Topological Materials : Some Basic Concepts

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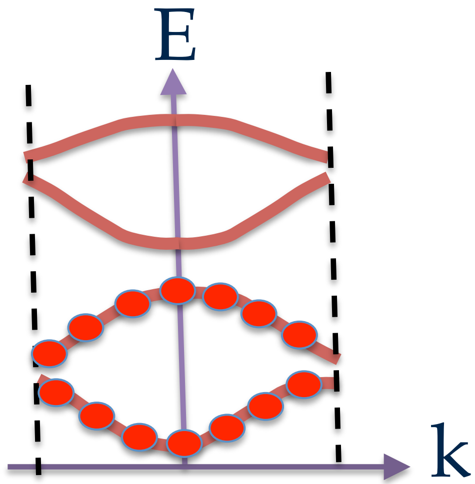
Introduction

Insulators (before 1980)



In insulators, an **energy gap** separates empty and filled electronic states at T=0.

(In contrast, metals have partially filled bands at T=0)

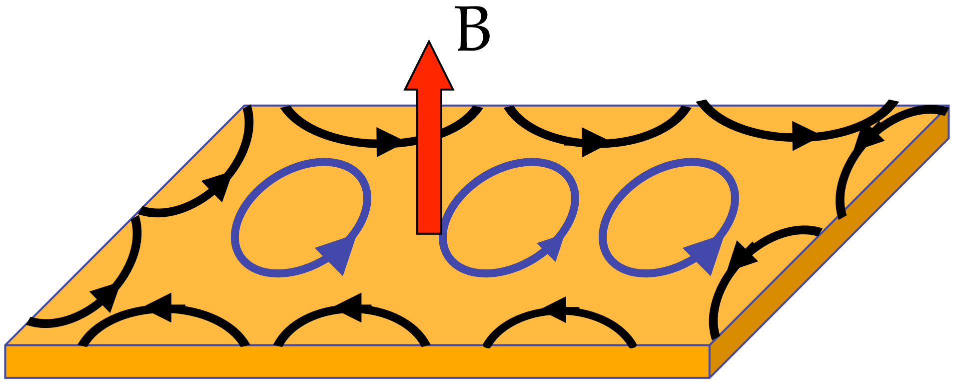
Examples:
Covalent insulators (e.g. GaAs),
atomic insulators (e.g. solid Ar),
vacuum.

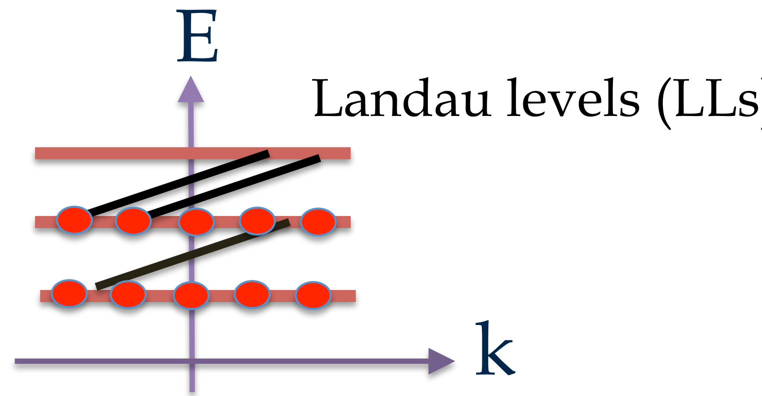
Due to the energy gap, insulators do not conduct electricity under weak, time-independent electric fields.

This talk is about gapped systems that *do* conduct electricity.

Insulators (after 1980)

Quantum Hall insulator



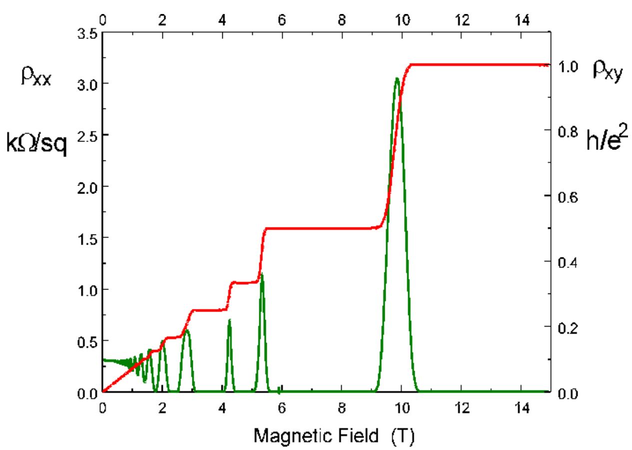


In spite of bulk energy gap, the **edges are metallic.**

Metallic edge states are *robust.*

integer (# of filled LLs)

Hall conductivity is *perfectly quantized.* $$\sigma_{xy}(B) = n\frac{e^2}{h}\mathrm{sgn}(B)$$

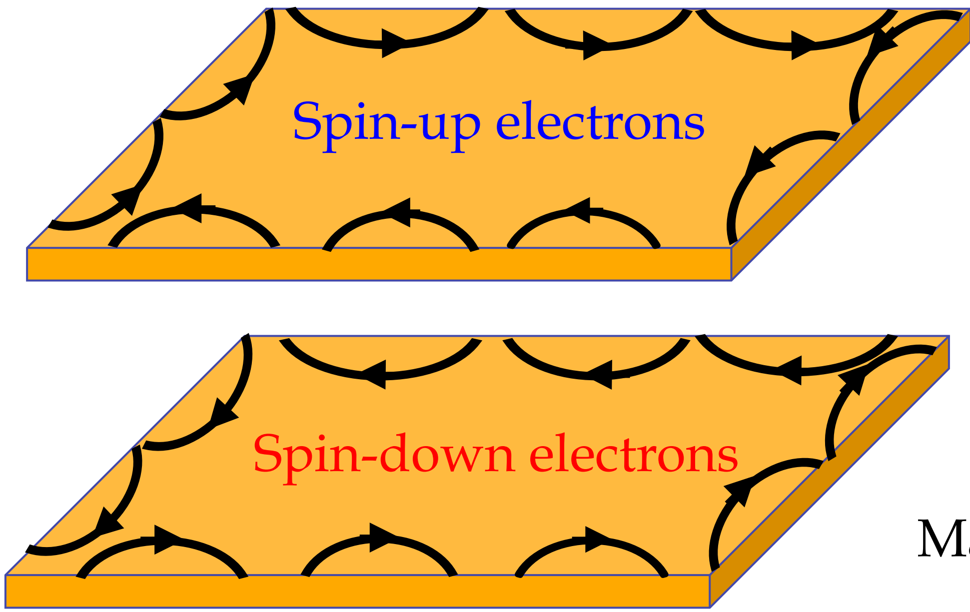


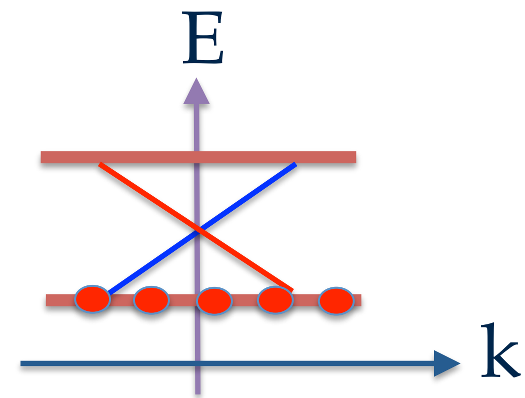
Why is the **quantization independent of sample details**?

Why can **some gapped systems conduct whereas other do not?**

Insulators (after 2005)

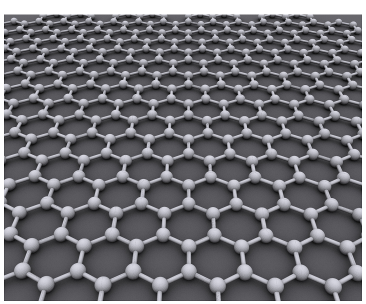
Quantum Spin Hall insulator (with time-reversal symmetry)

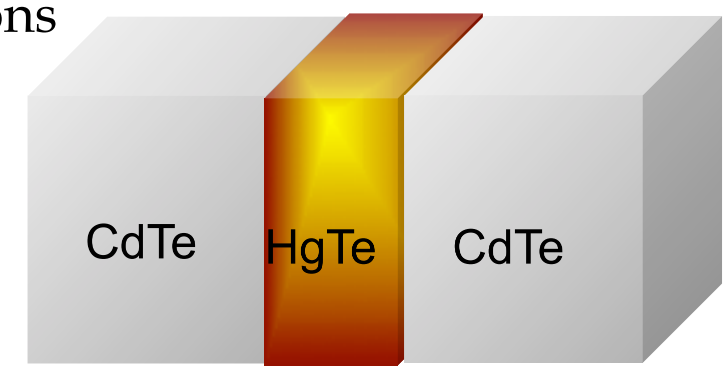




Made possible by spin-orbit coupling

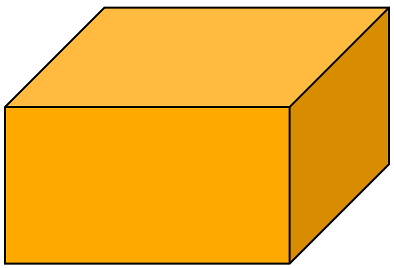
Metallic edge states (*massless 1D Dirac fermions*) are *robust* under non-magnetic perturbations





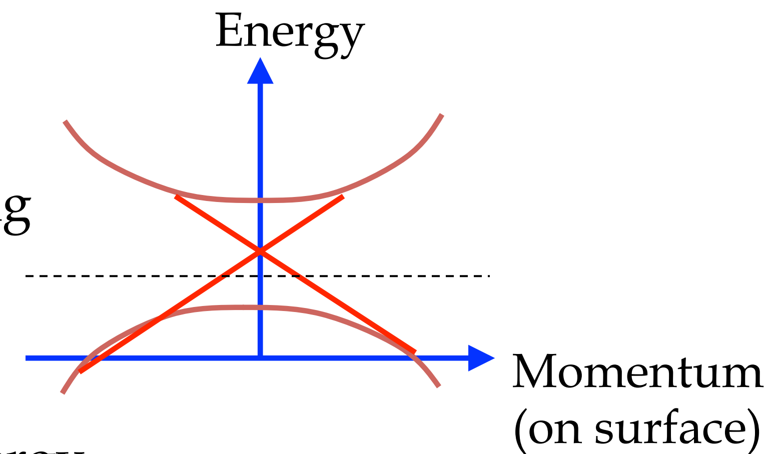
Insulators (after 2007)

3D topological insulators (with time-reversal symmetry)



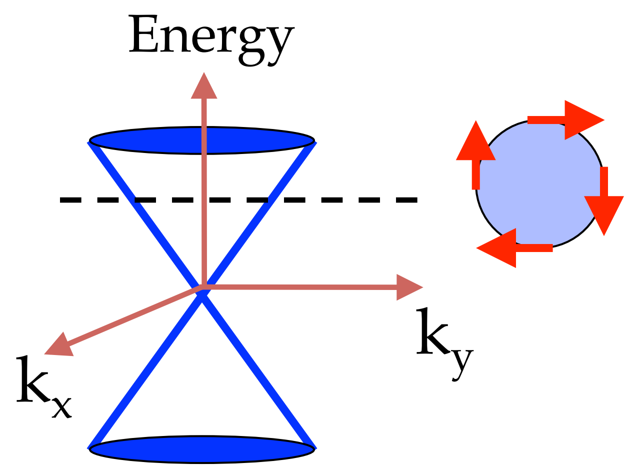
Bi_xSb_{1-x}, Bi_2Te_3, Bi_2Se_3…

Strong spin-orbit coupling



Surface states:

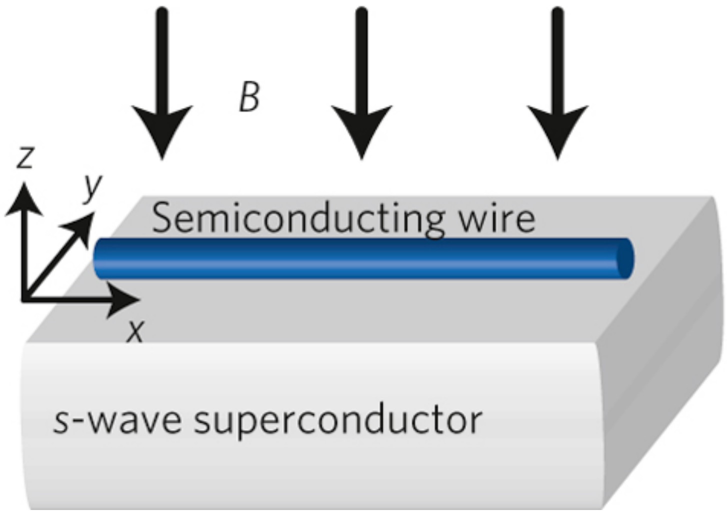
Massless 2D Dirac fermions



Dirac cones robust under non-magnetic perturbations

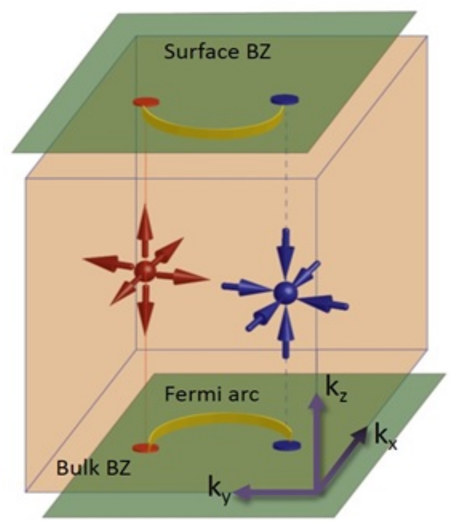
More recent developments

Topological superconductors



Surface states: Majorana fermions

Topological semimetals



3D massless Dirac fermions

Cd_2As_3, TaAs, NbP…

Band Theory

Elements of Traditional Band Theory

Non-interacting electrons moving in a perfectly periodic array of atoms

Eigenstate

$$\boxed{H|\Psi_{\mathbf{k}n}\rangle = E_{\mathbf{k}n}|\Psi_{\mathbf{k}n}\rangle}$$

Hamiltonian Eigen-energy

Crystal momentum *k* is a good quantum number

n is the **band** label

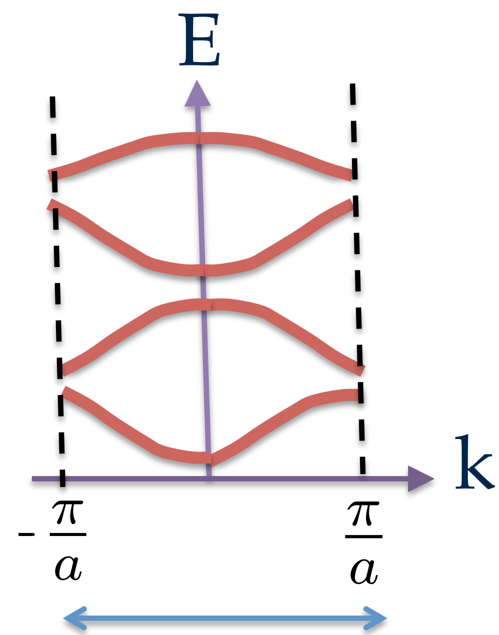
Energies and wave functions have the periodicity of the reciprocal lattice.

Bloch's theorem: Periodic part

$$|\Psi_{\mathbf{k}n}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{\mathbf{k}n}\rangle$$

Bloch Hamiltonian : $h(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}He^{i\mathbf{k}\cdot\mathbf{r}}$

$$h(\mathbf{k})|u_{\mathbf{k}n}\rangle = E_{\mathbf{k}n}|u_{\mathbf{k}n}\rangle$$



1st Brillouin zone (BZ)

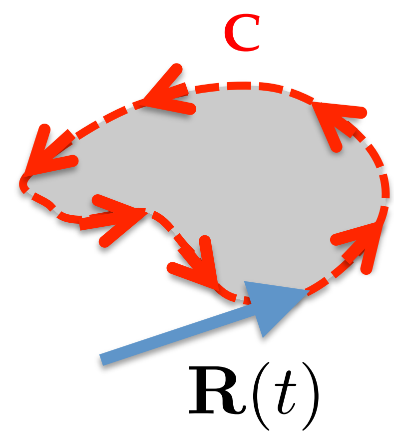
Elements of Topological Band Theory

Berry phase: [M. Berry, 1983]

Consider a Hamiltonian that depends on an external (vector) parameter ***R*.**

$$\boxed{H(\mathbf{R})}$$

Imagine that ***R*** changes in time adiabatically.



What is the time evolution of the wave function?

Initial state: $|\psi(t=0)\rangle = |n, \mathbf{R}(0)\rangle$

State at time *t*: $|\psi(t)\rangle = e^{i\theta(t)}|n, \mathbf{R}(t)\rangle$ (adiabaticity)

$$\boxed{\theta(t) = \frac{1}{\hbar}\int_0^t dt' E_n(\mathbf{R}(t')) - i\int_C d\mathbf{R}\cdot\langle n\mathbf{R}|\frac{d}{d\mathbf{R}}|n, \mathbf{R}\rangle}$$

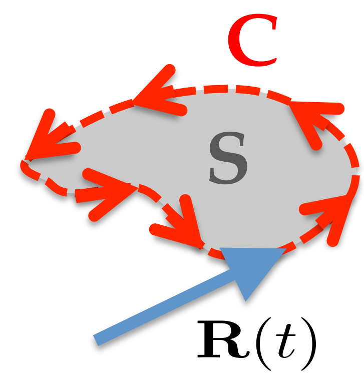
Dynamical phase.

Berry phase (Geometrical phase)

Elements of Topological Band Theory

Berry connection: $\boxed{\mathbf{A}_n(\mathbf{R}) = \langle n, \mathbf{R}|\boldsymbol{\nabla}_{\mathbf{R}}|n, \mathbf{R}\rangle}$

Berry phase: $\boxed{\gamma_n = \int_C \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R}}$



Reminiscent of phase of a particle in an EM field.

The Berry connection is analogue to a vector potential.
Thus, Berry phase is not gauge-invariant unless **C** is a closed loop.

Stokes' theorem: $\oint_C \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R} = \int_S d\mathbf{S} \cdot [\boldsymbol{\nabla}_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})]$

Berry curvature: $\boxed{\mathbf{F}_n(\mathbf{R}) = \boldsymbol{\nabla}_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})}$

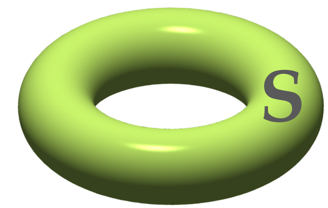
The Berry curvature is analogue to a magnetic field.
Thus, it is gauge-invariant

Elements of Topological Band Theory

Chern number:

Consider a closed surface **S**, such as

or



$$\boxed{n_{\text{Chern}} = \frac{1}{2\pi}\int_S \mathbf{F}_n(\mathbf{R})\cdot d\mathbf{S}}$$

The Chern number is an integer. It is also a **topological invariant**, i.e. independent of the details of the Hamiltonian.

Analogies:

Electric field

Electron's charge

Gauss' Law: $\oint_S \epsilon\mathbf{E}\cdot d\mathbf{S} = e \times \text{integer}$

Gauss-Bonnet theorem: $\frac{1}{4\pi}\oint_S \kappa\, dS = 1 - g$

Gaussian curvature

"Genus"= number of holes

Elements of Topological Band Theory

Example: two-level system (e.g. spin ½ particle in a magnetic field)

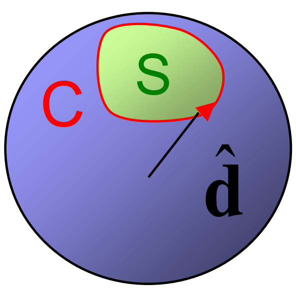
$$\boxed{h(\mathbf{R}) = \mathbf{R} \cdot \boldsymbol{\sigma}}$$

Eigenstates: $|\pm\rangle$ Eigenvalues: $E_\pm(\mathbf{R}) = \pm|\mathbf{R}|$

Berry curvature: $$\boxed{\mathbf{F}_\pm(\mathbf{R}) = \pm\frac{\mathbf{R}}{2R^3}}$$

Field of a monopole located at band degeneracy points.

Sum of Berry curvature over all bands is zero.



Berry phase = ½ (solid angle subtended by *C*)

Chern number= 2 x monopole charge enclosed inside a closed surface

Band Topology in 1D

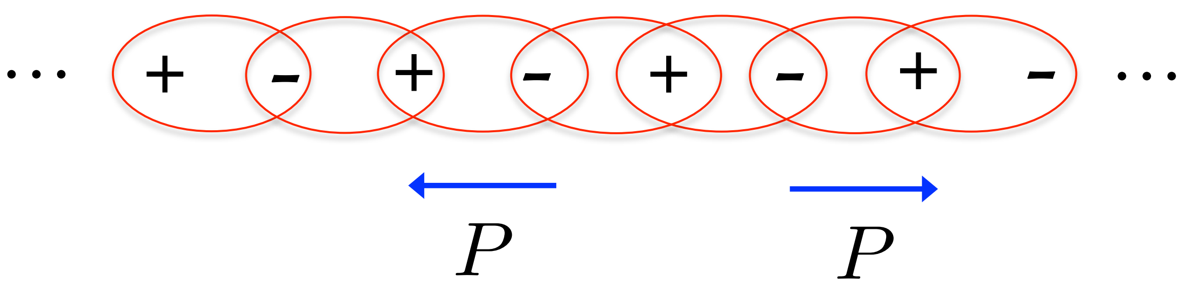
Electric Polarization of a 1D Insulator

Electrical polarization = dipole moment per unit volume.

Polarization charge $\rho = -\nabla \cdot \mathbf{P}$

Polarization current $\mathbf{j} = \partial \mathbf{P}/\partial t$

Electrical polarization defined only modulo $e \times$ integer

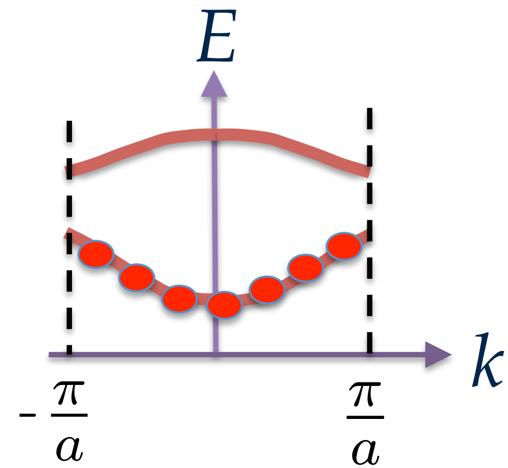


Relation between electric polarization and Berry phase

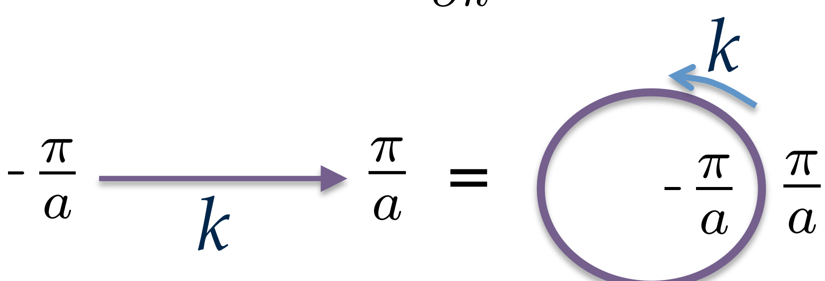
[Resta & Vanderbilt, 1994]

$$\boxed{P = \frac{e}{2\pi} \sum_{n \in \mathrm{occ}} \int_{BZ} A_n(k)\, dk}$$

Berry connection. k plays the role of R



$$A_n(k) = i \langle u_{kn} | \frac{\partial}{\partial k} | u_{kn} \rangle$$



Berry phase defined modulo 2pi → P defined only modulo $e \times$ integer

Link between quantum mechanics and classical electrostatics.

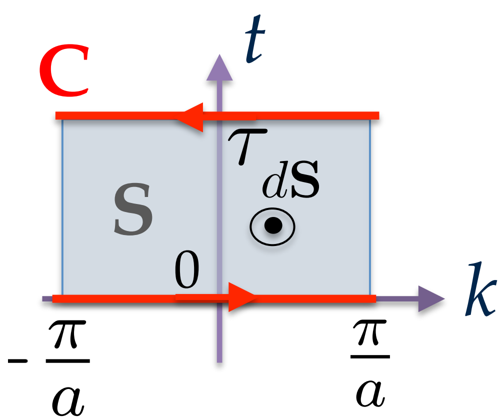
Thouless Charge Pump (1983)

1D insulator under a **time-periodic perturbation**.

Bloch Hamiltonian: $\boxed{h(k,t) = h(k,t+\tau)}$

What is the charge pumped in one cycle of the external perturbation?

$$Q = \int_0^\tau dt \frac{\partial P}{\partial t} = P(t=\tau) - P(t=0) \equiv \Delta P$$

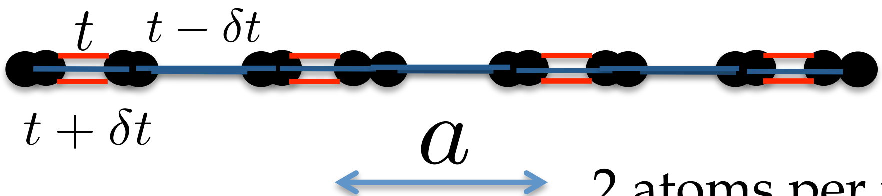


$$\mathbf{R} = (k,t)$$

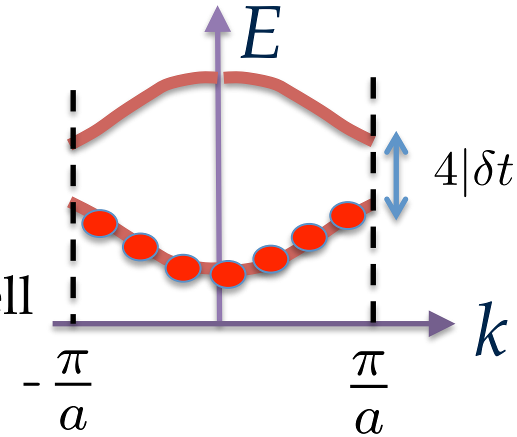
$$\boxed{\Delta P = \frac{e}{2\pi} \sum_{n\in\mathrm{occ}} \oint_C \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R}}$$

Su-Schrieffer-Heeger Model (1979)

1D lattice, spinless electrons, half filling.

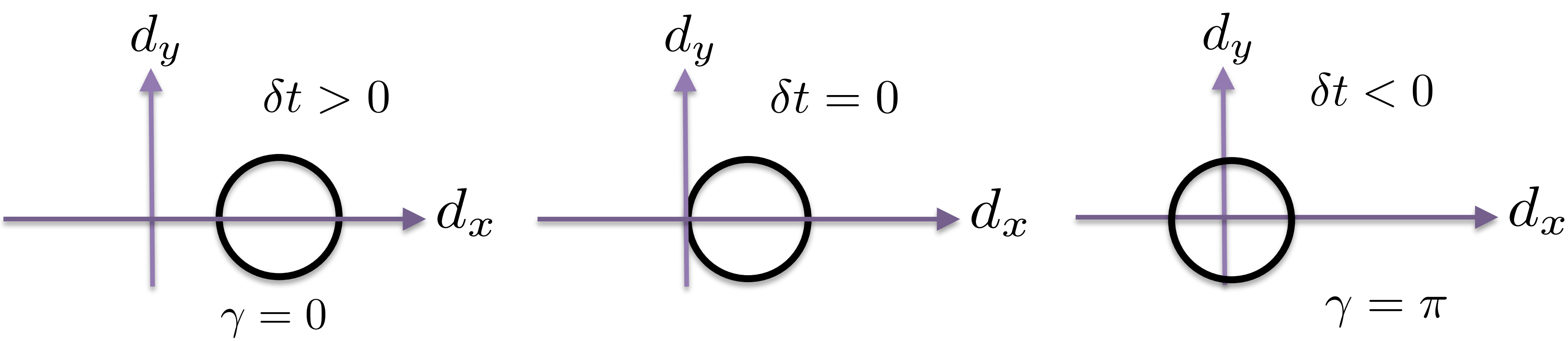


2 atoms per unit cell



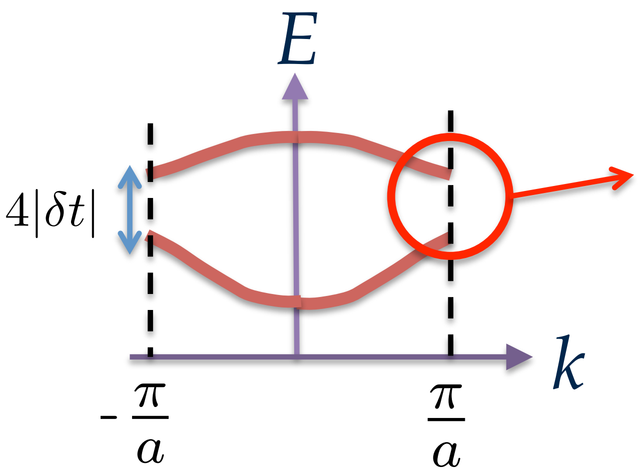
$$\boxed{h(k) = d_x(k)\sigma^x + d_y(k)\sigma^y}$$

How does ***d*** change as *k* runs from $-\pi/a$ to π/a ?



Particle-hole (PH) symmetry → $d_z=0$ → the bulk gap must close in order to go from one phase to another. If PH symmetry is broken, the two phases are no longer distinct. **Symmetry-protected topological phase**.

Emergence of Dirac Fermions at low energies:



$$k = \pi/a - q$$

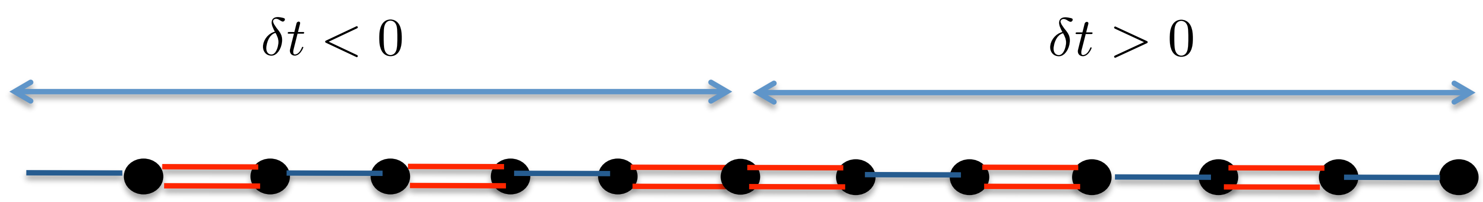
Assume: $|\delta t| \ll t$ and $qa \ll 1$

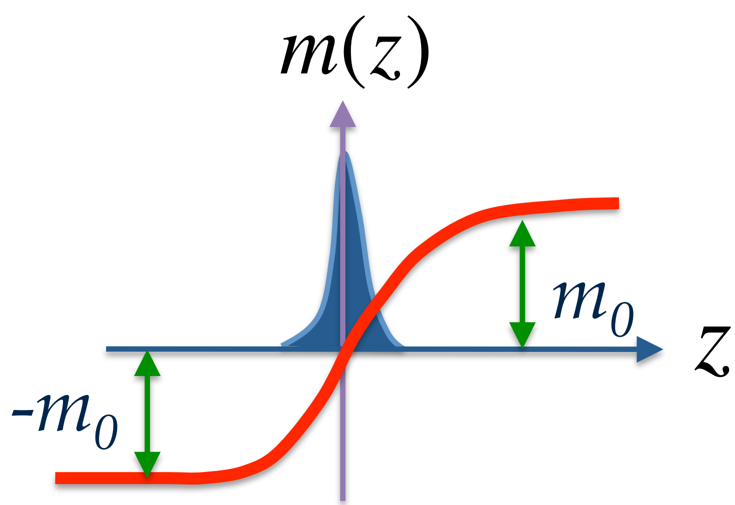
$$\boxed{h(q) \simeq m\sigma^x + vq\sigma^y}$$ 1D Dirac Hamiltonian

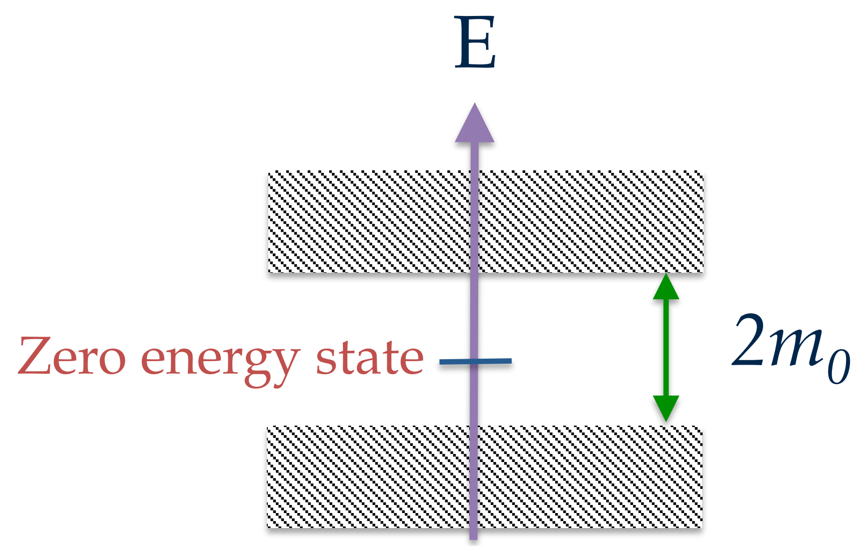
$$\boxed{m \equiv 2\delta t}$$ Dirac mass

$$\boxed{v \equiv at}$$ Velocity of Dirac fermion

Emergence of zero modes at “domain walls”







$$h(z) \simeq m(z)\sigma^x - iv\sigma^y\partial_z$$

Jackiw-Rebbi zero mode: localized at domain wall, decay length v/m_0

Insensitive to details of the Hamiltonian.

This result can be generalized to 2 and 3 dimensions.

Band Topology in 2D

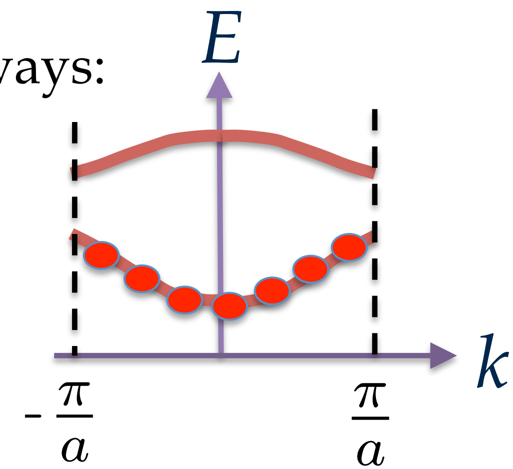
The Hall conductivity of a 2D band insulator is always quantized

$$\boxed{\mathbf{j} = e \sum_{\mathbf{k}n} \langle \psi_{\mathbf{k}n} | \mathbf{v} | \psi_{\mathbf{k}n} \rangle f_{\mathbf{k}n}}$$

Electric current in a crystal.

Vanishes in equilibrium.

An applied electric field can induce a current in two ways:



(i) By changing the population of the states: $\delta f_{\mathbf{k}n}$

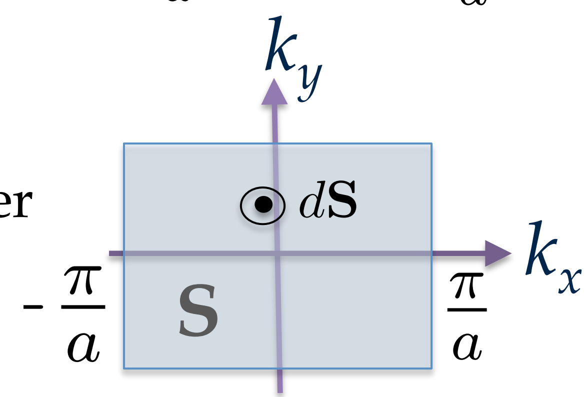
This effect vanishes in insulators
at low temperatures and under dc fields.

(ii) *By changing the eigenstates:* $\delta | \psi_{\mathbf{k}n} \rangle$

This leads to a Hall conductivity in insulators.

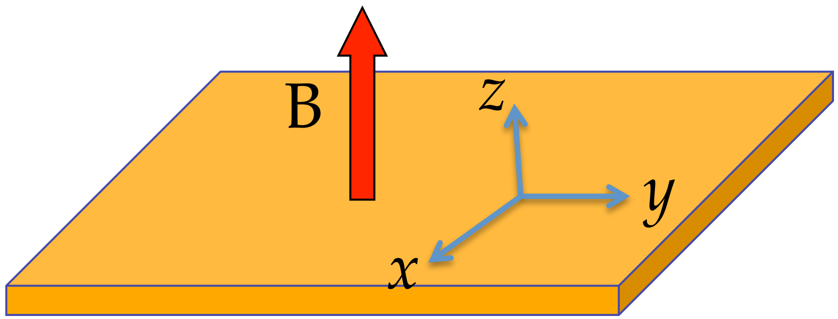
$$\sigma_{xy} = \frac{e^2}{h} \sum_{n \in \mathrm{occ}} \frac{1}{2\pi} \int_S d\mathbf{S} \cdot \mathbf{F}_n(\mathbf{k})$$

Chern number



Chern number vanishes in presence of time-reversal symmetry

Quantum Hall Insulator

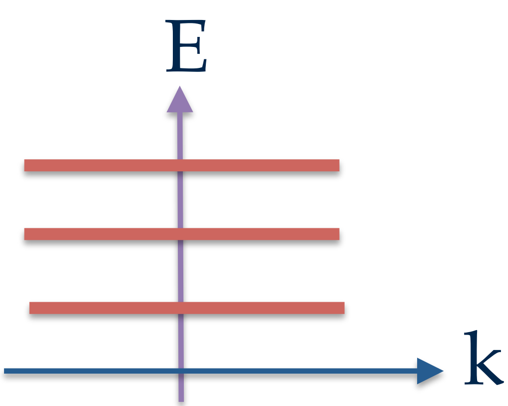


$$H = \frac{1}{2m}\left[p_x^2 + \left(p_y - \frac{eB}{c}x\right)^2\right]$$

(Landau gauge)

p_y is a good quantum number.

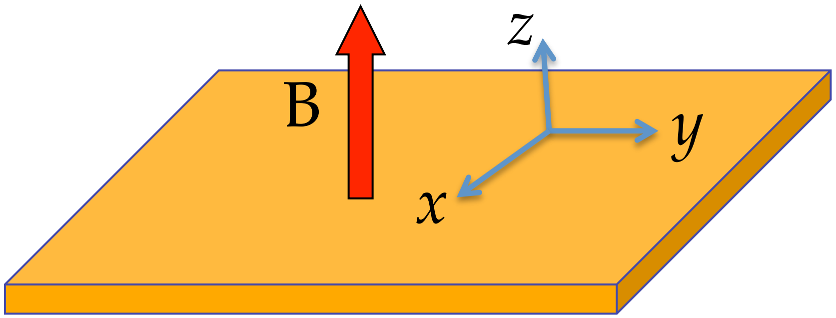
In the x-direction, a harmonic oscillator with frequency ω_c centered at $c\,p_y/(eB)$



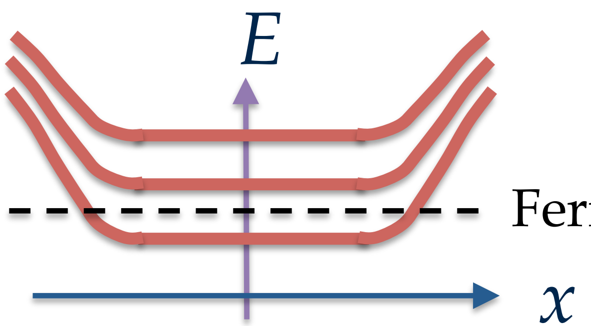
$$E_n = \omega_c(n + 1/2)$$

$$\omega_c = eB/(mc)$$

Edge states in quantum Hall insulators:



Assume infinite length along y, finite length along x.



LLs bend near sample edge.

Fermi level intersects LLs at the edge.

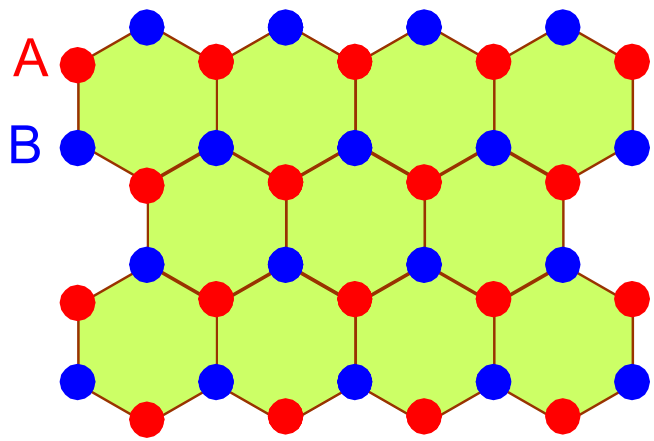
# of edge states at the Fermi level= # of occupied bulk LLs =sum over Chern numbers of occupied LLs

Electrons on same edge move along the same direction.

Electrons on opposite edges move along the opposite directions.

Robustness against backscattering

Graphene



One orbital per site

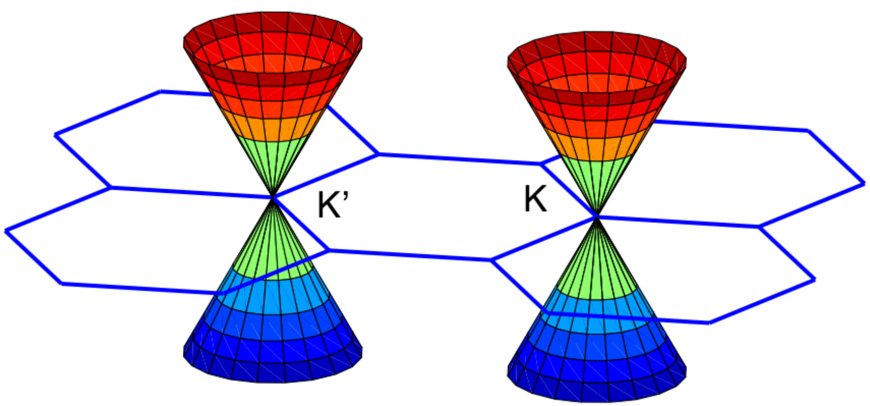
Two atoms per unit cell (A and B)

No spin (for now)

A/B pseudospin

$$\boxed{h(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}}$$

Emergence of massless Dirac fermions at low energies:



K/K' pseudospin

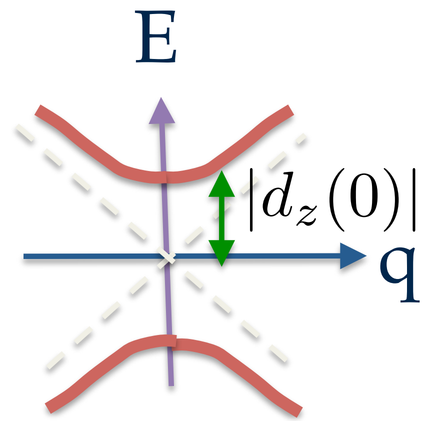
$$\boxed{h(\mathbf{q}) = v\tau^z\sigma^x q_x + v\sigma^y q_y}$$

Momentum measured from Dirac node

Due to time-reversal symmetry and inversion symmetry, $d_z=0$

How to make spinless graphene insulating

$$\boxed{h(\mathbf{q}) = v\,\tau^z\sigma^x\,q_x + v\,\sigma^y q_y + d_z(\mathbf{q})\sigma^z}$$



Need to break either time-reversal symmetry or inversion symmetry

(i) Break inversion symmetry

$$\boxed{d_z(\mathbf{q}) = m_S}$$

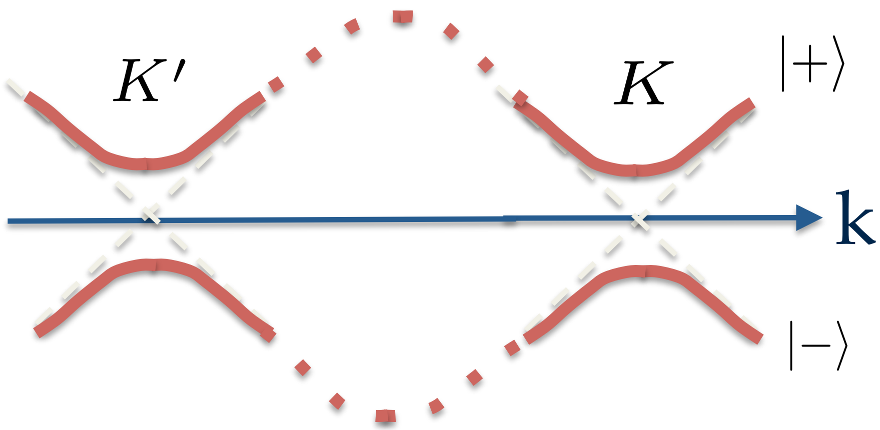
Semenoff insulator (1984)

(ii) Break time-reversal symmetry

$$\boxed{d_z(\mathbf{q}) = m_H\tau^z}$$

Haldane insulator (1988)
[a.k.a. Chern insulator]

Chern number in spinless graphene



"Chern number" for Dirac fermion at K:

$$\boxed{n_K = \frac{1}{2}\mathrm{sgn}(v_K^x v_K^y m_K)}$$

(similarly for K′)

Total Chern # of a band: $\boxed{n_{\mathrm{Chern}} = n_K + n_{K'}}$

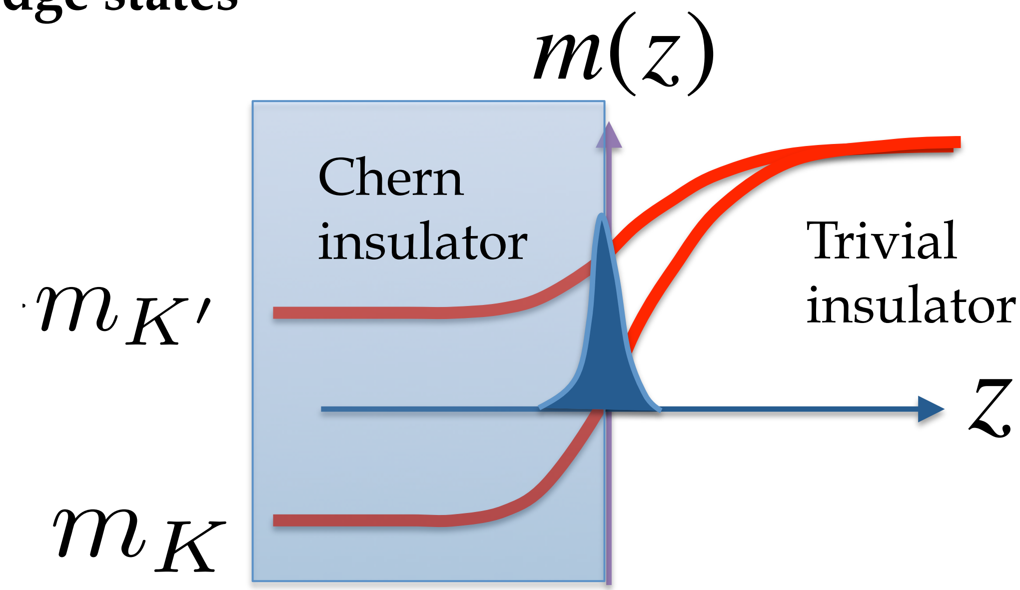
Semenoff insulator:

$m_K = m_{K'}$ $\boxed{n_{\mathrm{Chern}} = 0}$ Trivial insulator

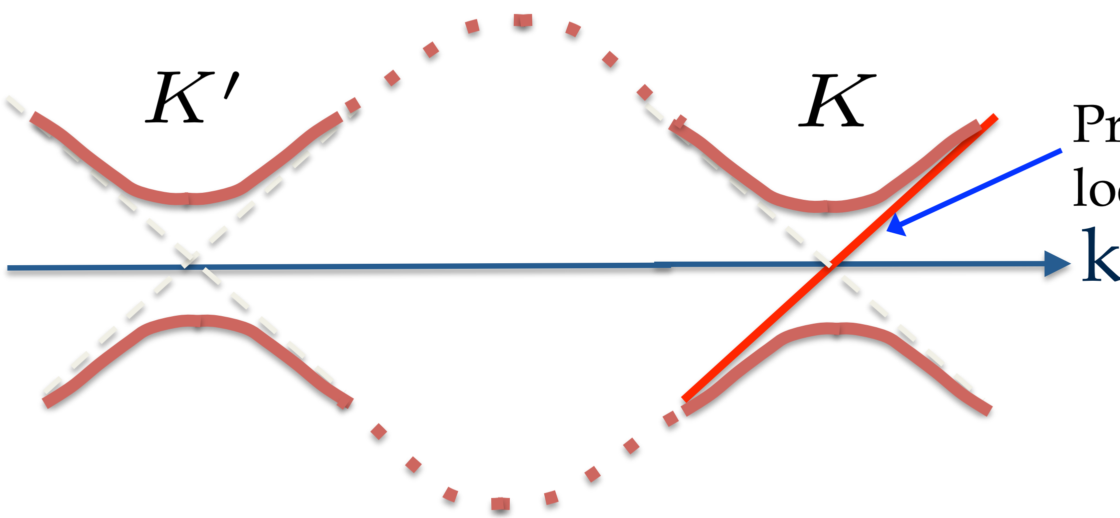
Haldane/Chern insulator:

$m_K = -m_{K'}$ $\boxed{n_{\mathrm{Chern}} = \mathrm{sgn}(m_H)}$ Topological insulator

Edge states



Jackiw-Rebbi mode

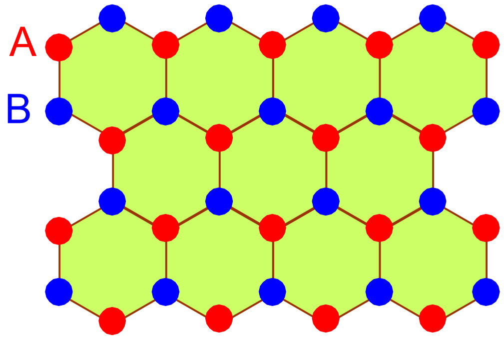


Propagating mode localized along edge

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

Quantum Hall effect without magnetic field (1988)

Kane-Mele model (2005)



One orbital per site

Two atoms per unit cell (A and B)

Include spin

Low-energy effective Hamiltonian:

spin

$$\boxed{h(\mathbf{q}) = v_x \tau^z \sigma^x q_x + v_y \sigma^y q_y + \lambda_{so} \tau^z \sigma^z s^z}$$

Opens a gap at K and K' **without breaking any symmetries**

s^z is conserved.

Spin-degenerate energy spectrum.

Two copies of a Haldane/Chern insulator

$$\boxed{h(\mathbf{q}) = v_x \tau^z \sigma^x q_x + v_y \sigma^y q_y + \lambda_{so} \tau^z \sigma^z s^z}$$

Spin-up electrons:

Haldane/Chern insulator with mass $\boxed{m_H = +\lambda_{so}}$

Spin-down electrons:

Haldane/Chern insulator with mass $\boxed{m_H = -\lambda_{so}}$

Total Chern number: $\boxed{n_\uparrow + n_\downarrow = 0}$

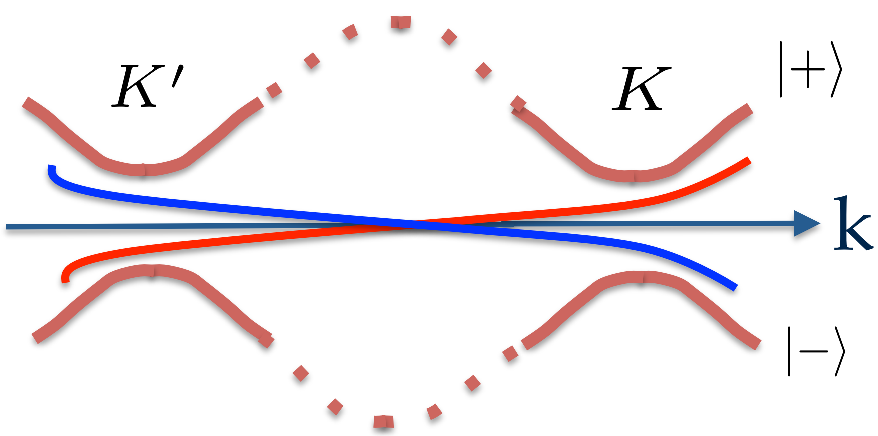
"Spin Chern number": $\boxed{n_\uparrow - n_\downarrow = 2\,\mathrm{sgn}(\lambda_{so})}$

Spin-Hall conductivity:

$$\boxed{\sigma^{s}_{xy} = \sigma^{\uparrow}_{xy} - \sigma^{\downarrow}_{xy} = (n_{\uparrow} - n_{\downarrow})\frac{e^2}{h}}$$

Quantum spin-Hall insulator

Edge states:



Spin-up edge state

Spin-down edge state

Time-reversal symmetry →

(i) spin-up and spin-down edge states counter-propagate.

(ii) edge states are degenerate at $k=0$ (Kramer's degeneracy).

Practical issue: $\lambda_{\rm so} < 1\mathrm{mK}$

Alternative systems : HgTe/CdTe quantum wells (2007)

InAs/GaSb quantum wells (2011)

Silicene and other organic materials (2011)

Fundamental issue: In general spin is not conserved along any direction

One can no longer think of two decoupled copies of a Chern insulator. Likewise, the spin-Chern number is ill-defined.

However, the **edges states remain robust so long as the bulk gap does not close.** This is another example of symmetry-protected topological phase (the symmetry in question is time-reversal)**.**

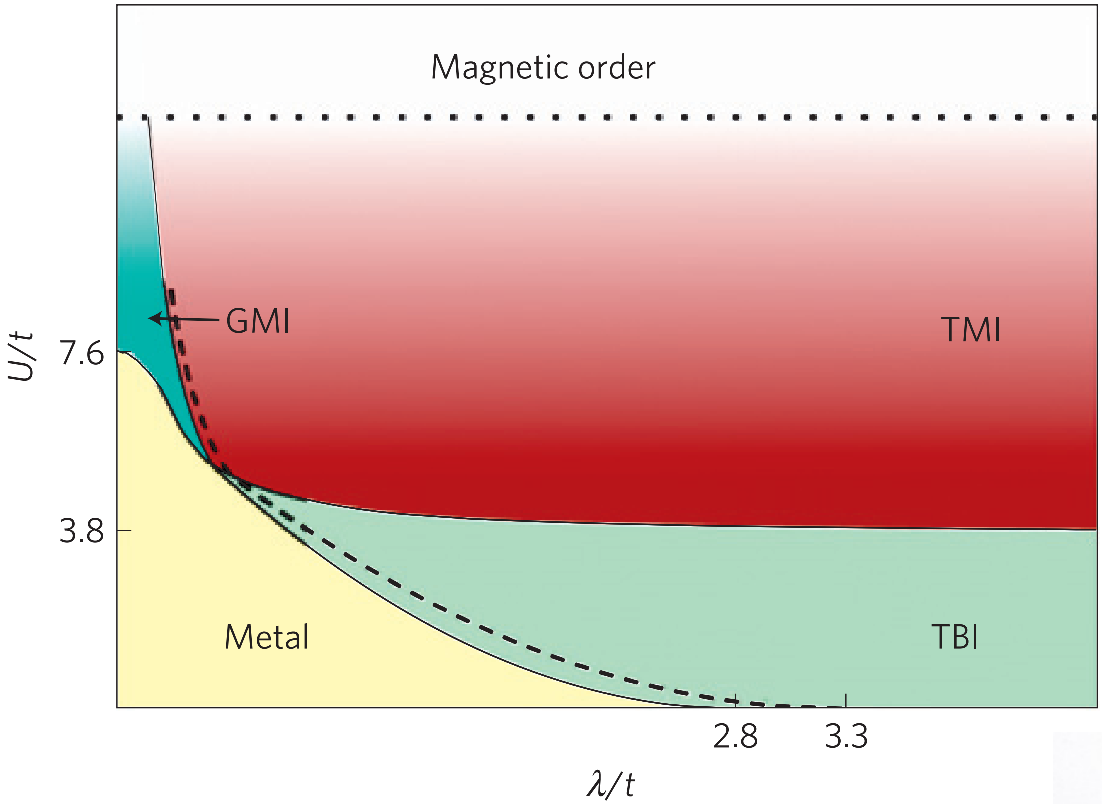
There is a **(non-Chern) topological invariant** that is responsible for this robustness. This is the **Z_2 invariant**. Its inception and development in 2D and 3D crystals (2005-2007) led to an explosion of research in topological insulators.

Non-interacting topological phases in any dimension

Symmetry				d							
AZ	Θ	Ξ	Π	1	2	3	4	5	6	7	8
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

[Kitaev, Ludwig, Schnyder, Ryu, 2008]

Interacting topological phases



Pesin and Balents, Nature Phys. **6**, 376 (2010)

Topological invariants in interacting systems

So far, we have discussed the band topology in terms of the single-particle wave functions.

How to capture the band topology of interacting systems beyond the mean field approximation?

Topological Hamiltonian

Non-interacting Hamiltonian

$$\boxed{h_{\text{eff}}(\mathbf{k}) \equiv -G^{-1}(0,\mathbf{k}) = h(\mathbf{k}) + \Sigma(0,\mathbf{k})}$$

Full Green's function
(zero Matsubara frequency)

Electron self-energy
(zero Matsubara frequency)

Use the eigenstates of $h_{\text{eff}}(\mathbf{k})$ to calculate the Chern number in interacting systems.

Wang *et al.*, PRX **2**, 031008 (2012)