Topological Insulators and Superconductors

Lecture #1: Topology and Band Theory

Lecture #2: Topological Insulators in 2 and 3 dimensions

Lecture #3: Topological Superconductors, Majorana Fermions an Topological quantum compuation

General References :

M.Z. Hasan and C.L. Kane, RMP in press, arXiv:1002.3895
X.L. Qi and S.C. Zhang, Physics Today 63 33 (2010).
J.E. Moore, Nature 464, 194 (2010).

My collaborators :

Gene Mele, Liang Fu, Jeffrey Teo, Zahid Hasan

Topology and Band Theory

I. Introduction

- Insulating State, Topology and Band Theory

II. Band Topology in One Dimension

- Berry phase and electric polarization
- Su Schrieffer Heeger model :

  domain wall states and Jackiw Rebbi problem
- Thouless Charge Pump

III. Band Topology in Two Dimensions

- Integer quantum Hall effect
- TKNN invariant
- Edge States, chiral Dirac fermions

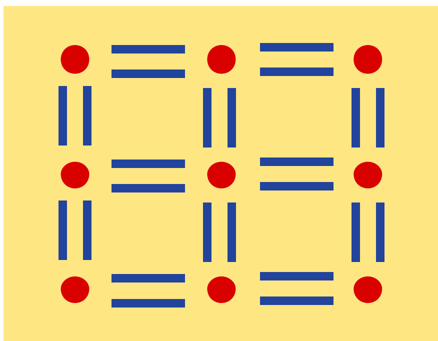
IV. Generalizations

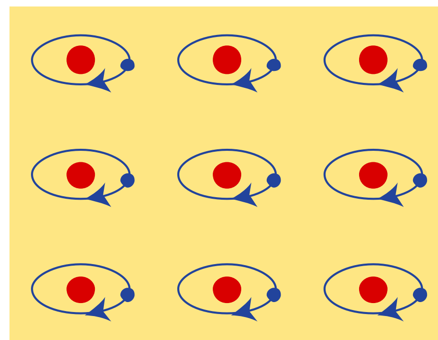
- Bulk-Boundary correspondence
- Higher dimensions
- Topological Defects

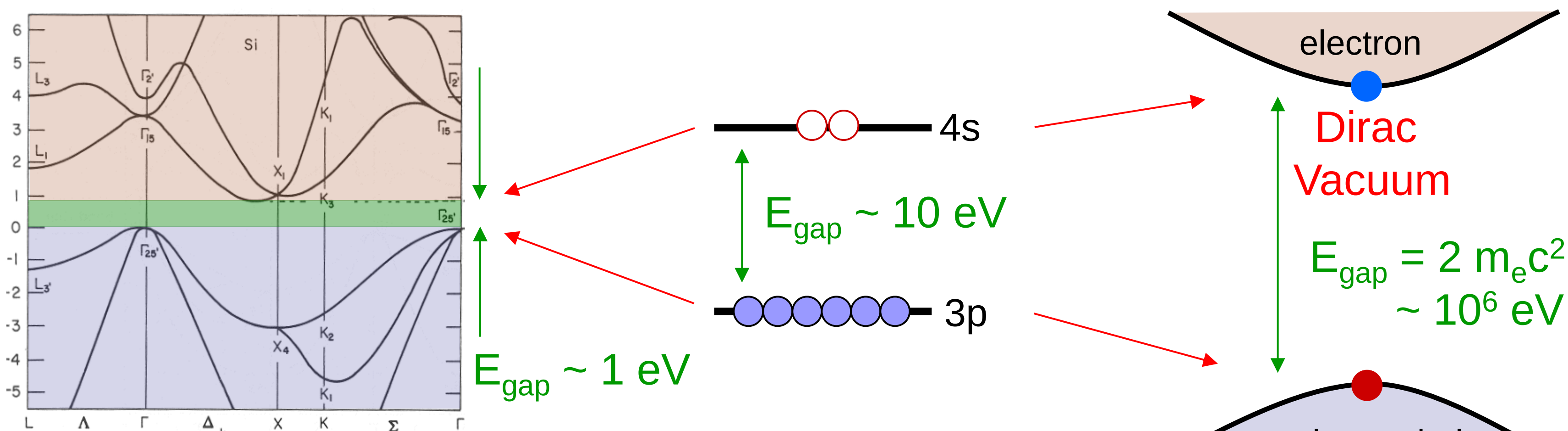
The Insulating State

Characterized by energy gap: absence of low energy electronic excitations

Covalent Insulator	Atomic Insulator	The vacuum
e.g. intrinsic semiconductor	e.g. solid Ar	



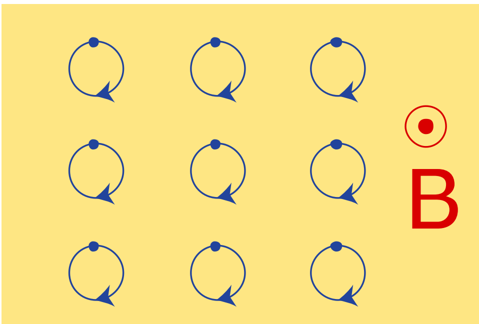


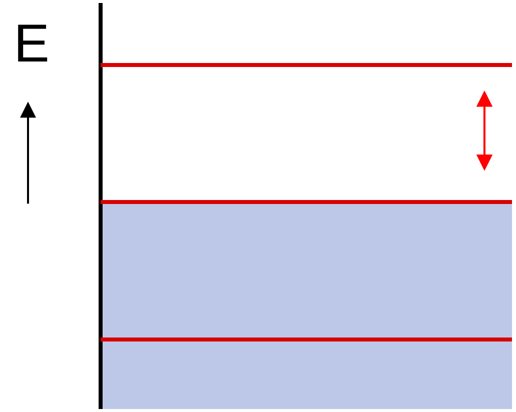


Silicon

The Integer Quantum Hall State

2D Cyclotron Motion, Landau Levels

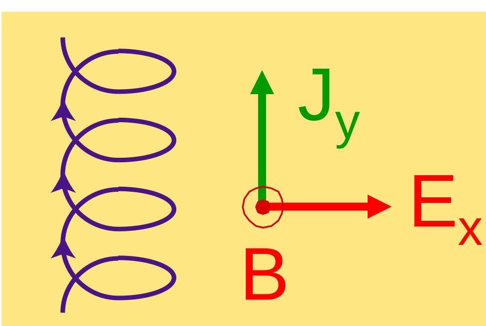




$$E_{gap} = \hbar\omega_c$$

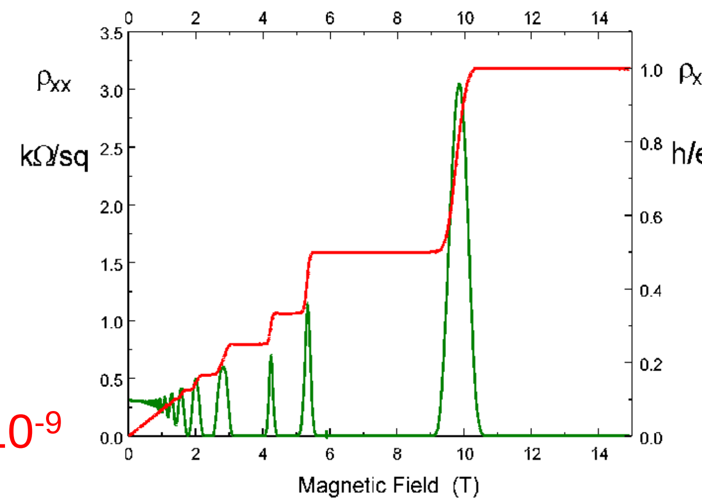
Energy gap, but NOT an insulator

Quantized Hall conductivity : $J_y = \sigma_{xy} E_x$



$$\sigma_{xy} = n\frac{e^2}{h}$$

Integer accurate to 10^{-9}



Topology

The study of geometrical properties that are insensitive to smooth deformations

Example: 2D surfaces in 3D

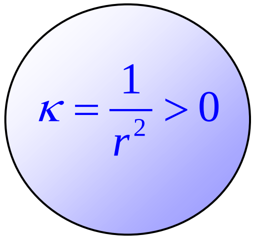
A closed surface is characterized by its genus, g = # holes

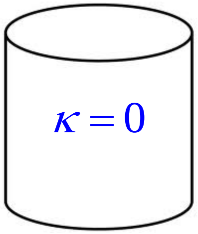
g=0

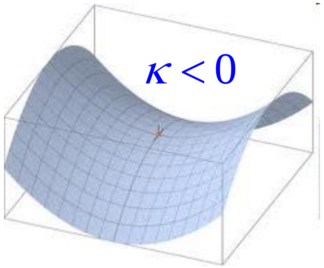
g=1

g is an integer topological invariant that can be expressed in terms of the gaussian curvature κ that characterizes the local radii of curvature

$$\kappa = \frac{1}{r_1 r_2}$$







Gauss Bonnet Theorem : $$\int_S \kappa dA = 4\pi(1-g)$$

A good math book : Nakahara, ‘Geometry, Topology and Physics’

Band Theory of Solids

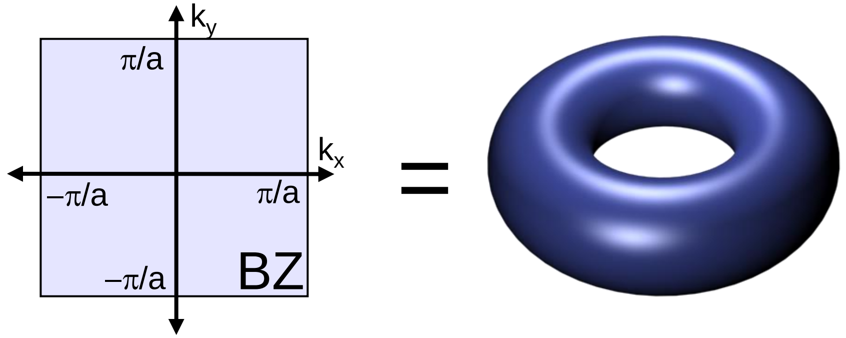
Bloch Theorem :

Lattice translation symmetry $T(\mathbf{R})|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}|\psi\rangle$ $\qquad |\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u(\mathbf{k})\rangle$

Bloch Hamiltonian $H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\mathrm{H}e^{i\mathbf{k}\cdot\mathbf{r}}$ $\qquad H(\mathbf{k})|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})|u_n(\mathbf{k})\rangle$

$\mathbf{k} \in$ Brillouin Zone

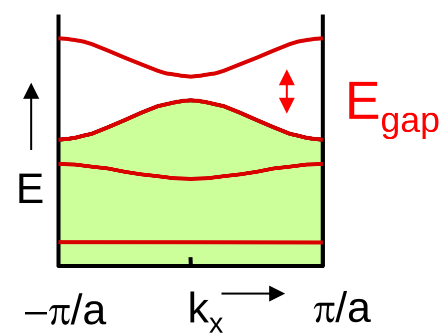
$=$ Torus, T^d



Band Structure :

A mapping $\mathbf{k} \mapsto H(\mathbf{k})$

(or equivalently to $E_n(\mathbf{k})$ and $|u_n(\mathbf{k})\rangle$)



Topological Equivalence : adiabatic continuity

Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap

Berry Phase

Phase ambiguity of quantum mechanical wave function

$$\left|u(\mathbf{k})\right\rangle \to e^{i\phi(\mathbf{k})}\left|u(\mathbf{k})\right\rangle$$

Berry connection : like a vector potential $\mathbf{A} = -i\left\langle u(\mathbf{k})\right|\nabla_{\mathbf{k}}\left|u(\mathbf{k})\right\rangle$

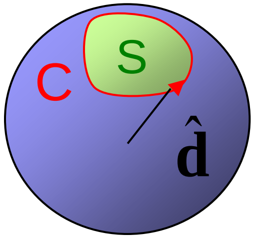
$$\mathbf{A} \to \mathbf{A} + \nabla_{\mathbf{k}}\phi(\mathbf{k})$$

Berry phase : change in phase on a closed loop C $\gamma_C = \oint_C \mathbf{A}\cdot d\mathbf{k}$

Berry curvature : $\mathbf{F} = \nabla_{\mathbf{k}} \times \mathbf{A}$ $\gamma_C = \int_S \mathbf{F}\, d^2k$

Famous example : eigenstates of 2 level Hamiltonian

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k})\cdot\vec{\sigma} = \begin{pmatrix} d_z & d_x - id_y \\ d_x + id_y & -d_z \end{pmatrix}$$



$$H(\mathbf{k})\left|u(\mathbf{k})\right\rangle = +\left|\mathbf{d}(\mathbf{k})\right|\left|u(\mathbf{k})\right\rangle$$

$$\gamma_C = \frac{1}{2}\left(\text{Solid Angle swept out by } \hat{\mathbf{d}}(\mathbf{k})\right)$$

Topology in one dimension : Berry phase and electric polarization

see, e.g. Resta, RMP 66, 899 (1994)

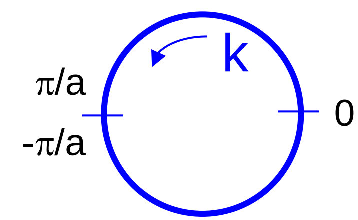
Electric Polarization

$$P = \frac{\text{dipole moment}}{\text{length}} \qquad \nabla \cdot P = \rho_b$$

The end charge is not completely determined by the bulk polarization P because integer charges can be added or removed from the ends :

$$Q = P \text{ mod } e$$

Polarization as a Berry phase : $$P = \frac{e}{2\pi} \oint A(k)dk$$



P is not gauge invariant under "large" gauge transformations.
This reflects the end charge ambiguity

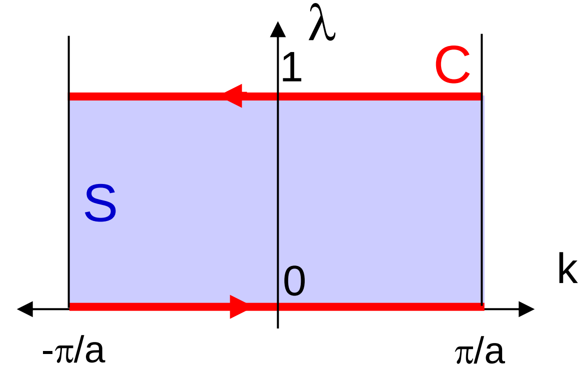
$$P \rightarrow P + en \quad \text{when} \quad |u(k)\rangle \rightarrow e^{i\phi(k)}|u(k)\rangle \quad \text{with} \quad \phi(\pi/a) - \phi(-\pi/a) = 2\pi n$$

Changes in P, due to adiabatic variation are well defined and gauge invariant

$$|u(k)\rangle \rightarrow |u(k,\lambda(t))\rangle$$

$$\Delta P = P_{\lambda=1} - P_{\lambda=0} = \frac{e}{2\pi}\oint_C \mathbf{A}dk = \frac{e}{2\pi}\int_S \mathbf{F}dkd\lambda$$

gauge invariant Berry curvature



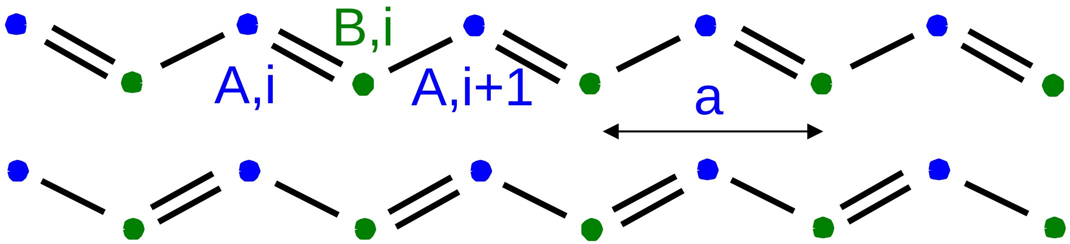
Su Schrieffer Heeger Model

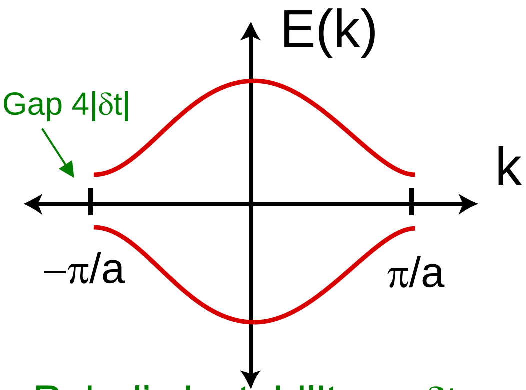
model for polyacetalene
simplest “two band” model

$$H = \sum_i (t+\delta t) c_{Ai}^\dagger c_{Bi} + (t-\delta t) c_{Ai+1}^\dagger c_{Bi} + h.c.$$

$\delta t > 0$

$\delta t < 0$





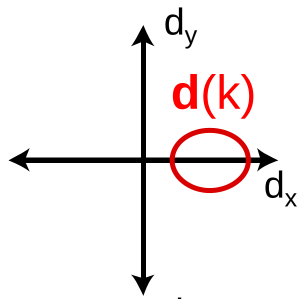
Peierl’s instability → δt

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

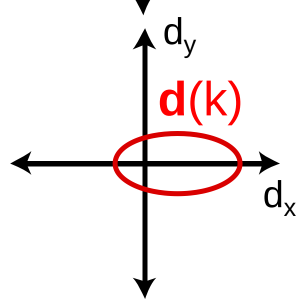
$$d_x(k) = (t+\delta t) + (t-\delta t)\cos ka$$

$$d_y(k) = (t-\delta t)\sin ka$$

$$d_z(k) = 0$$



δt>0 : Berry phase 0
P = 0

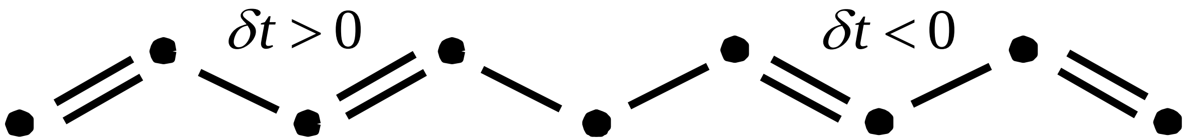


δt<0 : Berry phase π
P = e/2

Provided symmetry requires $d_z(k)=0$, the states with δt>0 and δt<0 are topologically distinct.
Without the extra symmetry, all 1D band structures are topologically equivalent.

Domain Wall States

An interface between different topological states has topologically protected midgap states



Low energy continuum theory :

For small δt focus on low energy states with k~π/a

$$k \rightarrow \frac{\pi}{a} + q \quad ; \quad q \rightarrow -i\partial_x$$

$$H = -i\mathrm{v}_F \sigma_x \partial_x + m(x)\sigma_y \qquad \mathrm{v}_F = ta \quad ; \quad m = 2\delta t$$

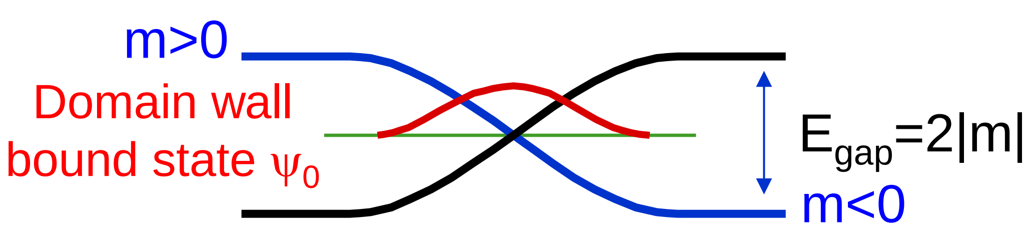
Massive 1+1 D Dirac Hamiltonian $\quad E(q) = \pm\sqrt{(\mathrm{v}_F q)^2 + m^2}$

"Chiral" Symmetry : $\quad \{\sigma_z, H\} = 0 \quad \rightarrow \quad \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$

Any eigenstate at +E has a partner at -E

Zero mode : topologically protected eigenstate at E=0

(Jackiw and Rebbi 76, Su Schrieffer, Heeger 79)

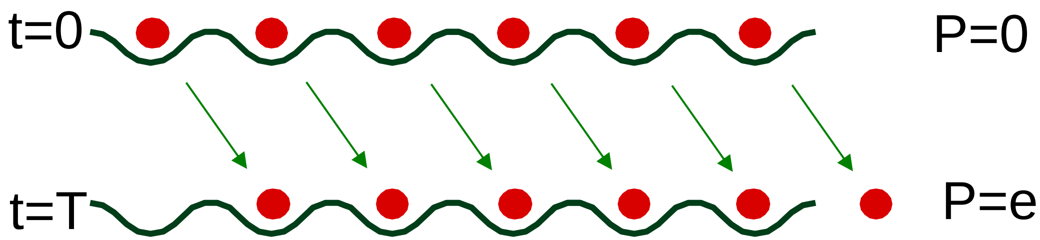


$$\psi_0(x) = e^{-\int_0^x m(x')dx'/\mathrm{v}_F} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

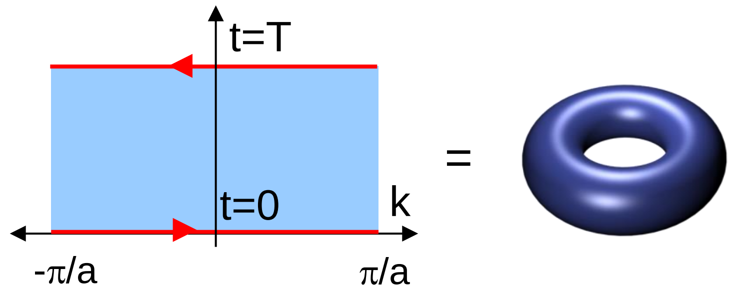
Thouless Charge Pump

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

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



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

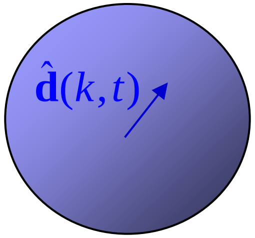


$$n=\frac{1}{2\pi}\int_{T^2}\mathbf{F}dkdt$$

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

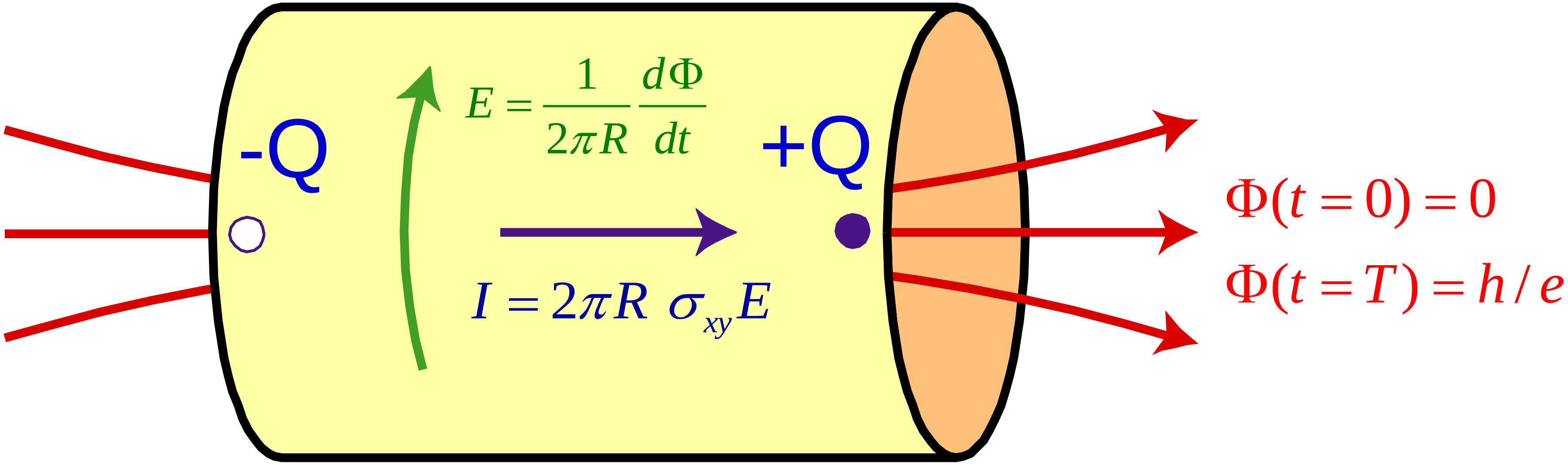
In the 2 band model, the Chern number is related to the solid angle swept out by $\hat{\mathbf{d}}(k,t)$, which must wrap around the sphere an integer n times.

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



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 : $H(T) = U^\dagger H(0) U$

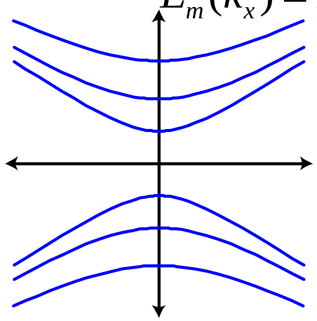
$$\Delta Q = ne \quad \rightarrow \quad \sigma_{xy} = n\frac{e^2}{h}$$

TKNN Invariant

Thouless, Kohmoto, Nightingale and den Nijs 82

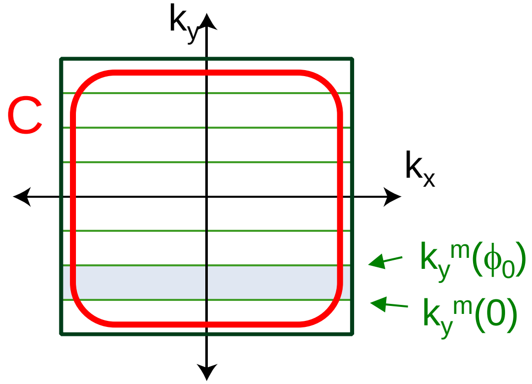
View cylinder as 1D system with subbands labeled by $k_y^m(\Phi) = \frac{1}{R}\left(m + \frac{\Phi}{\phi_0}\right)$

$$\Delta Q = \sum_m \frac{e}{2\pi}\int_0^{\phi_0} d\Phi \int dk_x \mathbf{F}\left(k_x, k_y^m(\Phi)\right) = ne$$



TKNN number = Chern number $\sigma_{xy} = n\frac{e^2}{h}$

$$n = \frac{1}{2\pi}\int_{BZ} d^2k \mathbf{F}(\mathbf{k}) = \frac{1}{2\pi}\oint_C \mathbf{A}\cdot d\mathbf{k}$$

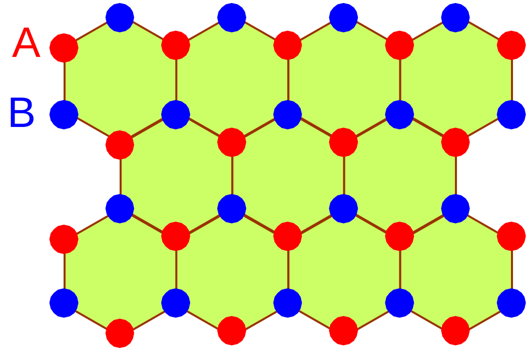


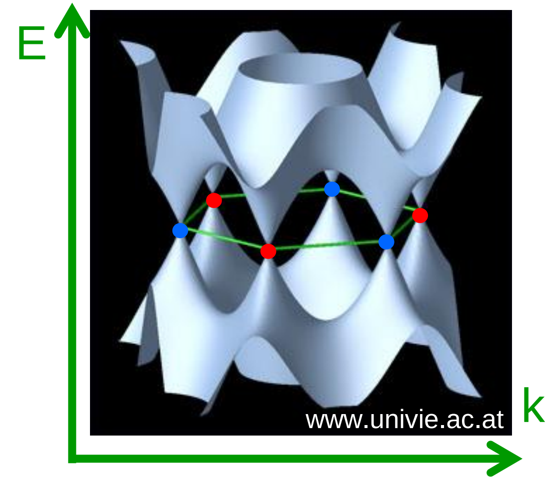
Distinguishes topologically distinct 2D band structures. Analogous to Gauss-Bonnet thm.

Alternative calculation: compute σ_{xy} via Kubo formula

Graphene

Novoselov et al. '05

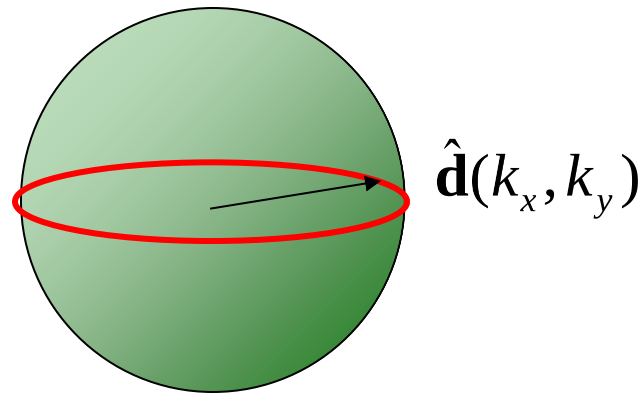




Two band model $H = -t \sum_{<ij>} c^{\dagger}_{Ai} c_{Bj}$

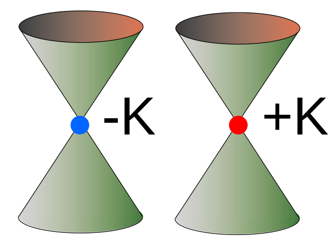
$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma}$$

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



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

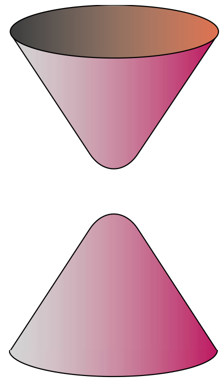
2D Dirac points at $\mathbf{k} = \pm\mathbf{K}$: point zeros in (d_x, d_y)



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

Berry's phase π around Dirac point

Topological gapped phases in Graphene



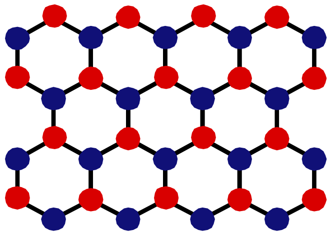
Break P or T symmetry : $H(\pm\mathbf{K}+\mathbf{q}) = v\,\mathbf{q}\cdot\sigma + m_\pm \sigma_z$

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

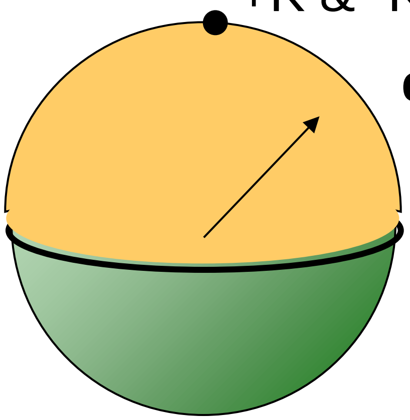
$n = \#$times $\hat{\mathbf{d}}(\mathbf{k})$ wraps around sphere

1. Broken P : eg Boron Nitride

$m_+ = m_-$

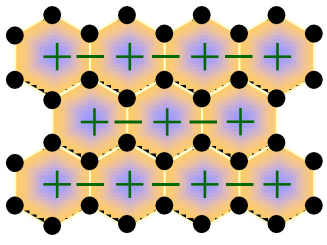


Chern number n=0 : Trivial Insulator

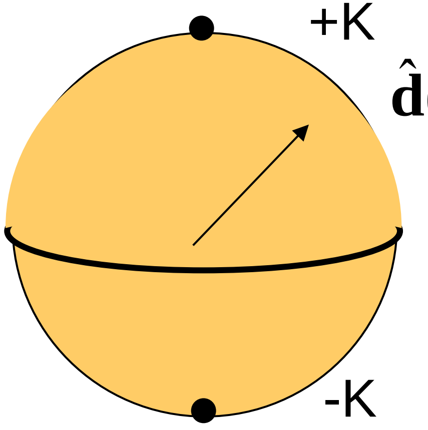


2. Broken T : Haldane Model '88

$m_+ = -m_-$

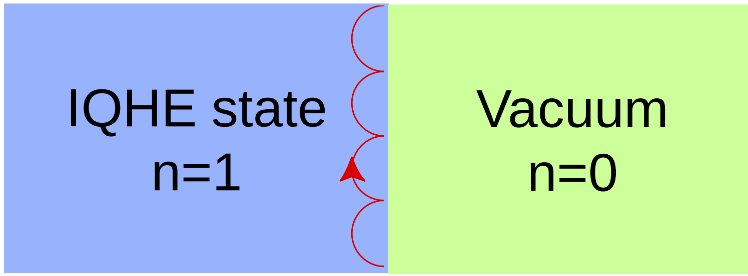


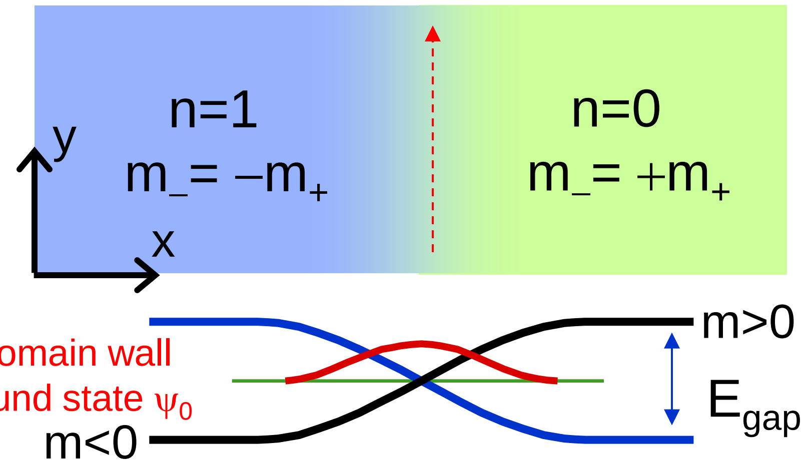
Chern number n=1 : Quantum Hall state



Edge States

Gapless states at the interface between topologically distinct phases



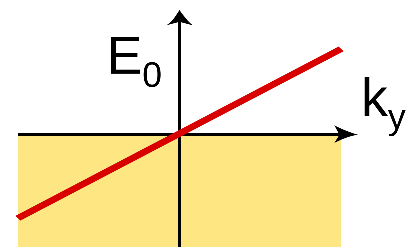


Edge states ~ skipping orbits
Lead to quantized transport

Band inversion transition : Dirac Equation

$$H = -i\mathrm{v}_F(\sigma_x\partial_x + \sigma_y\partial_y) + m(x)\sigma_z$$

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



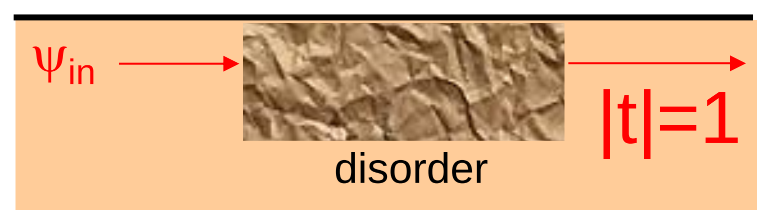
Chiral Dirac Fermions

Chiral Dirac fermions are unique 1D states :

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

Fermion Doubling Theorem :

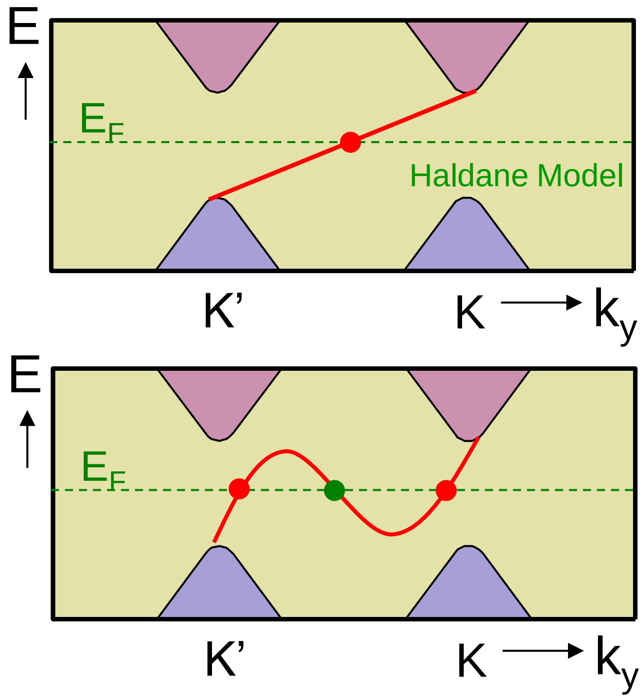
Chiral Dirac Fermions can not exist in a purely 1D system.



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

Generalizations

d=4 : 4 dimensional generalization of IQHE   Zhang, Hu '01

$$\mathbf{A}_{ij} = \langle u_i(\mathbf{k}) | \nabla_{\mathbf{k}} | u_j(\mathbf{k}) \rangle \cdot d\mathbf{k}$$

Non-Abelian Berry connection 1-form

$$\mathbf{F} = d\mathbf{A} + \mathbf{A} \wedge \mathbf{A}$$

Non-Abelian Berry curvature 2-form

$$n = \frac{1}{8\pi^2} \int_{T^4} \mathrm{Tr}[\mathbf{F} \wedge \mathbf{F}] \in \mathbb{Z}$$

2nd Chern number = integral of 4-form over 4D BZ

Boundary states : 3+1D Chiral Dirac fermions

Higher Dimensions : "Bott periodicity" d → d+2

	d							
	1	2	3	4	5	6	7	8
no symmetry	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
chiral symmetry	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0

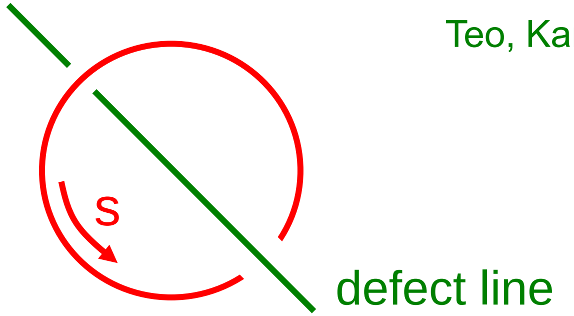
Topological Defects

Consider insulating Bloch Hamiltonians that vary slowly in real space

Teo, Kane '10

$$H = H(\mathbf{k}, s)$$

1 parameter family of 3D Bloch Hamiltonians



2nd Chern number : $n = \frac{1}{8\pi^2}\int_{T^3\times S^1} \mathrm{Tr}[\mathbf{F}\wedge\mathbf{F}]$

Generalized bulk-boundary correspondence :

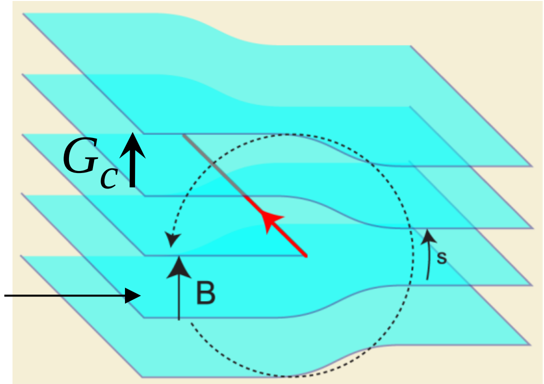
n specifies the number of chiral Dirac fermion modes bound to defect line

Example : dislocation in 3D layered IQHE

$$n = \frac{1}{2\pi}\mathbf{G}_c \cdot \mathbf{B}$$

3D Chern number (vector ⊥ layers)

Burgers' vector



Are there other ways to engineer 1D chiral dirac fermions?