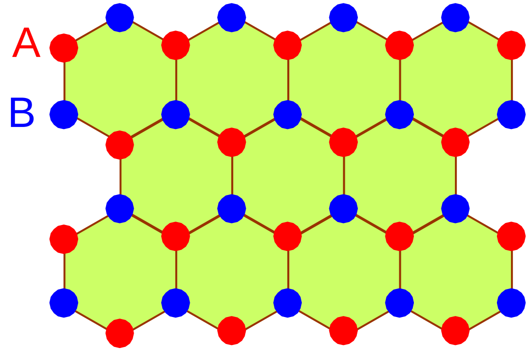
Topological Band Theory II: Time reversal symmetry

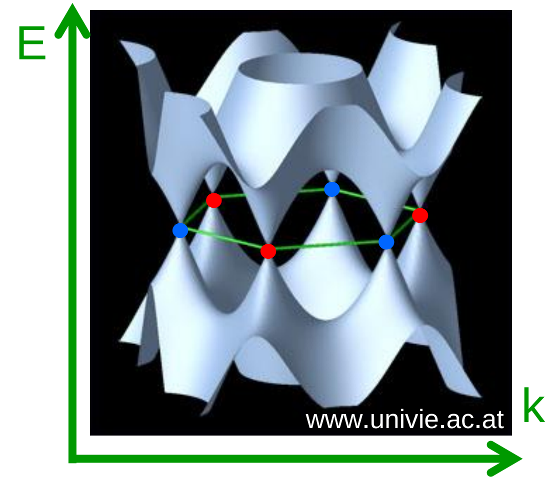
Lecture notes available at
https://www.lorentz.leidenuniv.nl/lorentzchair/

0. 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
   - Surface topological order

Graphene

Novoselov et al. '05



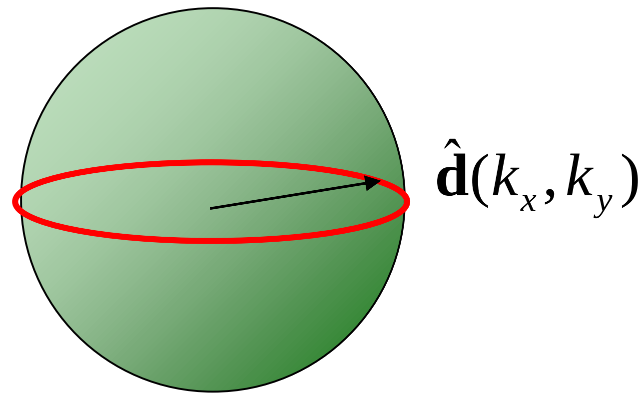


Two band model $H = -t \sum_{<ij>} c_{Ai}^{\dagger} c_{Bj}$

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

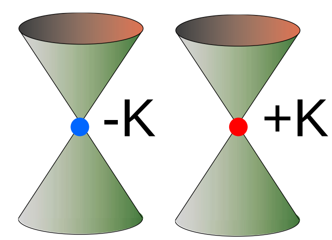
$$E(\mathbf{k}) = \pm |\mathbf{d}(\mathbf{k})|$$

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



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

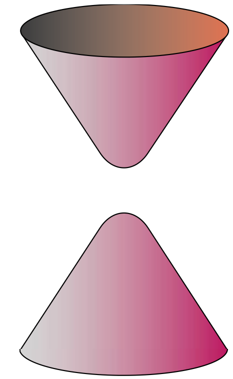
2D Dirac points at $\mathbf{k} = \pm\mathbf{K}$ point vortices in (d_x, d_y)



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

Berry's phase π around Dirac point

Topological gapped phases in Graphene



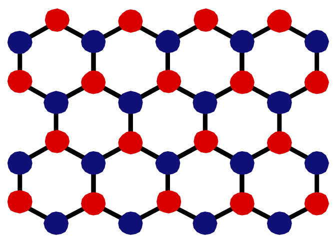
Break P or T symmetry : $H(\pm\mathbf{K}+\mathbf{q}) = \mathrm{v}\mathbf{q}\cdot\sigma + m_{\pm}\sigma_z$

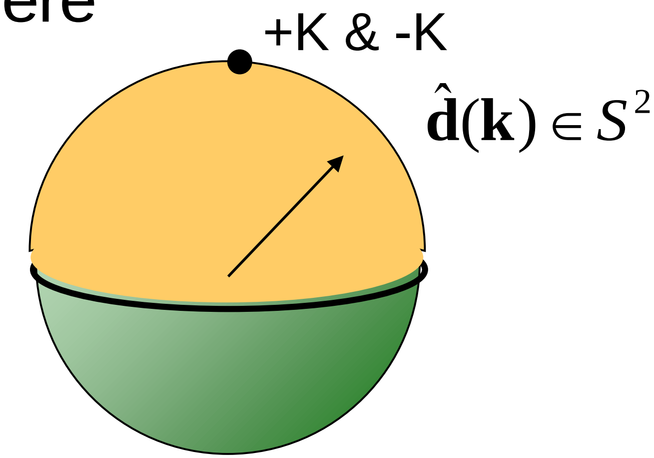
$$E(\mathbf{q}) = \pm\sqrt{\mathrm{v}^2|\mathbf{q}|^2 + m_{\pm}^2}$$

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

1. Broken P : eg Boron Nitride

$m_+ = m_-$

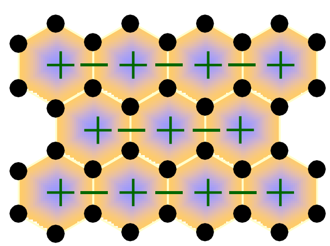


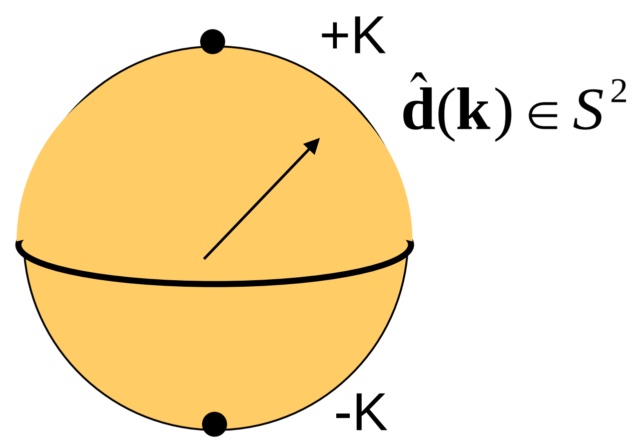


Chern number n=0 : Trivial Insulator

2. Broken T : Haldane Model ’88

$m_+ = -m_-$

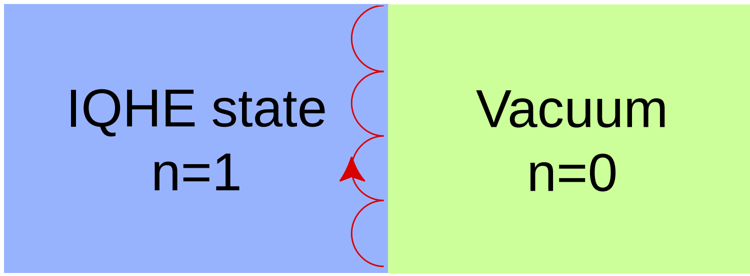


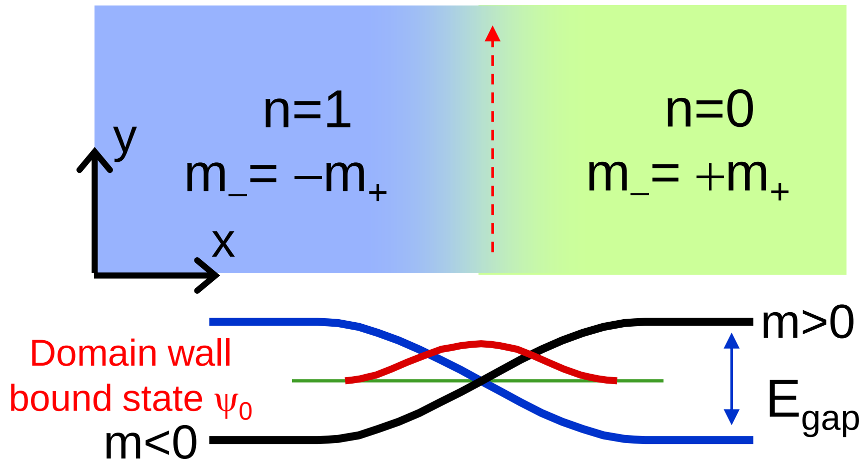


Chern number n=1 : Quantum Hall state

Edge States

Gapless states at the interface between topologically distinct phases



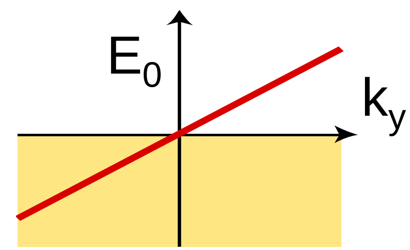


Edge states ~ skipping orbits
Lead to quantized transport

Band inversion transition : Dirac Equation

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

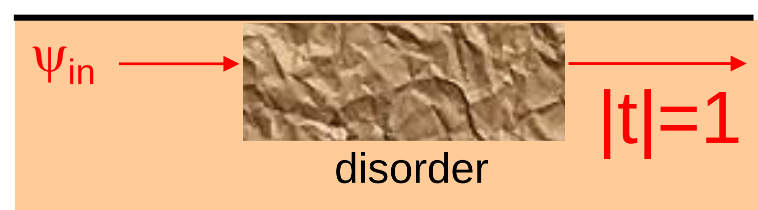
$$\psi_0(x) \sim e^{ik_y y} e^{-\int_0^x m(x')dx'/v_F} \qquad E_0(k_y) = v_F k_y$$



Chiral Dirac Fermions

Chiral Dirac fermions are unique 1D states :

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



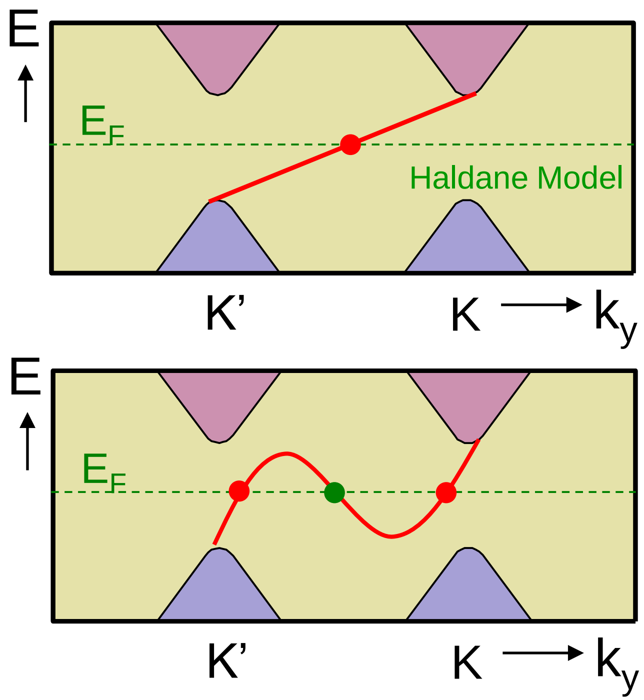
Fermion Doubling Theorem :

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

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

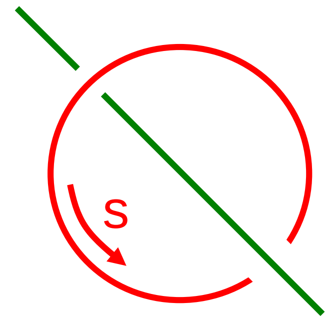
Topological Defects

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 :

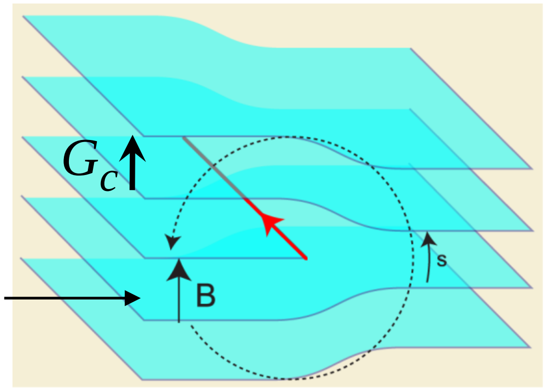
n specifies the number of chiral Dirac fermion modes bound to defect line

Example : dislocation in 3D layered IQHE

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

3D Chern number (vector ⊥ layers)

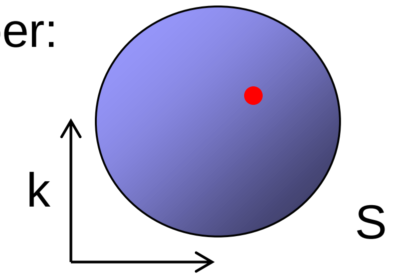
Burgers' vector



Weyl Semimetal

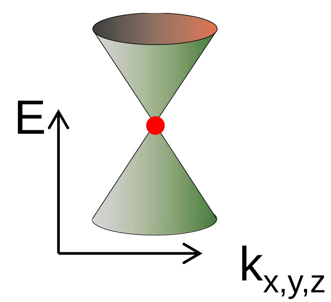
Gapless "Weyl points" in momentum space are topologically protected in 3D

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



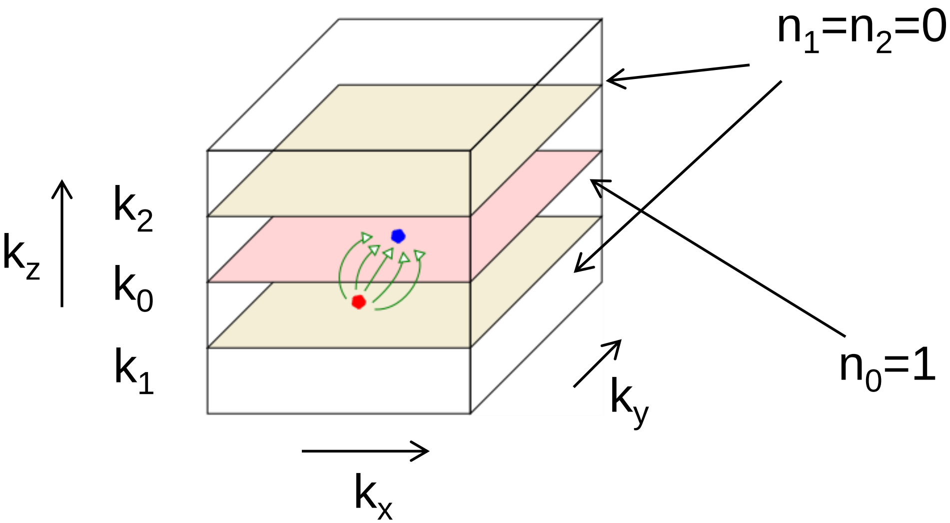
$$H(k_0 + q) = \mathrm{v}(q_x\sigma_x + q_y\sigma_y + q_z\sigma_z)$$

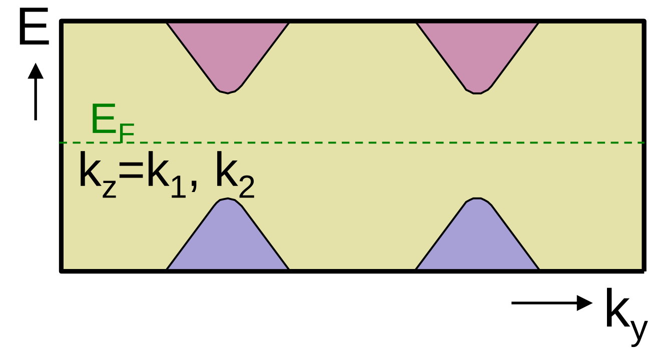
(or $\mathrm{v}_{ia} q_i \sigma_a$ with $\det[\mathrm{v}_{ia}] > 0$)

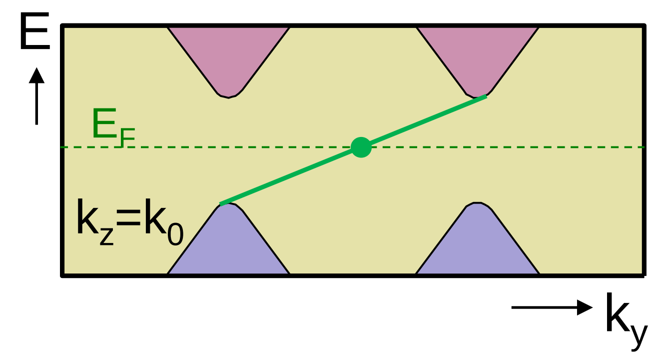
Total magnetic charge in Brillouin zone must be zero: Weyl points must come in +/- pairs.

Weyl point *requires* broken PT

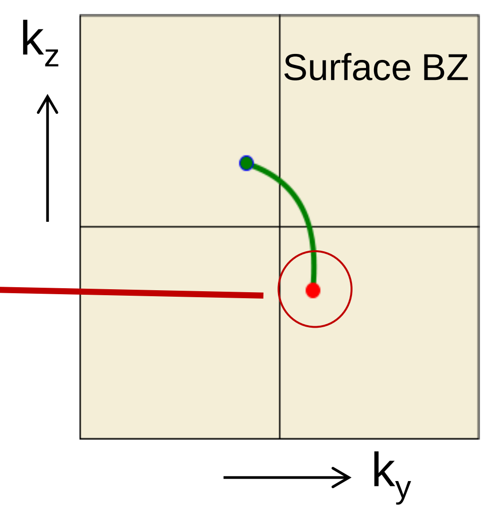
Surface Fermi Arc







http://www.todayifoundout.com/index.php/2013/10/bloody-history-barber-pole/



Energy gaps in graphene:

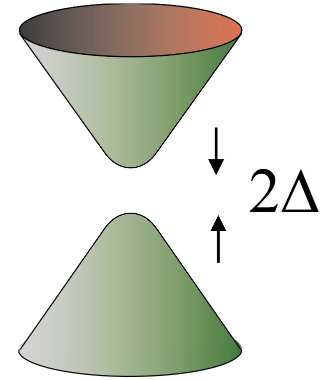
σ_z ~ sublattice

τ_z ~ valley

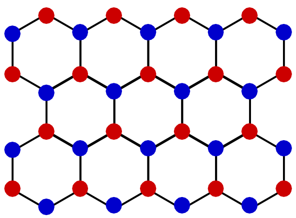
s_z ~ spin

$$H = v_F \sigma \cdot p + V$$

$$E(p) = \pm\sqrt{v_F^2 p^2 + \Delta^2}$$



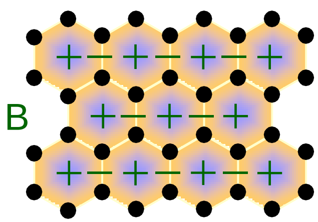
1. Staggered Sublattice Potential (e.g. BN)



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

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

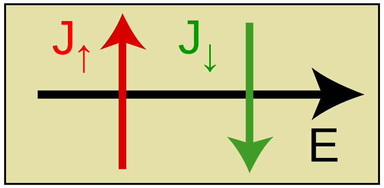
Quantum Spin-Hall Effect

Quantum Spin Hall Effect in Graphene

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

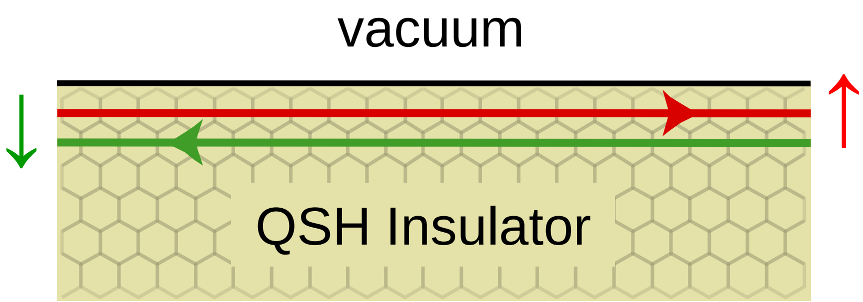
Simplest model:
|Haldane|^2
(conserves S_z)

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

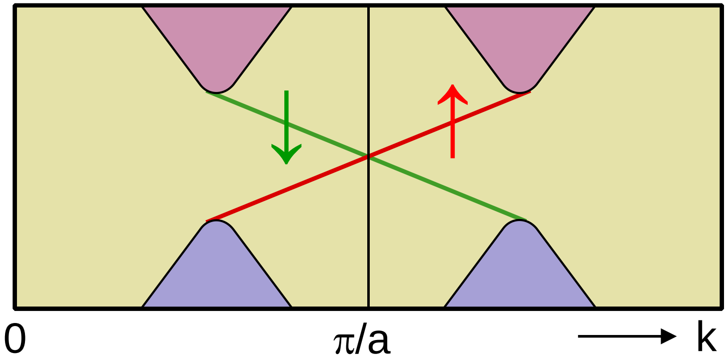


Bulk energy gap, but gapless edge states

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

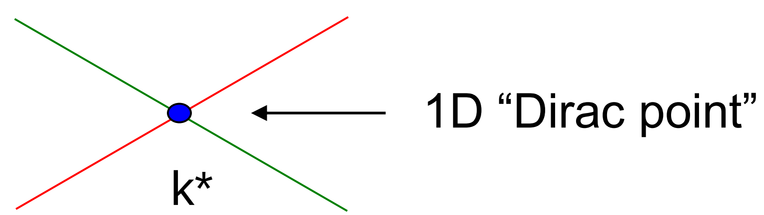
Spin ½ : $\Theta\begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix} = \begin{pmatrix}\psi^*_\downarrow \\ -\psi^*_\uparrow\end{pmatrix}$ $\quad\Theta^2 = -1$

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

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

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

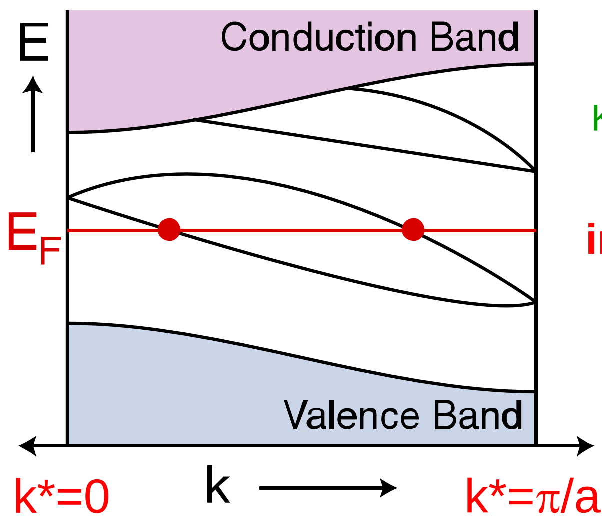
Time Reversal Invariant $\mathbb{Z}_2$ Topological Insulator

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 $0<k<\pi/a$

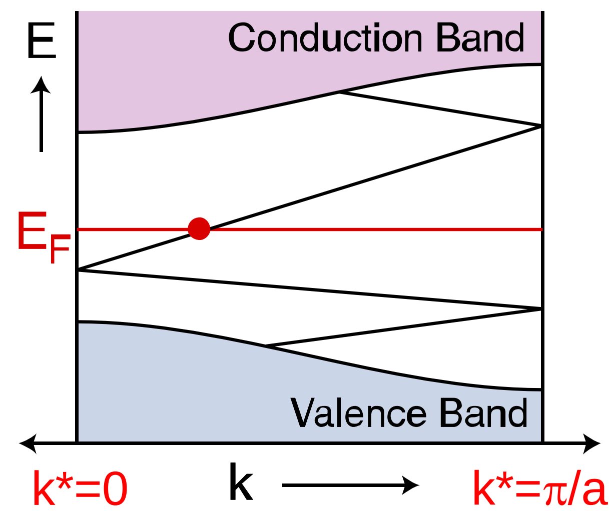
ν=0 : Conventional Insulator



Even number of bands
crossing Fermi energy

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

ν=1 : Topological Insulator

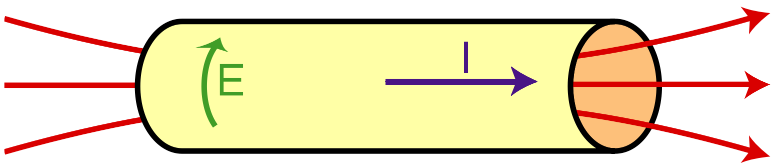


Odd number of bands
crossing Fermi energy

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

Sensitivity to boundary conditions in a multiply connected geometry

ν=N IQHE on cylinder: Laughlin Argument

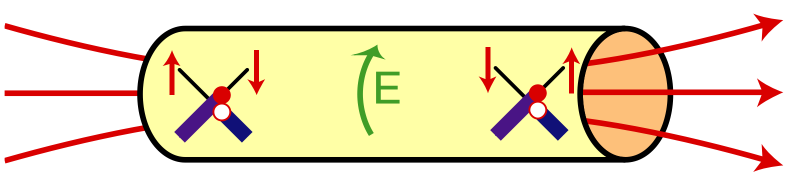


$\Delta\Phi = \phi_0 = h/e$

$\Delta Q = \; N e$

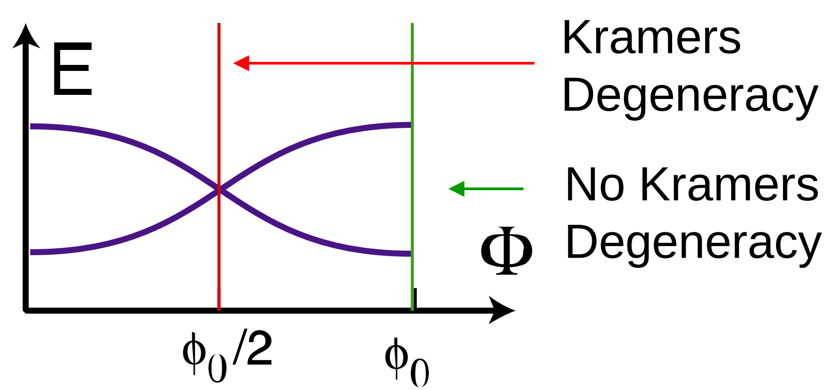
Flux $\phi_0 \Rightarrow$ Quantized change in Electron Number at the end.

Quantum Spin Hall Effect on cylinder



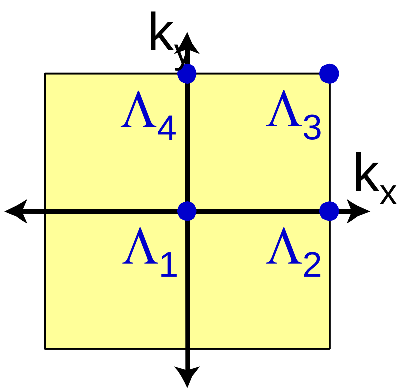
$\Delta\Phi = \phi_0 / 2$

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



Bulk 2D Brillouin Zone

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

  "time reversal polarization" analogous to $\frac{e}{2\pi}\oint A(k)dk$
- Z_2 invariant : $(-1)^\nu = \prod_{a=1}^{4} \delta(\Lambda_a) = \pm 1$

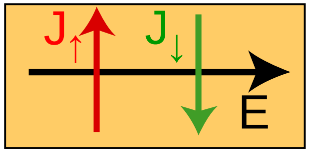
  Gauge invariant, but requires continuous gauge

ν is easier to determine if there is extra symmetry:

1. S_z conserved : independent spin Chern integers :

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

Quantum spin Hall Effect :



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

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

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

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

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

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

Allows a straightforward determination of ν from band structure calculations.