Organizing Principles for Understanding Matter

Symmetry

- Conceptual simplification
- Conservation laws
- Distinguish phases of matter by pattern of broken symmetries

symmetry group p4

symmetry group p31m

Topology

- Properties insensitive to smooth deformation
- Quantized topological numbers
- Distinguish *topological* phases of matter

genus = 0

genus = 1

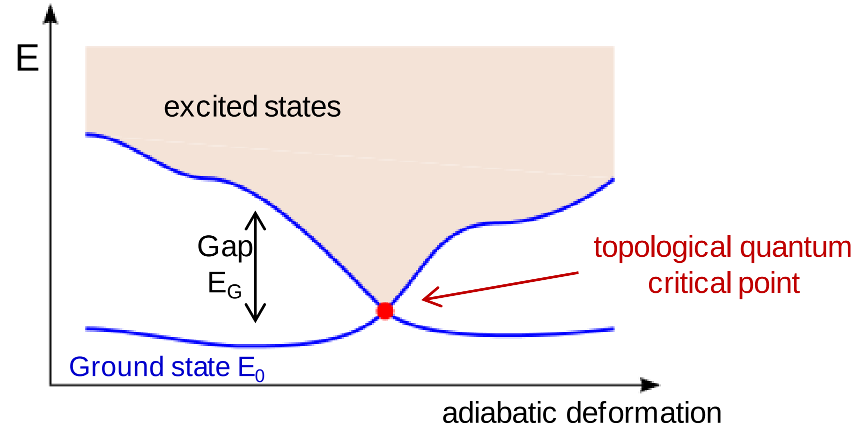
Interplay between symmetry and topology has led to a new understanding of electronic phases of matter.

Topology and Quantum Phases

Topological Equivalence : Principle of Adiabatic Continuity

Quantum phases with an energy gap are topologically equivalent if they can be smoothly deformed into one another without closing the gap.

Topologically distinct phases are separated by quantum phase transition.

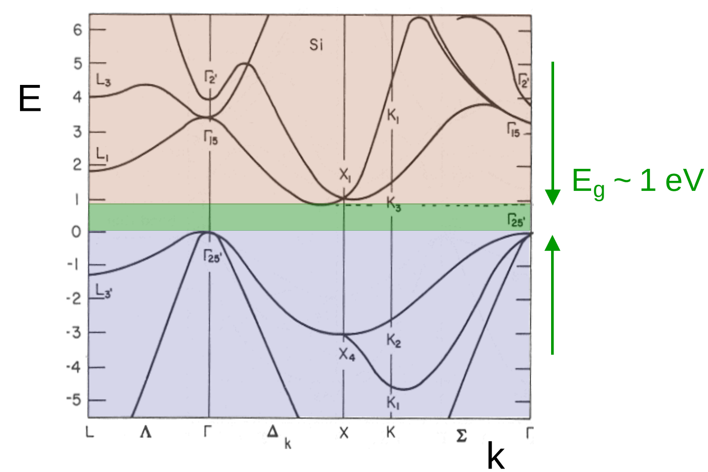


Topological Band Theory

Describe states that are adiabatically connected to non interacting fermions

Classify single particle Bloch band structures

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



Band Theory of Solids
e.g. Silicon

Topological Electronic Phases

Many examples of topological band phenomena

States adiabatically connected to independent electrons:

- Quantum Hall (Chern) insulators
- Topological insulators
- Weak topological insulators
- Topological crystalline insulators
- Topological (Fermi, Weyl and Dirac) semimetals …..

Many real materials
and experiments

Beyond Band Theory: Strongly correlated states

State with intrinsic topological order

- fractional quantum numbers
- topological ground state degeneracy
- quantum information

- Symmetry protected topological states
- Surface topological order ……

Much recent conceptual
progress, but theory is
still far from the real electrons

Topological Superconductivity

Proximity induced topological superconductivity

Majorana bound states, quantum information

Tantalizing recent
experimental progress

Topological Band Theory

Lecture #1: Topology and Band Theory

Lecture #2: Topological Insulators in 2 and 3 dimensions
Topological Semimetals

Lecture #3: Topological Superconductivity
Majorana Fermions
Topological quantum computation

General References :

"Colloquium: Topological Insulators"
M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010)

"Topological Band Theory and the Z2 Invariant,"
C. L. Kane in "Topological insulators"
edited by M. Franz and L. Molenkamp, Elsevier, 2013.

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

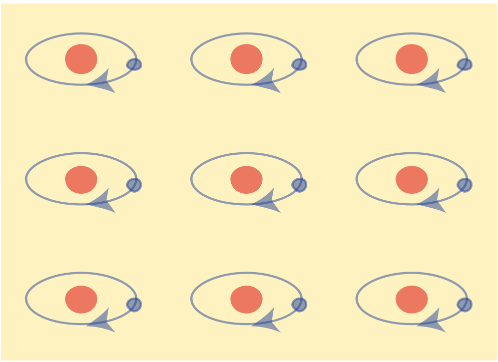
IV. Generalizations

- Bulk-Boundary correspondence
- Weyl semimetal
- Higher dimensions
- Topological Defects

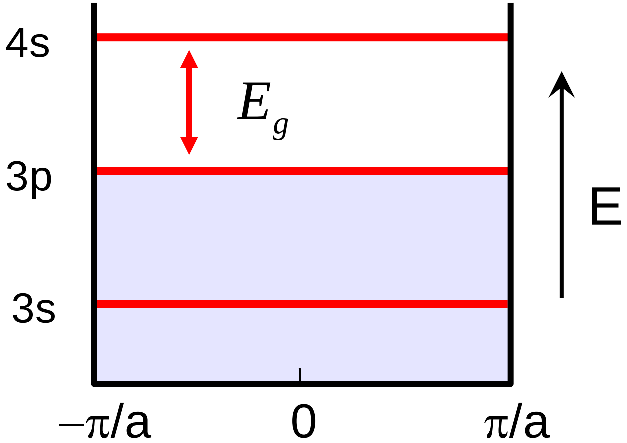
Insulator vs Quantum Hall state

The Insulating State

atomic insulator

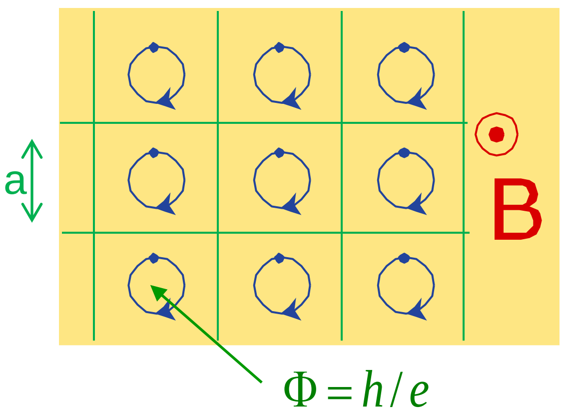


atomic energy levels

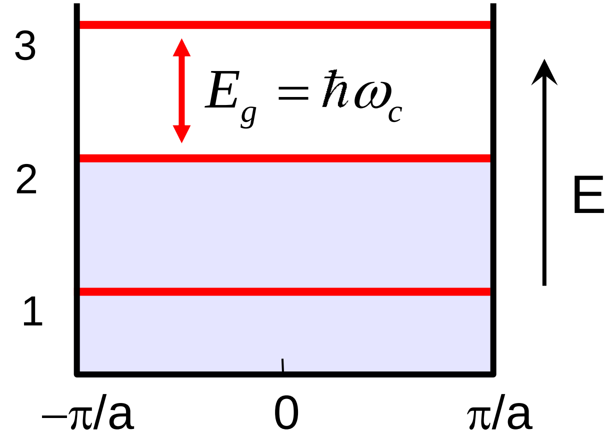


The Integer Quantum Hall State

2D Cyclotron Motion, $\sigma_{xy} = e^2/h$



Landau levels



What's the difference? Distinguished by Topological Invariant

Topology

The study of geometrical properties that are insensitive to smooth deformations

Example: 2D surfaces in 3D

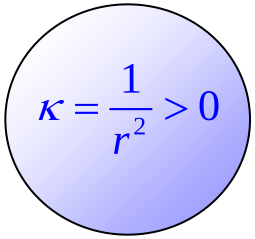
A closed surface is characterized by its genus, g = # holes

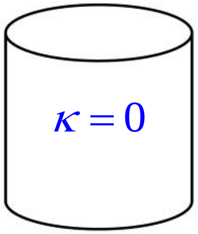
g=0

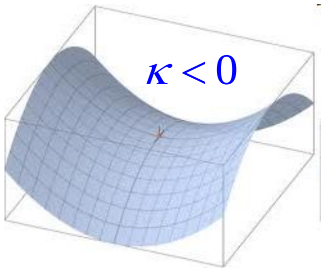
g=1

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

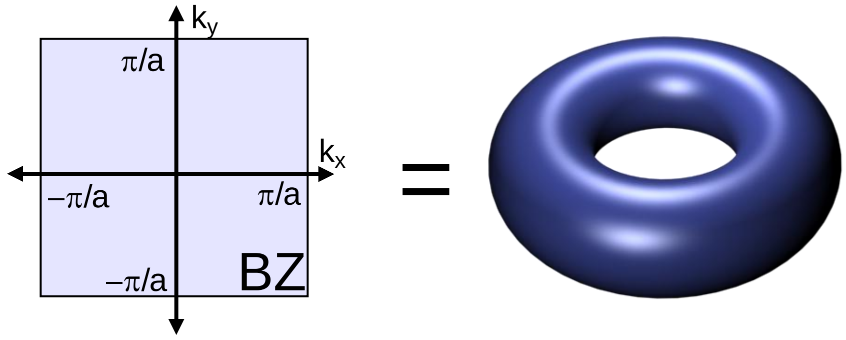
Bloch Theorem :

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

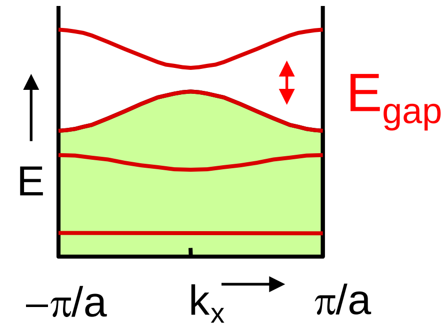
$=$ Torus, T^d



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

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

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

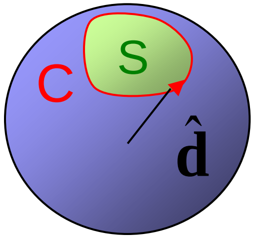
$$\mathbf{A} \to \mathbf{A} + \nabla_{\mathbf{k}}\phi(\mathbf{k})$$

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

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



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

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

Topology in one dimension : Berry phase and electric polarization

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

Classical electric polarization :

$$P = \frac{\text{dipole moment}}{\text{length}}$$

Bound charge density $\rho_{bound} = \nabla \cdot P$

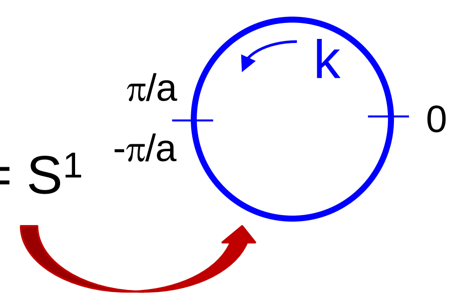
End charge $Q_{end} = P \cdot \hat{n}$

Proposition: The quantum polarization is a Berry phase

$$P = \frac{e}{2\pi} \oint_{BZ} A(k)\,dk$$

$$\mathbf{A} = -i \langle u(\mathbf{k}) | \nabla_{\mathbf{k}} | u(\mathbf{k}) \rangle$$

BZ = 1D Brillouin Zone = S^1



Circumstantial evidence #1 :

The polarization and the Berry phase share the same ambiguity:

They are both only defined modulo an integer.

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

$$Q_{\text{end}} = P \text{ mod } e$$

- The Berry phase is gauge invariant under continuous gauge transformations, but is not gauge invariant under "large" gauge transformations.

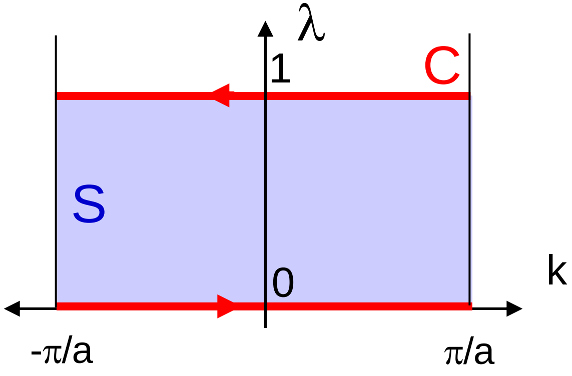
$$P \to P + en \quad \text{when} \quad |u(k)\rangle \to e^{i\phi(k)}|u(k)\rangle \quad \text{with} \quad \phi(\pi/a) - \phi(-\pi/a) = 2\pi n$$

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

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

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

gauge invariant Berry curvature



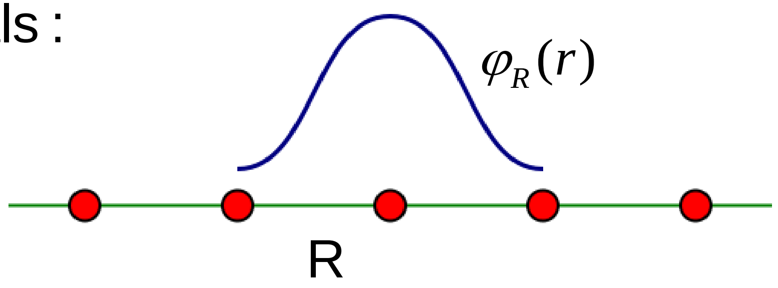
Circumstantial evidence #2 : $r \sim i\,\nabla_k$

$$“\; P = e\oint_{BZ}\frac{dk}{2\pi}\langle u(k)|r|u(k)\rangle = \frac{ie}{2\pi}\oint_{BZ}\langle u(k)|\nabla_k|u(k)\rangle \;”$$

A slightly more rigorous argument:

Construct Localized Wannier Orbitals :

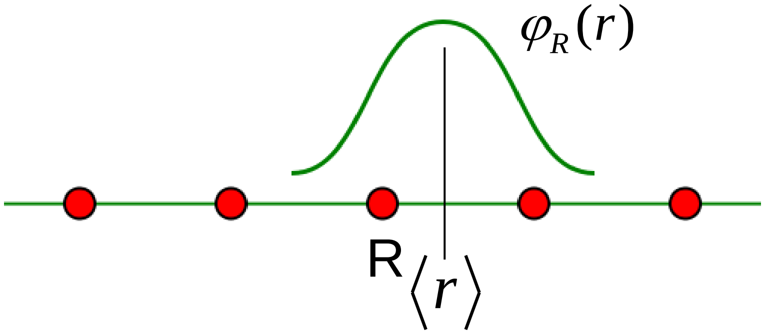
$$|\varphi(R)\rangle = \oint_{BZ}\frac{dk}{2\pi}e^{-ik(R-r)}|u(k)\rangle$$



Wannier states are gauge dependent, but for a sufficiently smooth gauge, they are localized states associated with a Bravais Lattice point R

$$P = e\langle\varphi(R)|r-R|\varphi(R)\rangle$$

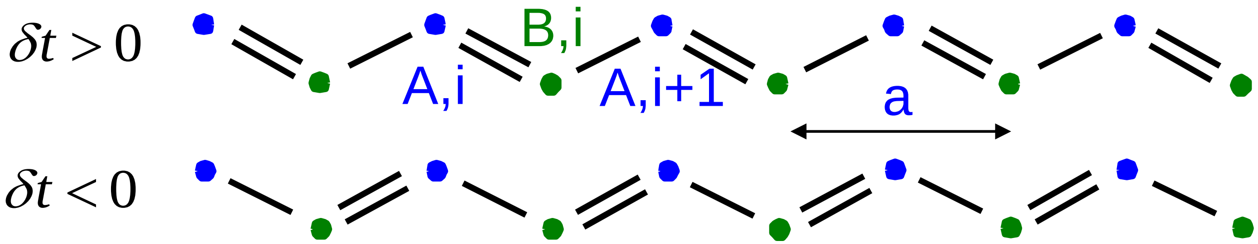
$$= \frac{ie}{2\pi}\oint_{BZ}\langle u(k)|\nabla_k|u(k)\rangle$$

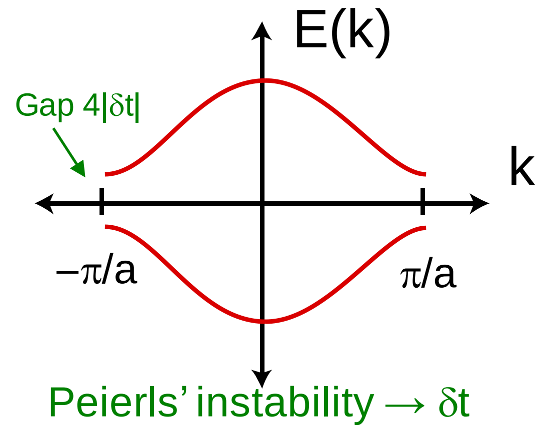


Su Schrieffer Heeger Model

model for polyacetylene
simplest “two band” model

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



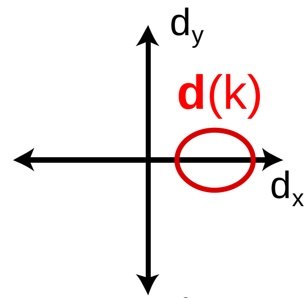


$$H(k) = \mathbf{d}(k) \cdot \vec{\sigma}$$

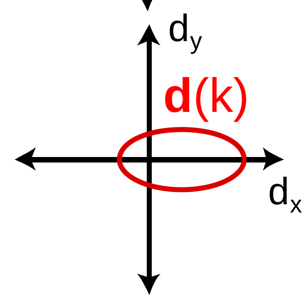
$$d_x(k) = (t+\delta t) + (t-\delta t)\cos ka$$

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

$$d_z(k) = 0$$



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 distinguished by an integer winding number. Without extra symmetry, all 1D band structures are topologically equivalent.

Symmetries of the SSH model

"Chiral" Symmetry : $\{H(k), \sigma_z\} = 0$ (or $\sigma_z H(k) \sigma_z = -H(k)$)

- Artificial symmetry of polyacetylene. Consequence of bipartite lattice with only A-B hopping: $c_{iA} \to c_{iA}$, $c_{iB} \to -c_{iB}$

- Requires $d_z(k)=0$: integer winding number

- Leads to particle-hole symmetric spectrum:

$$H\sigma_z |\psi_E\rangle = -E\sigma_z |\psi_E\rangle \quad \Rightarrow \quad \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$$

Reflection Symmetry : $H(-k) = \sigma_x H(k) \sigma_x$

- Real symmetry of polyacetylene.

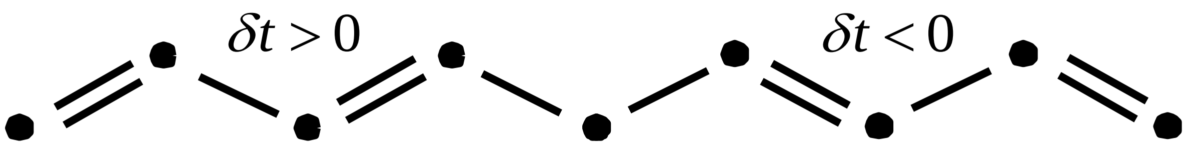
- Allows $d_z(k) \neq 0$, but constrains $d_x(-k) = d_x(k)$, $d_{y,z}(-k) = -d_{y,z}(k)$

- No p-h symmetry, but polarization is quantized: Z_2 invariant

P = 0 or e/2 mod e

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

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

$$H = -i v_F \sigma_x \partial_x + m(x)\sigma_y \qquad v_F = ta \quad ; \quad m = 2\delta t$$

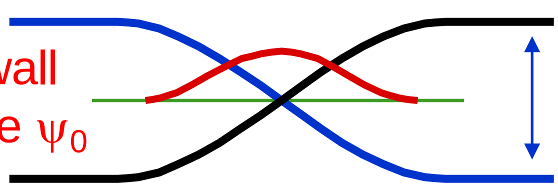
Massive 1+1 D Dirac Hamiltonian $\quad E(q) = \pm\sqrt{(v_F q)^2 + m^2}$

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

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)

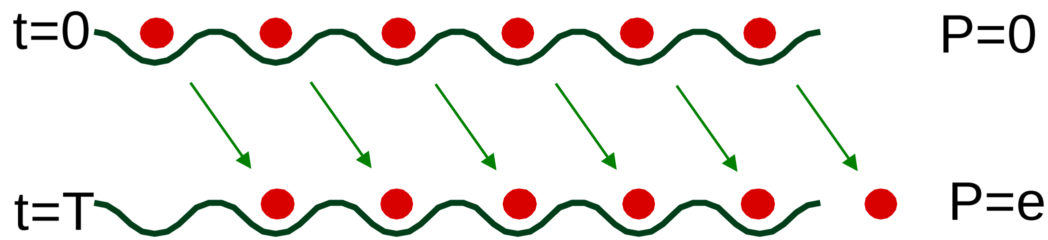


$$\psi_0(x) = e^{-\int_0^x m(x')dx'/v_F} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

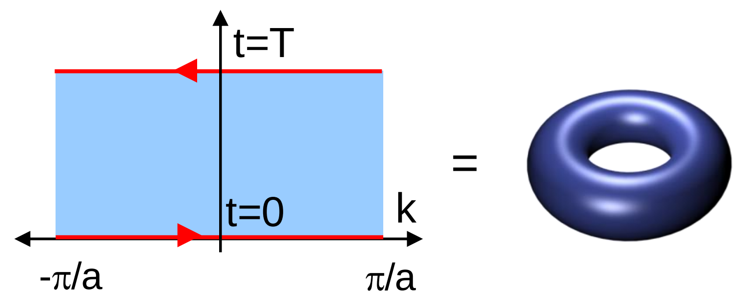
Thouless Charge Pump

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

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



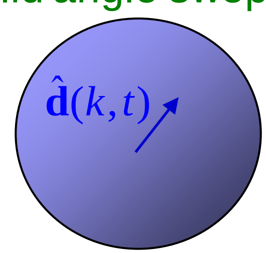
$$\Delta P=\frac{e}{2\pi}\left(\oint A(k,T)dk-\oint A(k,0)dk\right)=ne$$



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

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

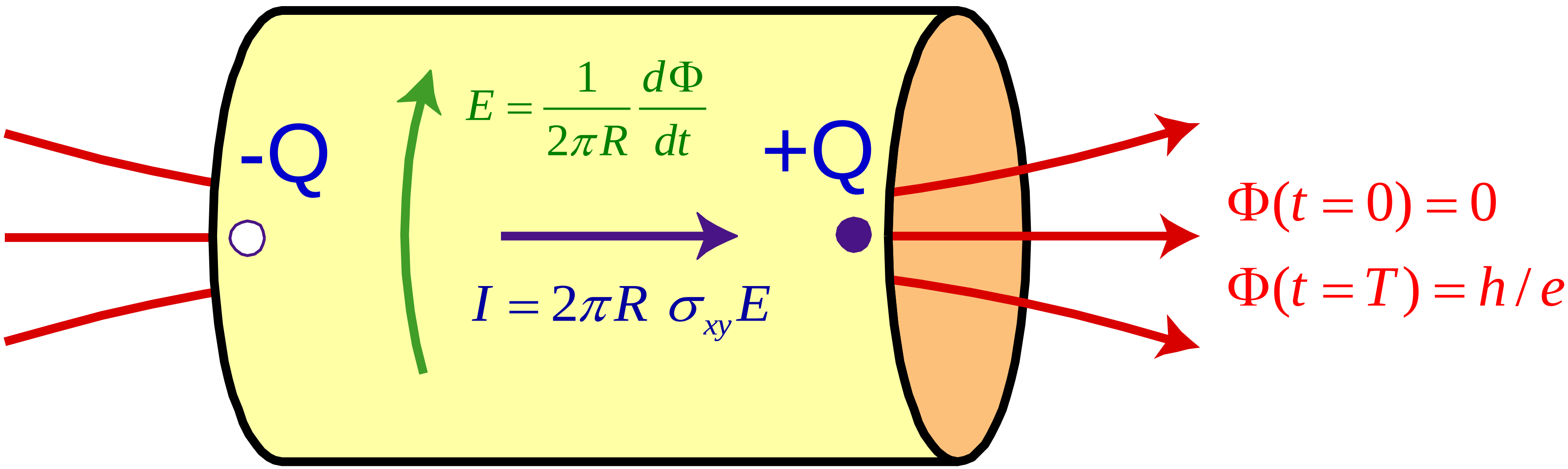
In the 2 band model, the Chern number is related to the solid angle swept out by $\hat{\mathbf{d}}(k,t)$, which must wrap around the sphere an integer n times.



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

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

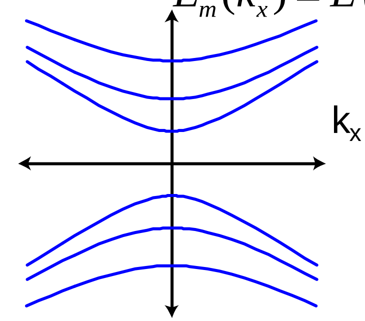
$$\Delta Q = ne \quad \rightarrow \quad \sigma_{xy} = n\frac{e^2}{h}$$

TKNN Invariant

Thouless, Kohmoto, Nightingale and den Nijs 82

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

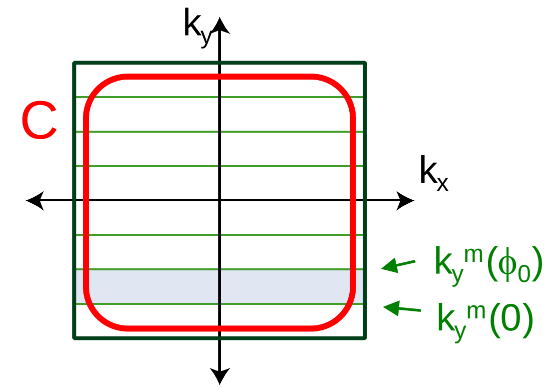
$E_m(k_x) = E\left(k_x, k_y^m(\Phi)\right)$



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

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

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



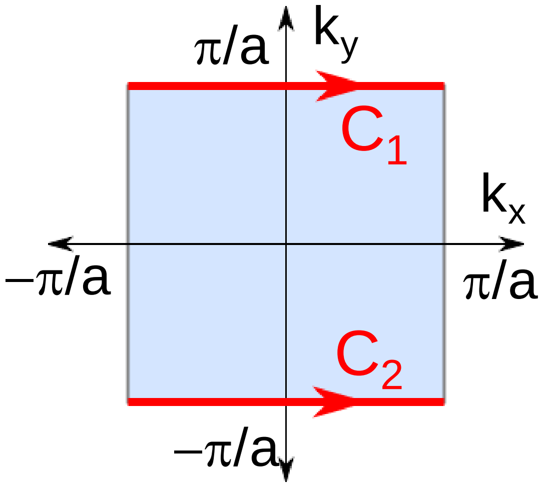
Distinguishes topologically distinct 2D band structures. Analogous to Gauss-Bonnet thm.

Alternative calculation: compute σ_{xy} via Kubo formula

TKNN Invariant

Thouless, Kohmoto, Nightingale and den Nijs 82

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

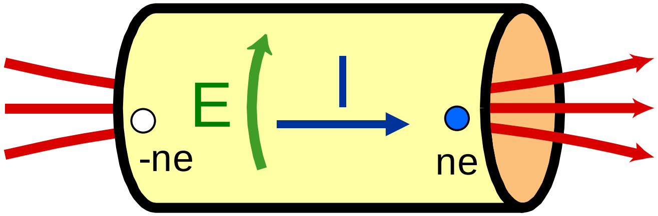


$$n = \frac{1}{2\pi}\oint_{C_1}\mathbf{A}\cdot d\mathbf{k} - \frac{1}{2\pi}\oint_{C_2}\mathbf{A}\cdot d\mathbf{k} \in \mathbb{Z}$$

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

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

Laughlin Argument: Thread magnetic flux ϕ_0 = h/e through a 1D cylinder
Polarization changes by $\sigma_{xy}\,\phi_0$

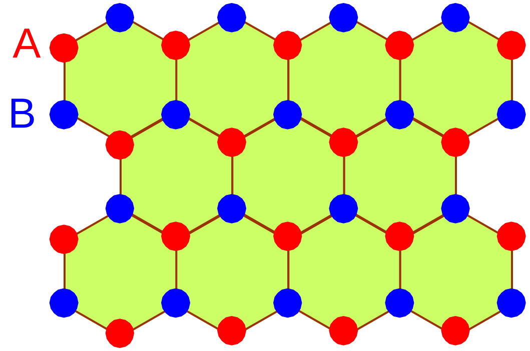


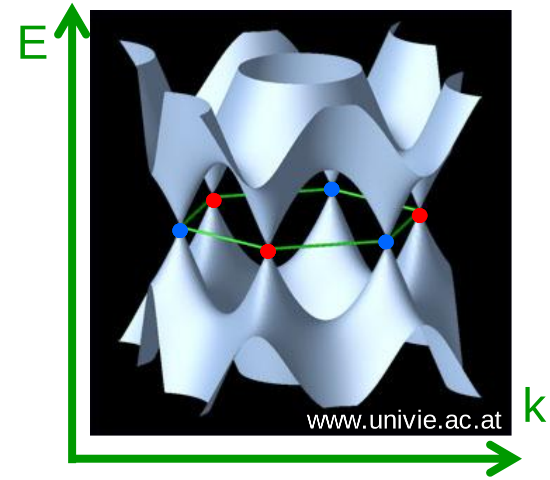
$$\Phi \propto k_y$$

$$\Delta P = ne$$

Graphene

Novoselov et al. '05



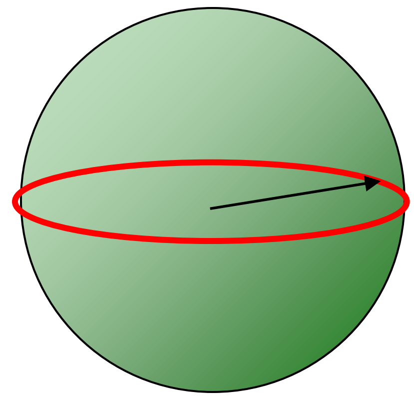


Two band model $H = -t \sum_{<ij>} c_{Ai}^{\dagger} c_{Bj}$

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

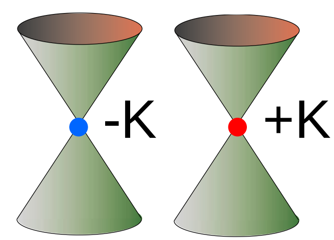
$$E(\mathbf{k}) = \pm |\mathbf{d}(\mathbf{k})|$$

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



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

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

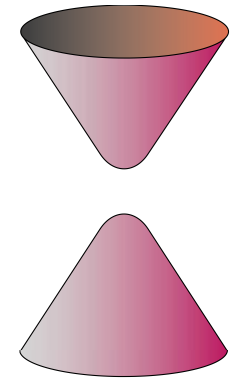


2D Dirac points at $\mathbf{k} = \pm\mathbf{K}$ point vortices in (d_x, d_y)

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

Berry's phase π around Dirac point

Topological gapped phases in Graphene



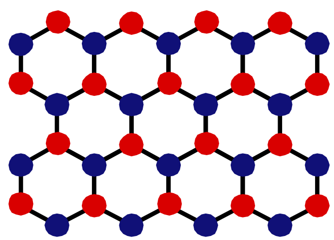
Break P or T symmetry : $H(\pm\mathbf{K}+\mathbf{q}) = \mathrm{v}\,\mathbf{q}\bullet\sigma + m_{\pm}\sigma_z$

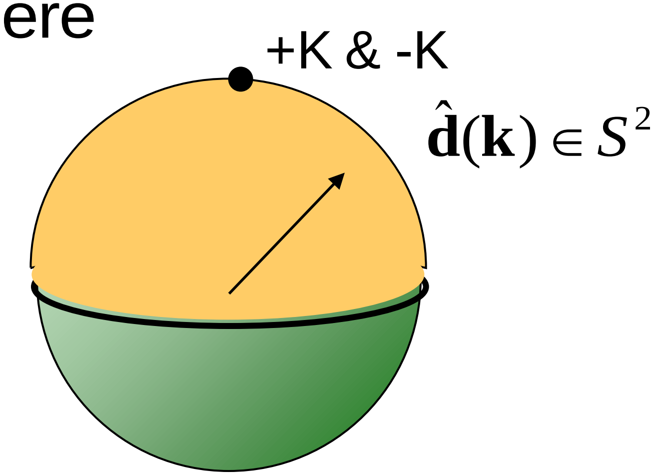
$$E(\mathbf{q}) = \pm\sqrt{\mathrm{v}^2\,|\,\mathbf{q}\,|^2 + m_{\pm}^2}$$

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

1. Broken P : eg Boron Nitride

$m_+ = m_-$

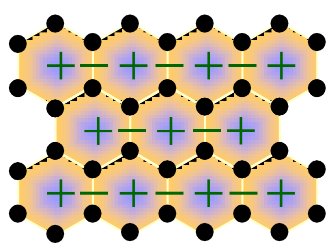


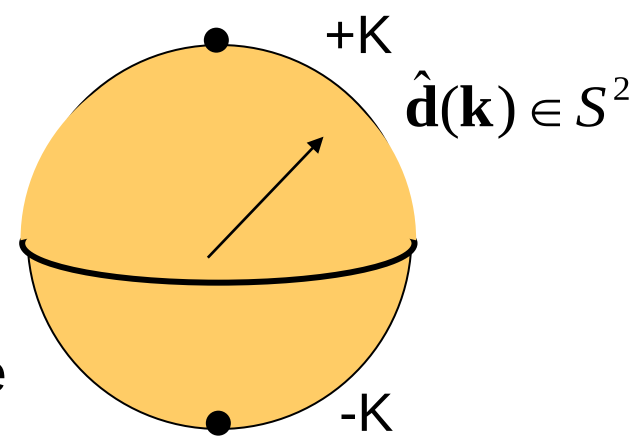


Chern number n=0 : Trivial Insulator

2. Broken T : Haldane Model '88

$m_+ = -m_-$

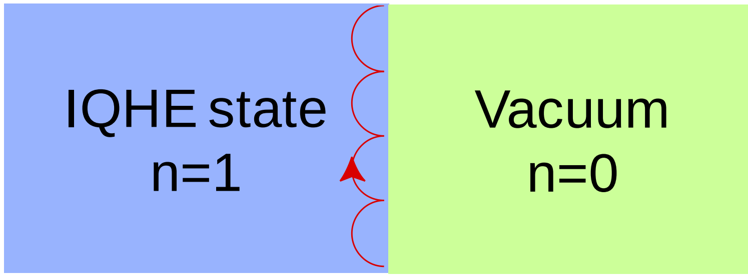




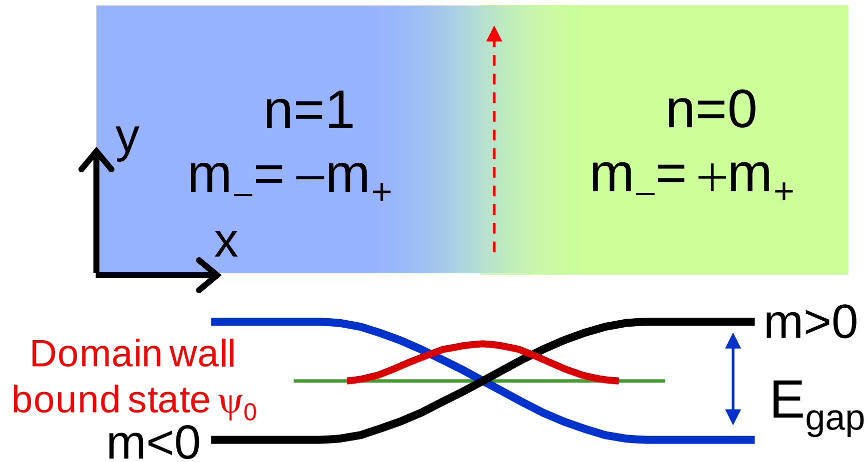
Chern number n=1 : Quantum Hall state

Edge States

Gapless states at the interface between topologically distinct phases



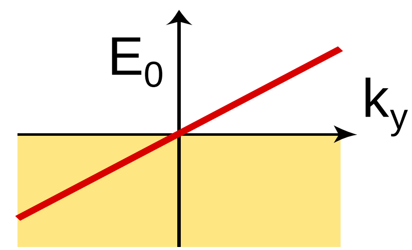
Edge states ~ skipping orbits
Lead to quantized transport



Band inversion transition : Dirac Equation

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

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



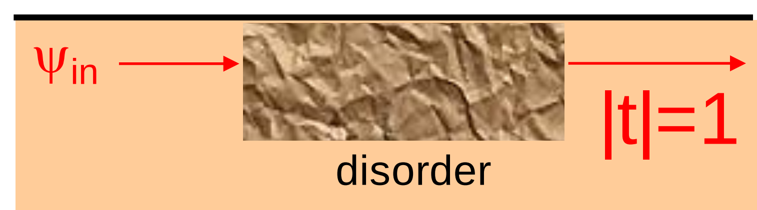
Chiral Dirac Fermions

Chiral Dirac fermions are unique 1D states :

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

Fermion Doubling Theorem :

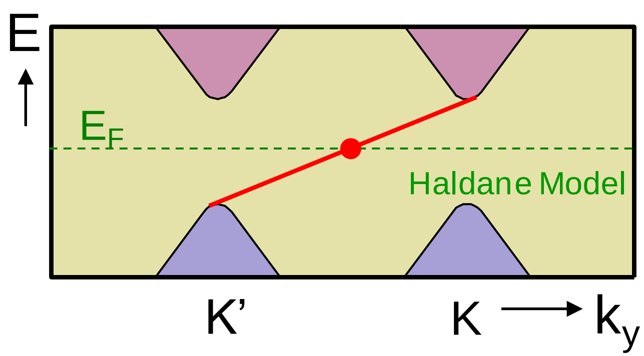
Chiral Dirac Fermions can not exist in a purely 1D system.



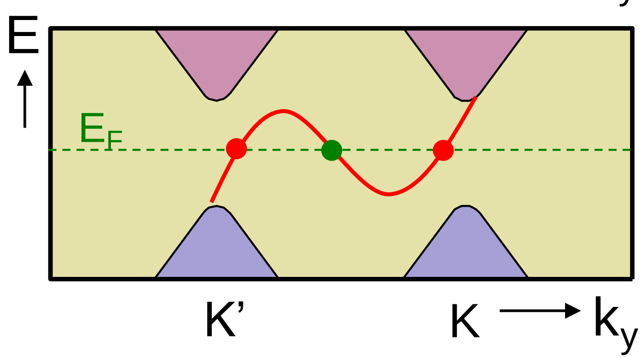
Bulk - Boundary Correspondence

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

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



$\Delta N = 1 – 0 = 1$



$\Delta N = 2 – 1 = 1$

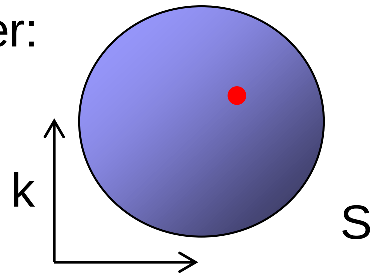
Bulk – Boundary Correspondence :

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

Weyl Semimetal

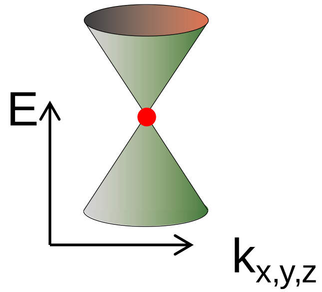
Gapless “Weyl points” in momentum space are topologically protected in 3D

A sphere in momentum space can have a Chern number:



$$n_S = \int_S d^2k\,\mathbf{F}(\mathbf{k}) \in \mathbb{Z}$$

n_S=+1: S must enclose a degenerate Weyl point:
Magnetic monopole for Berry flux

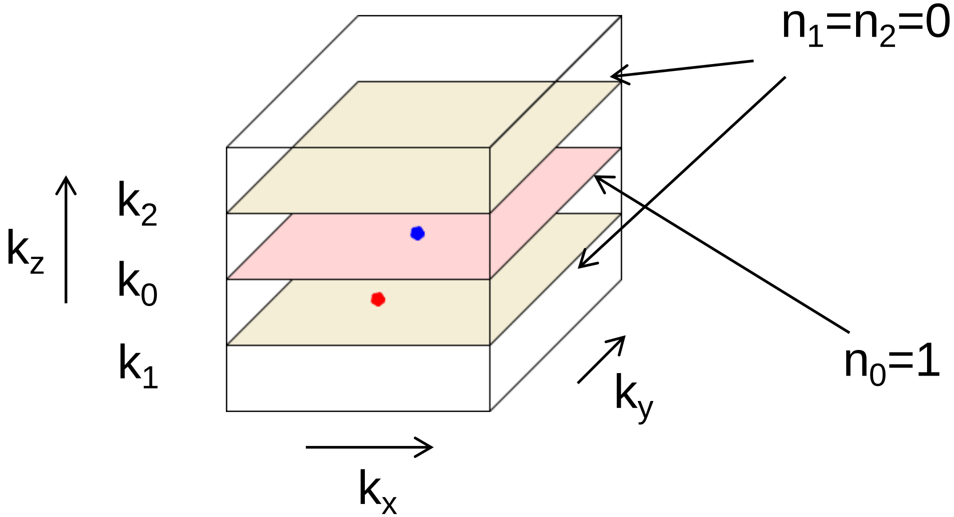


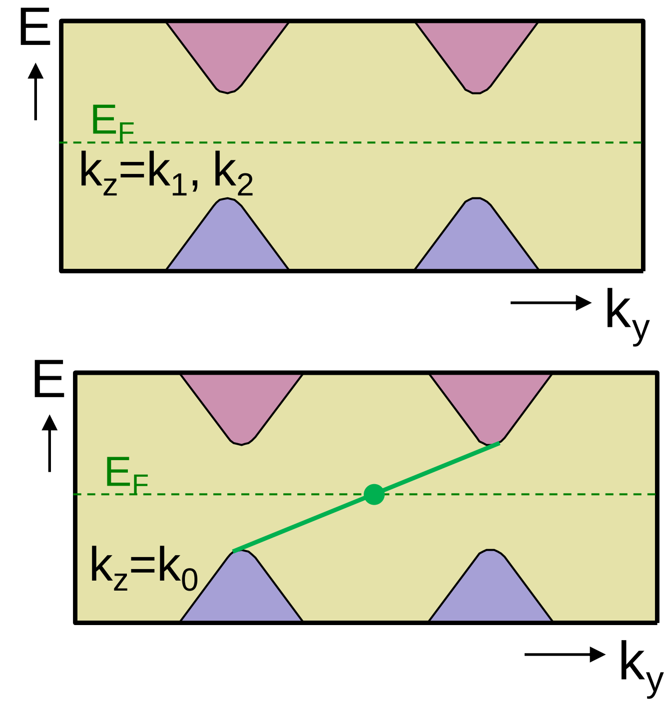
$$H(k_0+q) = \mathrm{v}(q_x\sigma_x + q_y\sigma_y + q_z\sigma_z)$$

(or $\mathrm{v}_{ia} q_i \sigma_a$ with $\det[\mathrm{v}_{ia}] > 0$)

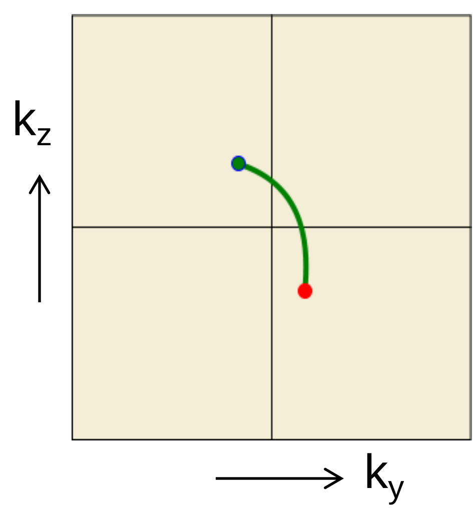
Total magnetic charge in Brillouin zone must be zero: Weyl points must come in +/- pairs.

Surface Fermi Arc





Surface BZ



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

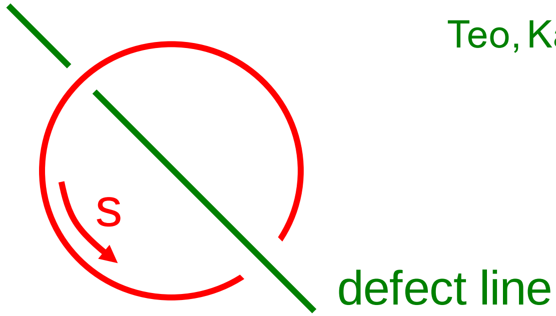
Topological Defects

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



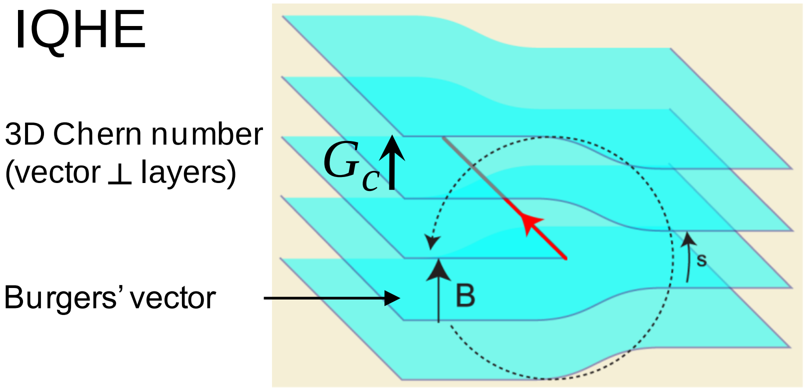
2nd Chern number : $n = \dfrac{1}{8\pi^2}\displaystyle\int_{T^3\times S^1} \mathrm{Tr}[\mathbf{F}\wedge\mathbf{F}]$

Generalized bulk-boundary correspondence :

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

Example : dislocation in 3D layered IQHE

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



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