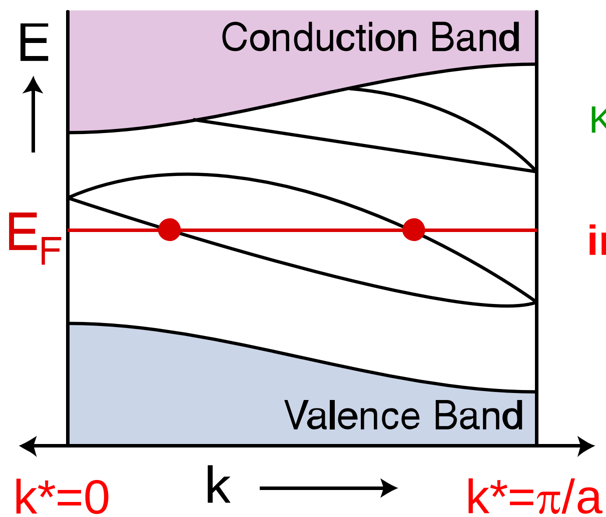
Absence of backscattering, even for strong disorder. No Anderson localization

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 $0<k<\pi/a$

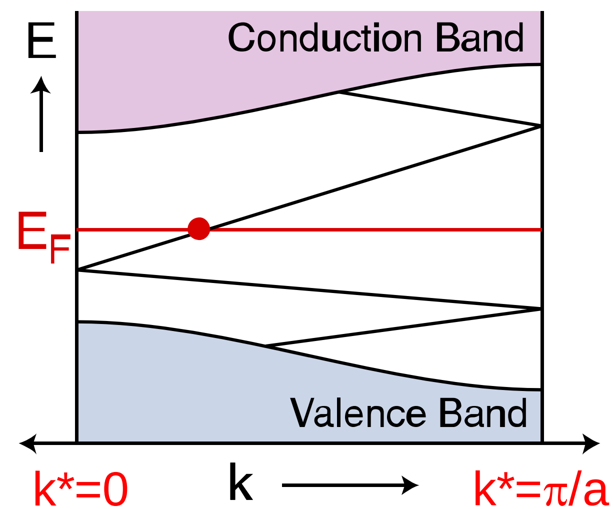
ν=0 : Conventional Insulator



Even number of bands
crossing Fermi energy

Kramers degenerate at
time reversal
invariant momenta
k* = −k* + G

ν=1 : Topological Insulator

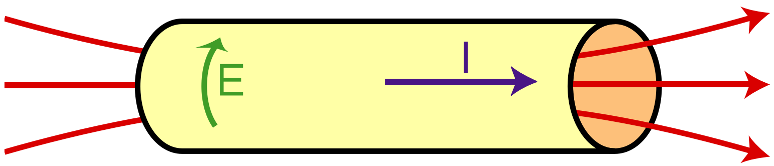


Odd number of bands
crossing Fermi energy

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

Sensitivity to boundary conditions in a multiply connected geometry

ν=N IQHE on cylinder: Laughlin Argument

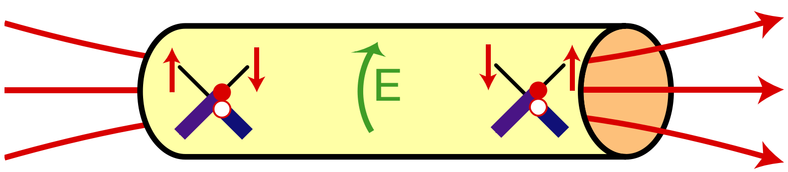


$\Delta\Phi = \phi_0 = h/e$

$\Delta Q = N e$

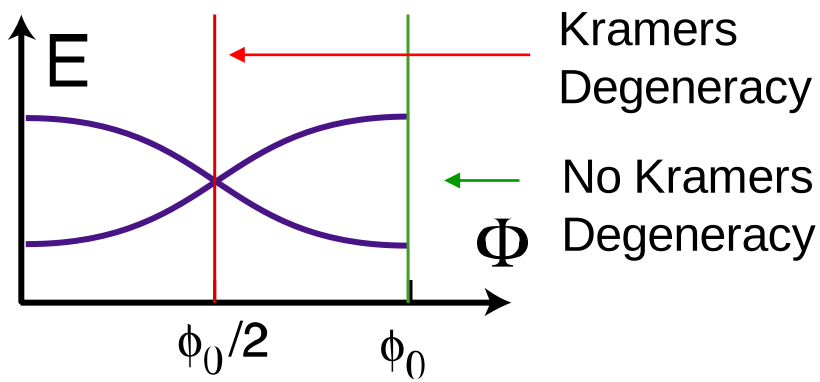
Flux $\phi_0 \Rightarrow$ Quantized change in Electron Number at the end.

Quantum Spin Hall Effect on cylinder



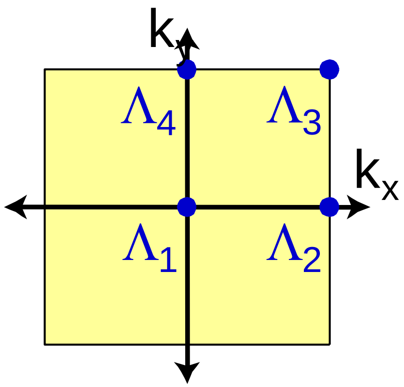
$\Delta\Phi = \phi_0 / 2$

Flux ϕ_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 : $\det[w(\Lambda_a)] = (\mathrm{Pf}[w(\Lambda_a)])^2$ 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 : $(-1)^\nu = \prod_{a=1}^{4} \delta(\Lambda_a) = \pm 1$

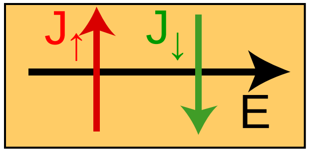
  Gauge invariant, but requires continuous gauge

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 :



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

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

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

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

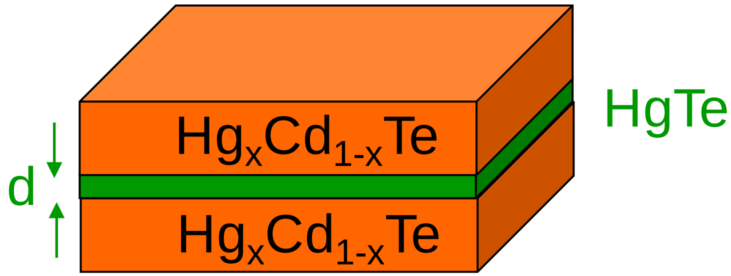
In a special gauge: $\delta(\Lambda_a) = \prod_n \xi_n(\Lambda_a)$

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

Allows a straightforward determination of ν from band structure calculations.

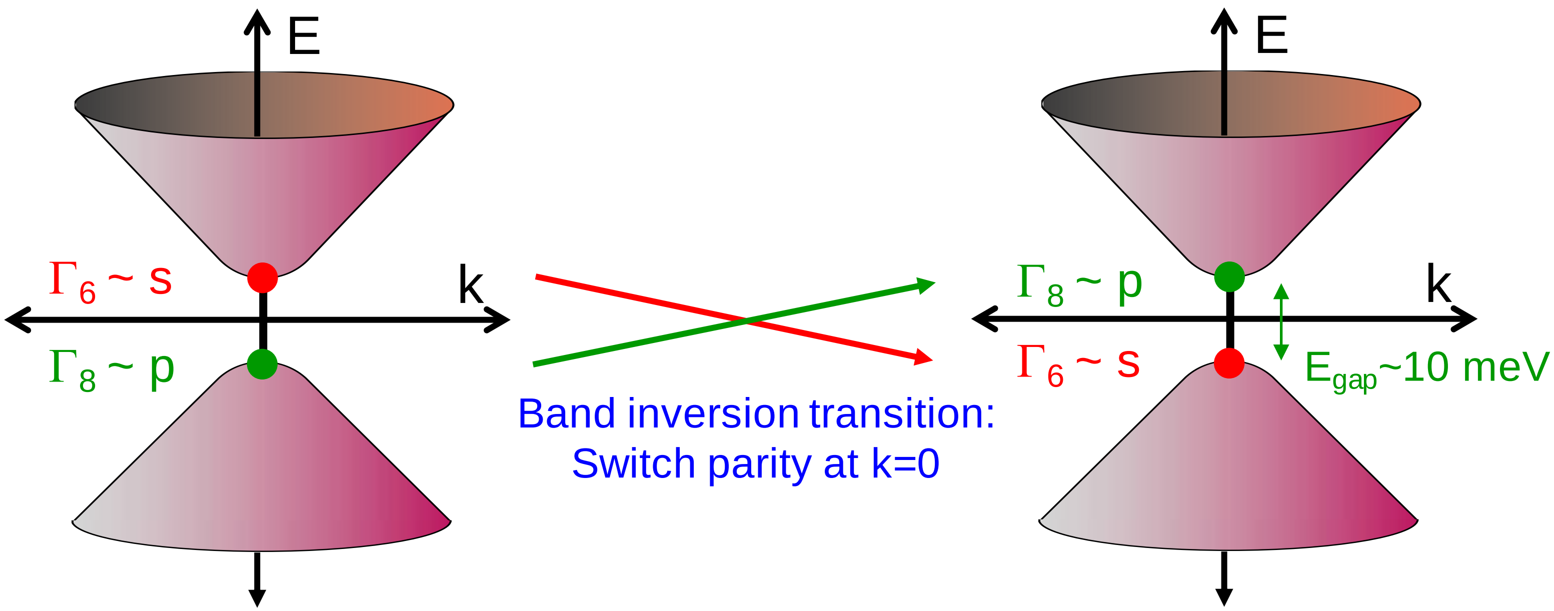
Quantum Spin Hall Effect in HgTe quantum wells

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

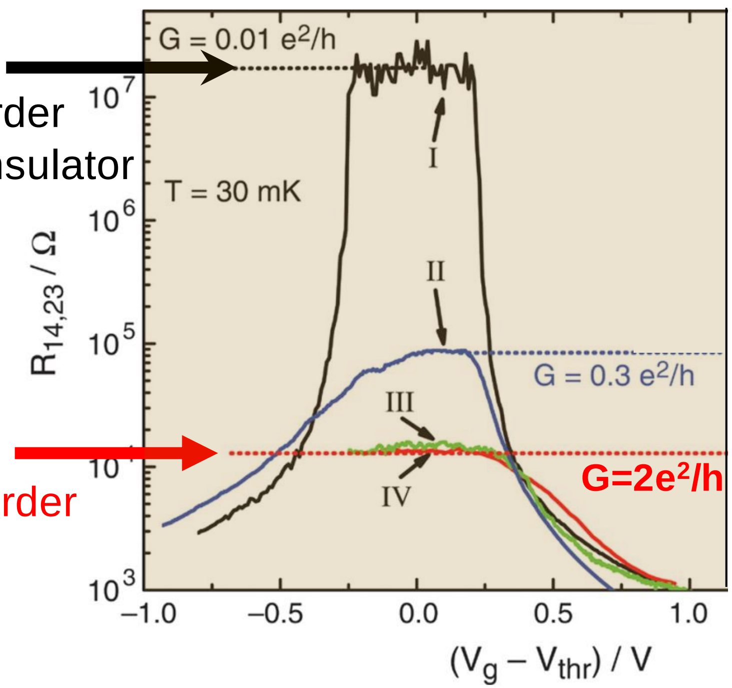
$$\prod \xi_{2n}(\Lambda_a) = -1$$

Experiments on HgCdTe quantum wells

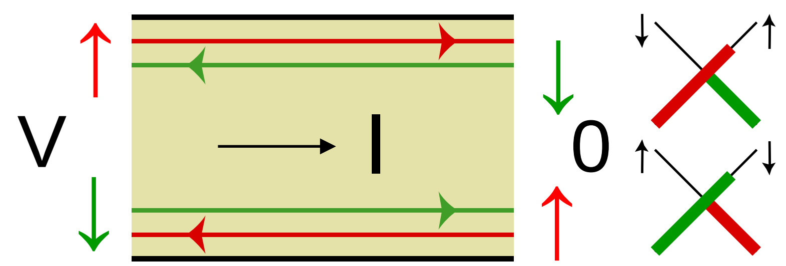
Expt: Konig, Wiedmann, Brune, Roth, Buhmann, Molenkamp, Qi, Zhang Science 2007

d< 6.3 nm
normal band order
conventional insulator

d> 6.3nm
inverted band order
QSH insulator



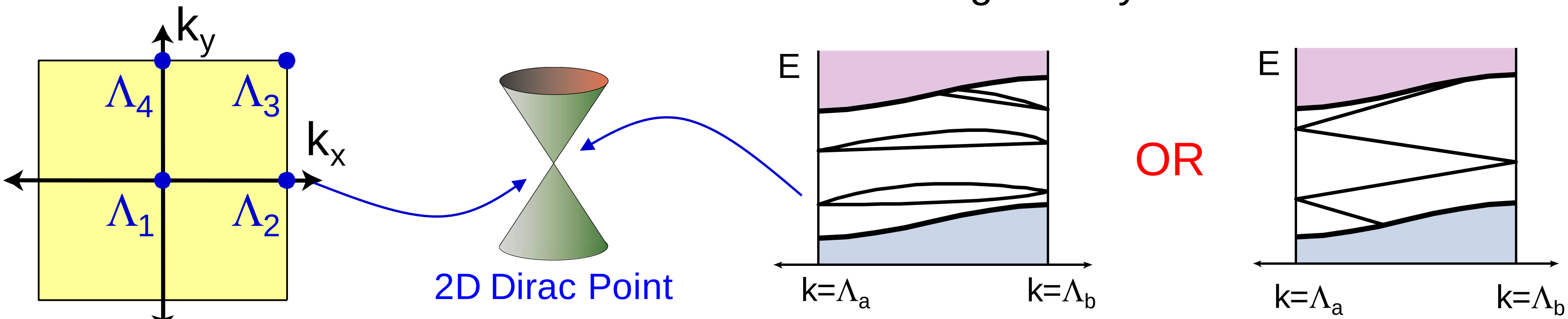
Landauer Conductance $G=2e^2/h$



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

3D Topological Insulators

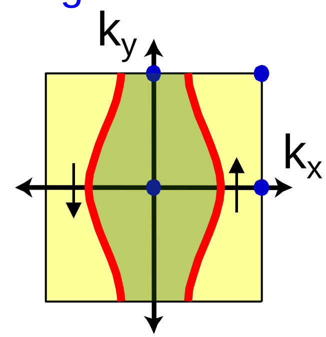
There are 4 surface Dirac Points due to Kramers degeneracy



Surface Brillouin Zone

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

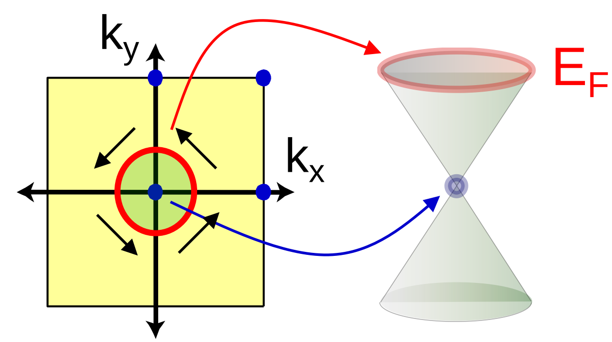
$\nu_0 = 0$: Weak Topological Insulator



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



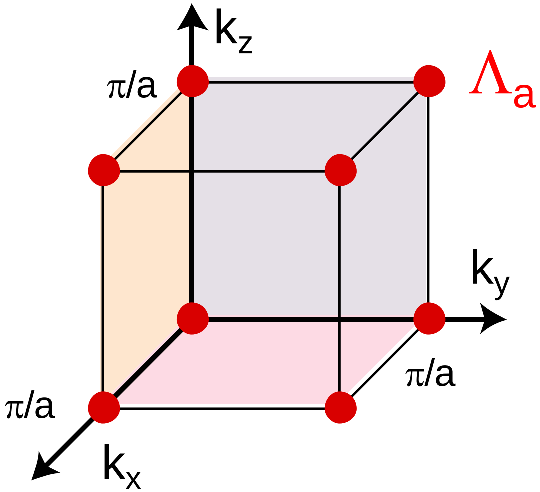
Fermi circle encloses odd number of Dirac points

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

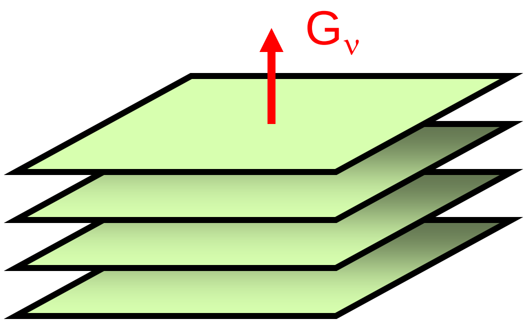


The 2D invariant

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

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)

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

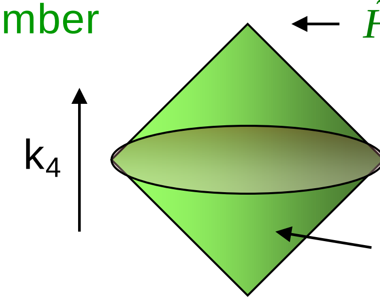
Topological Invariants in 3D

2. 4D → 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

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



$\tilde{H}(\mathbf{k},1) = H_0$ (Trivial insulator)

$\tilde{H}(\mathbf{k},0) = H(\mathbf{k})$

$\tilde{H}(\mathbf{k},-k_4) = \Theta\tilde{H}(\mathbf{k},k_4)\Theta^{-1}$

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 : $\mathrm{Tr}[\mathbf{F}\wedge\mathbf{F}] = dQ_3$

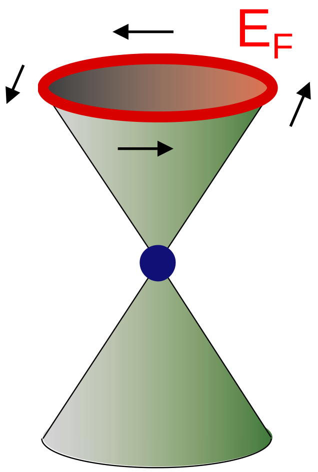
$$\nu_0 = \frac{1}{4\pi^2}\int \mathrm{d}^3k\, Q_3(\mathbf{k}) \bmod 2$$

$$Q_3(\mathbf{k}) = \mathrm{Tr}[\mathbf{A}\wedge d\mathbf{A} + \frac{2}{3}\mathbf{A}\wedge\mathbf{A}\wedge\mathbf{A}]$$

Gauge invariant up to an even integer.

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

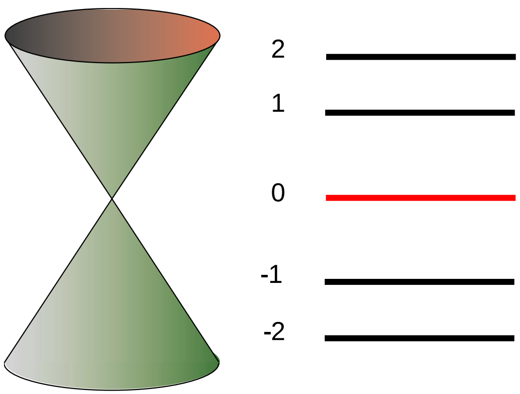
  Fu, Kane '07; Qi, Hughes, Zhang '08, Essin, Moore, Vanderbilt '09

- Superconducting state

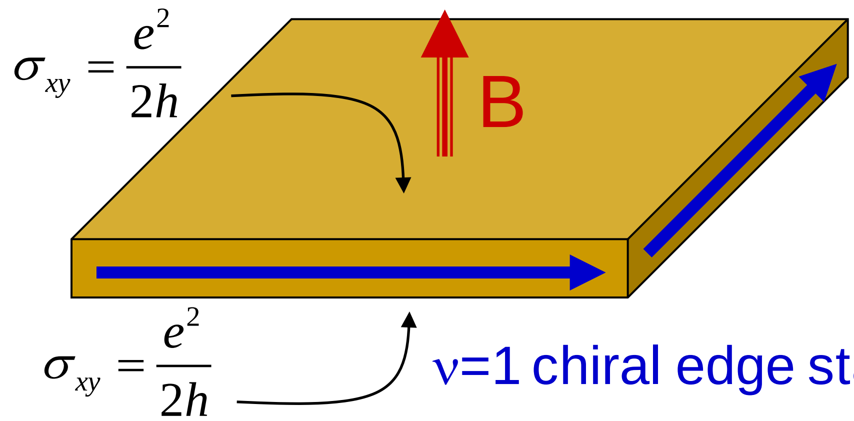
  Fu, Kane '08

Surface Quantum Hall Effect

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



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

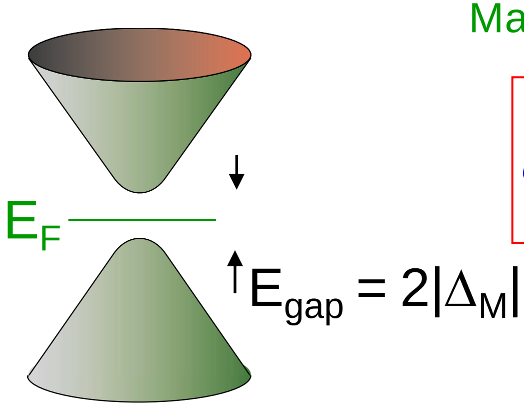


ν=1 chiral edge state

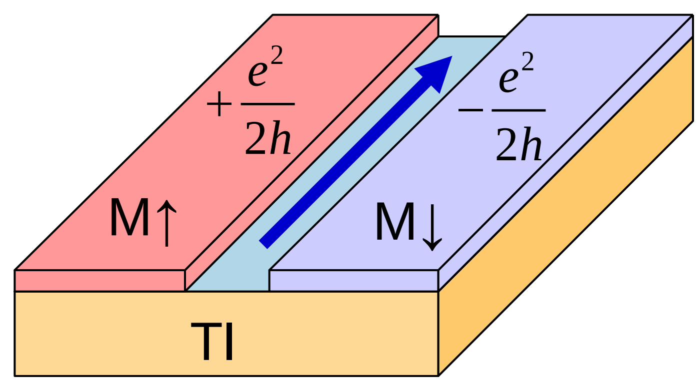
Anomalous QHE : Induce a surface gap by depositing magnetic material

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

Mass due to Exchange field



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

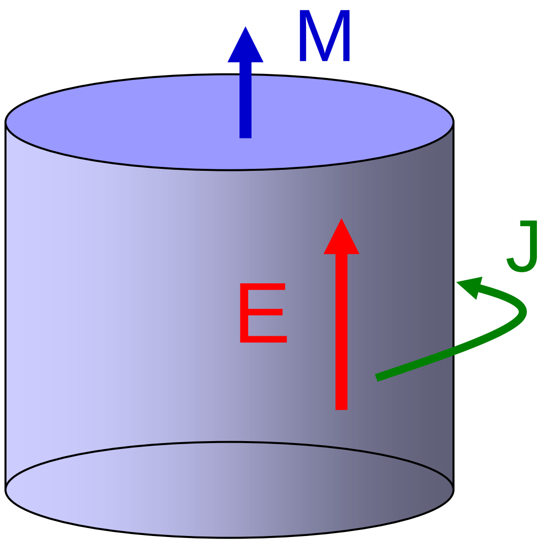


Chiral Edge State at Domain Wall : $\Delta_M \leftrightarrow -\Delta_M$

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)