Modern Topics in Solid-State Theory: Topological insulators and superconductors

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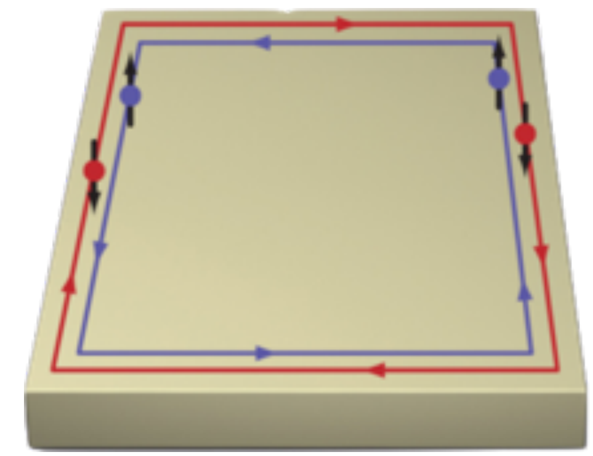
January 2016

Lecture Three: Topological superconductors

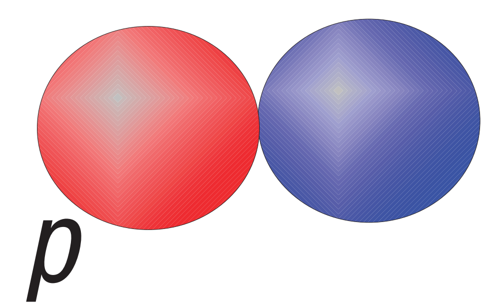
1. Topological insulators

- Z_2 bulk invariants
- Three-dimensional topological insulator



2. Topological superconductors

- Topological SCs in 1D: Kitaev model
- Topological SCs in 2D: chiral p-wave SC



Sr_2RuO_4

[picture courtesy S. Zhang et al.]

2D topological insulator: First bulk Z_2 invariant

[Kane Mele 05]

[Fu and Kane]

Bulk Z_2 invariant as an obstruction to define a "TR-smooth gauge":

- $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs
- TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta|u_n^{(2)}(\mathbf{k})\rangle$

$\Longrightarrow$ consider anti-symmetric "t-*matrix*":

$$t_{mn}(\mathbf{k}) = \left\langle u_m^-(\mathbf{k})\right| \Theta \left|u_n^-(\mathbf{k})\right\rangle$$

antisymmetry property: $t^{\mathrm{T}}(\mathbf{k}) = -t(\mathbf{k})$

$\Longrightarrow$ Pfaffian can be defined: $\mathrm{Pf}\,[t(\mathbf{k})]$

e.g.: $\mathrm{Pf}\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z$

$$(\mathrm{Pf}\,[\omega(\Lambda_a)])^2 = \det\,[\omega(\Lambda_a)]$$

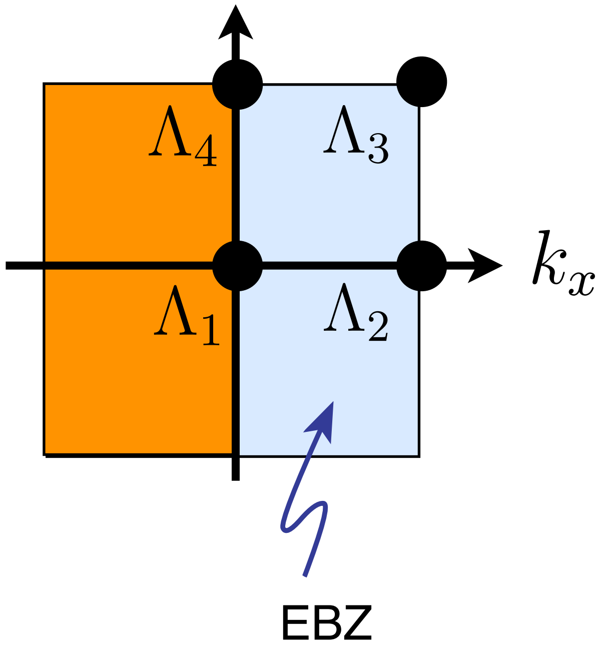
- Zeroes of $\mathrm{Pf}\,[t(\mathbf{k})]$ occur in isolated points, carry phase winding

- Due to time-reversal symmetry:

(i) $|\mathrm{Pf}[t(\mathbf{k})]| = |\mathrm{Pf}[t(-\mathbf{k})]| \Rightarrow$ zeros come in pairs

(ii) At TRI momenta Λ_a we have $|\mathrm{Pf}[t(\Lambda_a)]| = 1$

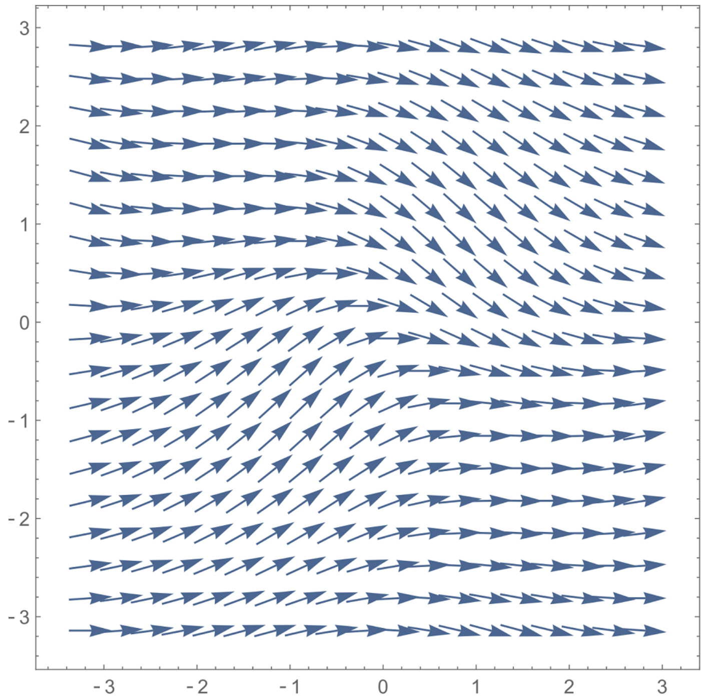
$\Rightarrow$ zeros cannot be brought to TRI momenta



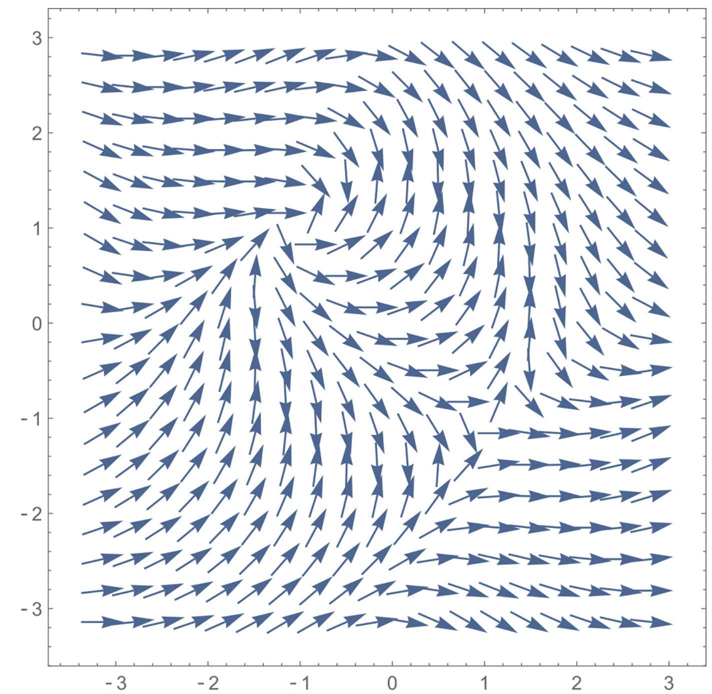
2D topological insulator: First bulk Z_2 invariant

Topological invariant = number or zeros of $\mathrm{Pf}\,[t(\mathbf{k})]$ in EBZ modulo 2

conventional insulator



topological insulator



$$I = \frac{1}{2\pi i}\int_{\partial(\mathrm{EBZ})} d\mathbf{k}\cdot\nabla\log\left(\mathrm{Pf}\left[\langle u_m^-(\mathbf{k})|\Theta|u_n^-(\mathbf{k})\rangle\right]\right) \mod 2$$

It follows from **bulk-boundary correspondence**: edge Z_2 invariant = bulk Z_2 invariant

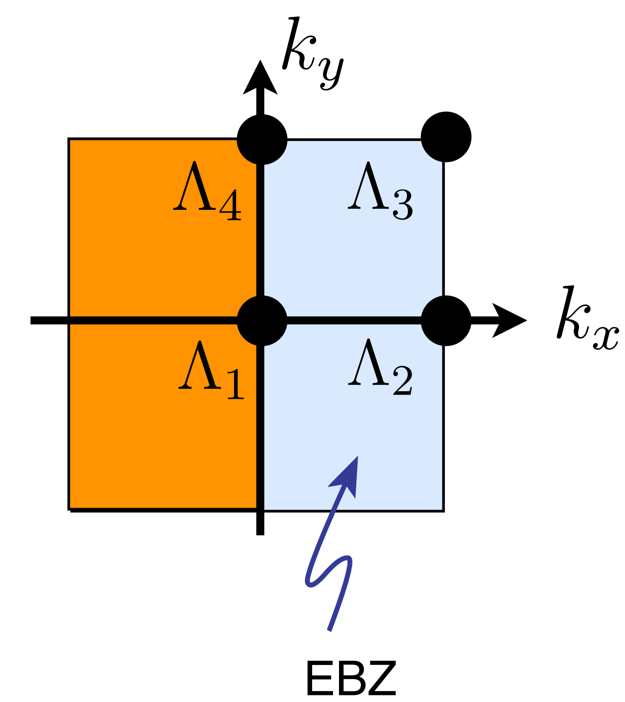
2D topological insulator: Second bulk Z_2 invariant

Bulk Z_2 invariant as an obstruction to define a "TR-smooth gauge":

[Kane Mele 05]

[Fu and Kane]

- $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs
- TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta|u_n^{(2)}(\mathbf{k})\rangle$



$\Rightarrow$ consider unitary *sewing matrix:*

$$\omega_{mn}(\mathbf{k}) = \langle u_m^-(-\mathbf{k})|\Theta|u_n^-(\mathbf{k})\rangle$$

antisymmetry property: $\omega^T(\mathbf{k}) = -\omega(-\mathbf{k})$

at TRI momenta: $\Lambda_a = -\Lambda_a \Rightarrow \omega^T(\Lambda_a) = -\omega(\Lambda_a)$ is antisymmetric

$\Rightarrow$ Pfaffian can be defined: $\mathrm{Pf}\,[\omega(\Lambda_a)]$ e.g.: $\mathrm{Pf}\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z$

$$(\mathrm{Pf}\,[\omega(\Lambda_a)])^2 = \det\,[\omega(\Lambda_a)]$$

Bulk Z_2 invariant (ν= 0,1):

$$(-1)^\nu = \prod_{a=1}^{4} \frac{\mathrm{Pf}\,[\omega(\Lambda_a)]}{\sqrt{\det\,[\omega(\Lambda_a)]}} = \pm 1$$

(gauge invariant, but smooth gauge needed)

It follows from **bulk-boundary correspondence**: edge Z_2 invariant = bulk Z_2 invariant

2D topological insulator: Bulk Z_2 invariants

Three equivalent definitions for **bulk Z_2 topological invariant:**

(A) in terms of sewing matrix:

$$(-1)^{\nu} = \prod_{a=1}^{4} \frac{\mathrm{Pf}\,[\omega(\Lambda_a)]}{\sqrt{\det\,[\omega(\Lambda_a)]}} = \pm 1$$

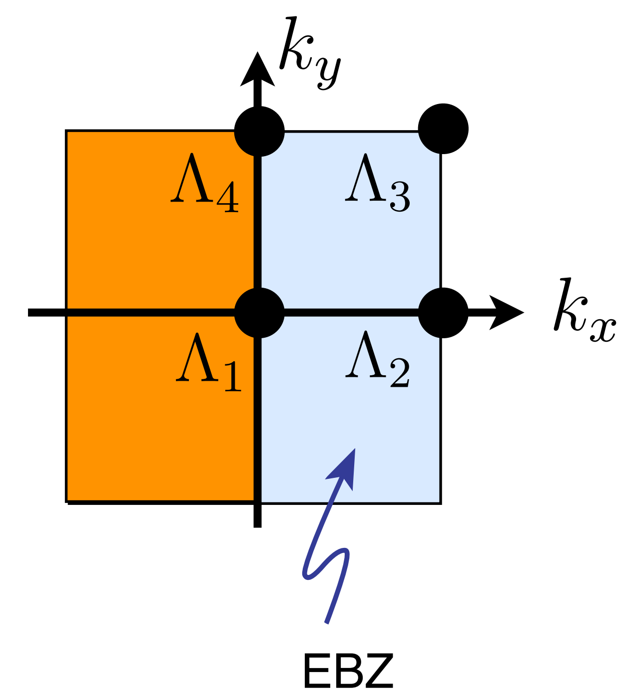
(gauge invariant, but smooth gauge needed)

sewing matrix: $\omega_{mn}(\mathbf{k}) = \langle u^{-}_{m}(-\mathbf{k})|\Theta|u^{-}_{n}(\mathbf{k})\rangle$ (is unitary, and anti-symmetric at TRI momenta)

(B) count number of zeroes of $\mathrm{Pf}\left[\langle u^{-}_{m}(\mathbf{k})|\Theta|u^{-}_{n}(\mathbf{k})\right]$ in EBZ

$$I = \frac{1}{2\pi i}\int_{\partial(\mathrm{EBZ})} d\mathbf{k}\cdot\nabla\log\left(\mathrm{Pf}\left[\underbrace{\langle u^{-}_{m}(\mathbf{k})|\Theta|u^{-}_{n}(\mathbf{k})}\right]\right)\ \mathrm{mod}\ 2$$

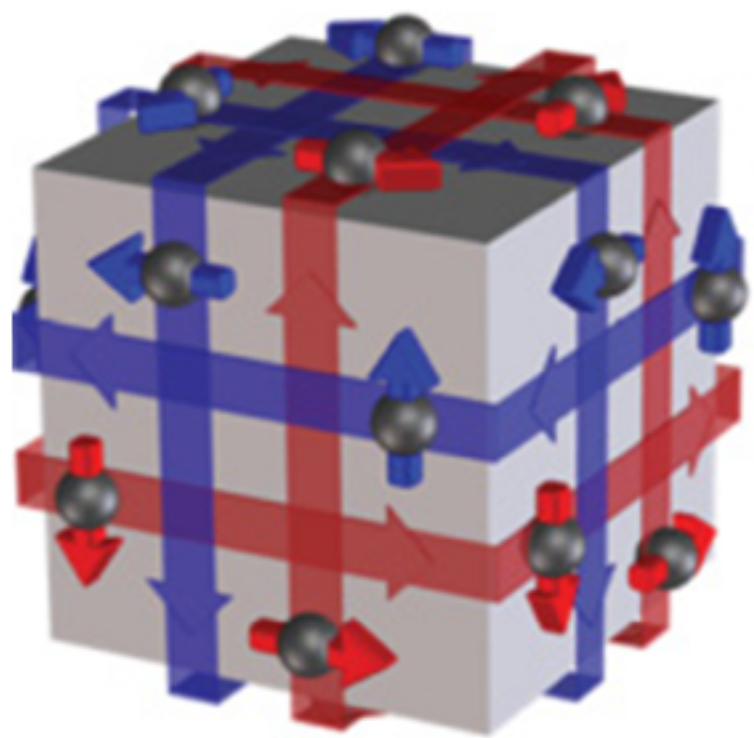
(antisymmetric at all momenta, but not unitary)



(C) in terms of Berry connection:

$$\nu = \frac{1}{2\pi}\left[\oint_{\partial(EBZ)} d\boldsymbol{k}\cdot\mathcal{A} - \int_{\mathrm{EBZ}} d^2\boldsymbol{k}\,\mathcal{F}\right] \mathrm{mod}\ \ 2$$

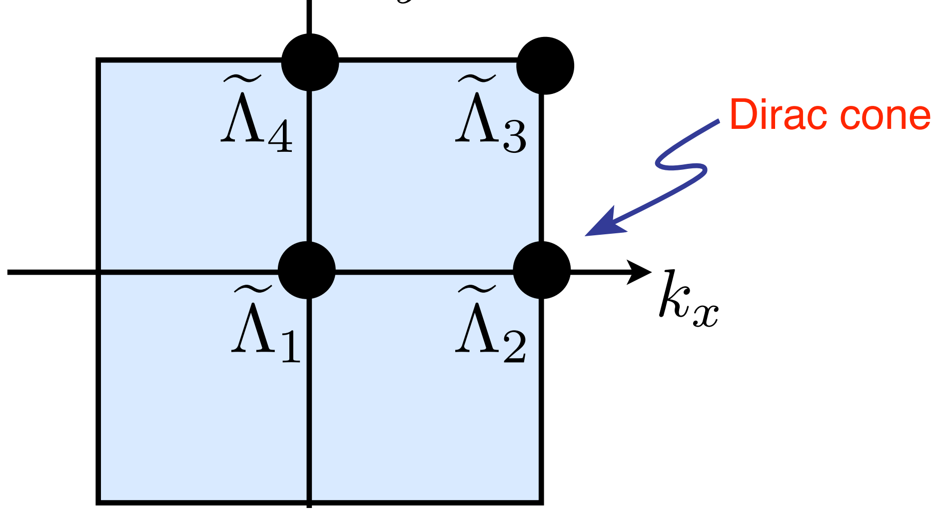
Three-dimensional topological insulators



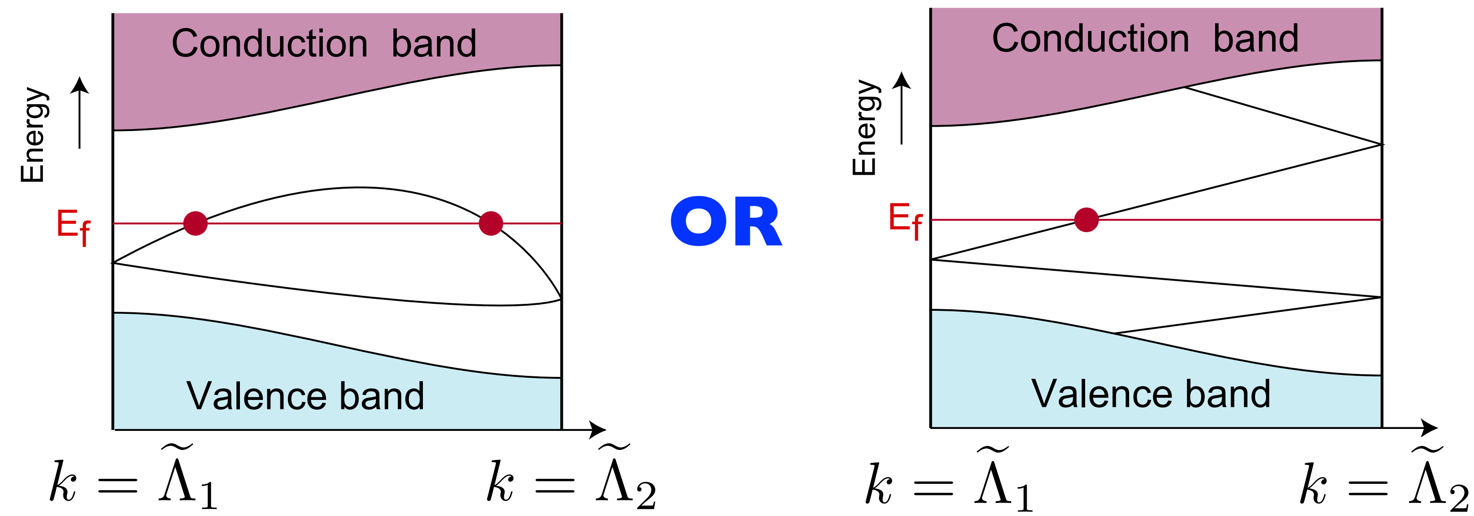
3D topological insulator: Surface Z_2 invariant

- How do surface states connect between TRI momenta? **[after Hasan & Kane, RMP 2010]**

(4 time-reversal invariant momenta in surface BZ)



surface Brillouin zone



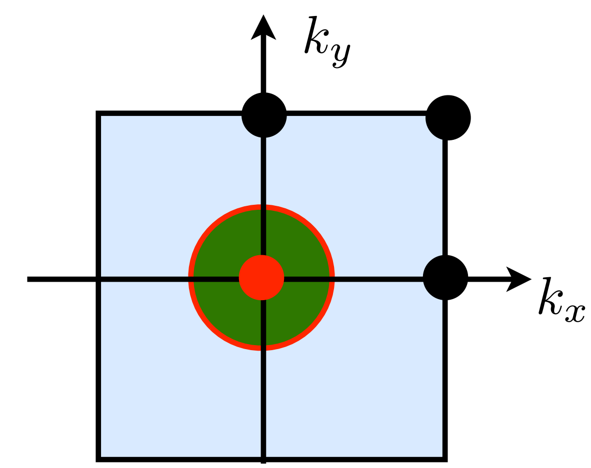
- **Surface Z_2 invariant:**

$\nu = 1$: **Strong topological insulator**

— Fermi surface encloses *odd* number of TRI momenta

— independent of surface orientation

— protected by time-reversal symmetry

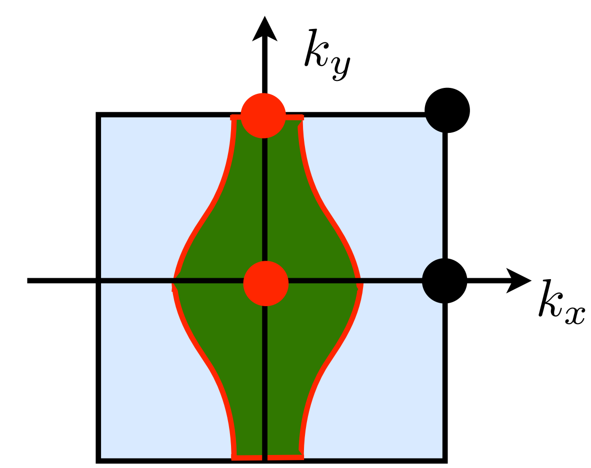


$\nu = 0$: **Weak topological insulator**

— Fermi surface encloses *even* number of TRI momenta

— depends on surface orientation (quasi-2D topological insulator)

— protected by time-reversal *and* translation symmetry



3D topological insulator: Bulk Z_2 invariant

[Kane-Mele, Moore-Balents, Roy, Fu-Kane-Mele (06-07)]

- **Bulk Z_2 invariant:**

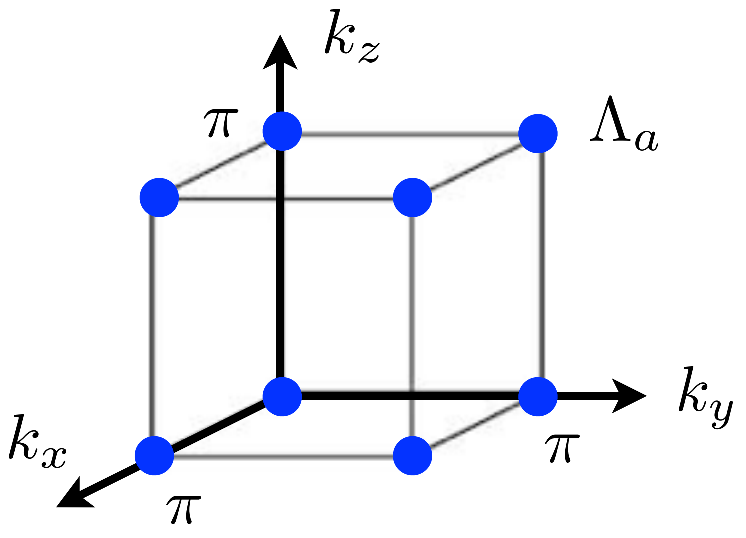
$$t_{mn}(\mathbf{k}) = \langle u_m^-(\mathbf{k}) | \Theta | u_n^-(\mathbf{k}) \rangle$$

– Zeros of $\mathrm{Pf}[t(\mathbf{k})]$ are lines

— Due to time-reversal symmetry there are only 16 possibilities for the arrangement of the lines:

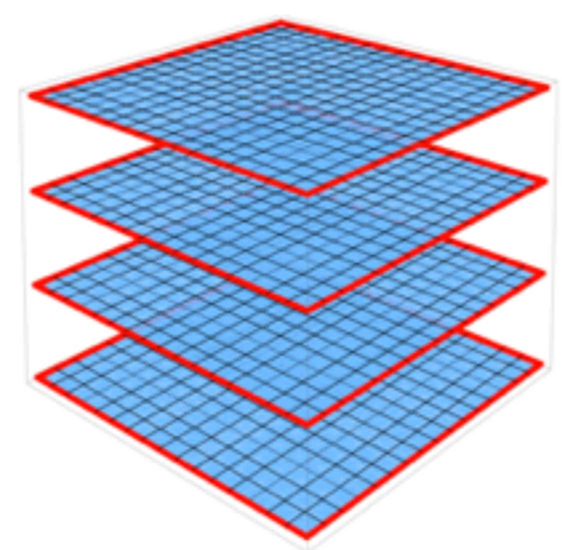
$$(\nu_0; \nu_1, \nu_2, \nu_3)$$

8 TRI momenta in bulk BZ



— Strong Z_2 invariant

$$(-1)^{\nu_0} = \prod_{a=1}^{8} \frac{\mathrm{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} = \pm 1$$



— Weak Z_2 invariant

$$(-1)^{\nu_i} = \prod_{a=1}^{4} \frac{\mathrm{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}}\Bigg|_{k_i=0}$$

Bulk-boundary correspondence: edge Z_2 invariant = bulk Z_2 invariant

Experimental detection of 3D topological insulators

▶ observed in certain band insulators with strong spin-orbit coupling

BiSb alloy, Bi_2Se_3, Bi_2Te_3, $TlBiTe_2$, $TlSbSe_2$, etc ....

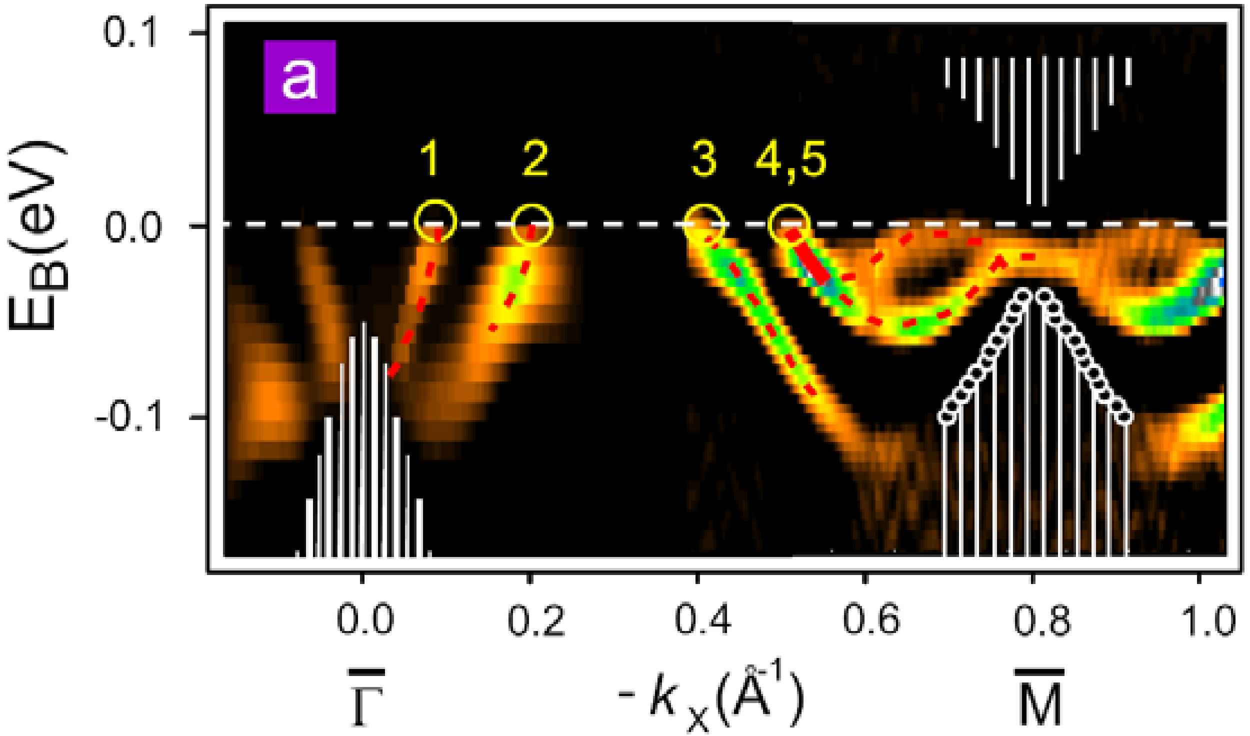
stable surface states cross a gap, that is opened up by spin-orbit coupling

- $\mathrm{Bi}_{1-x}\ \mathrm{Sb}_x$:

[Fu, Kane, PRL 2007]

[Hsieh, Hasan et al, Nature 2008]

momentum resolved photoemission (ARPES)



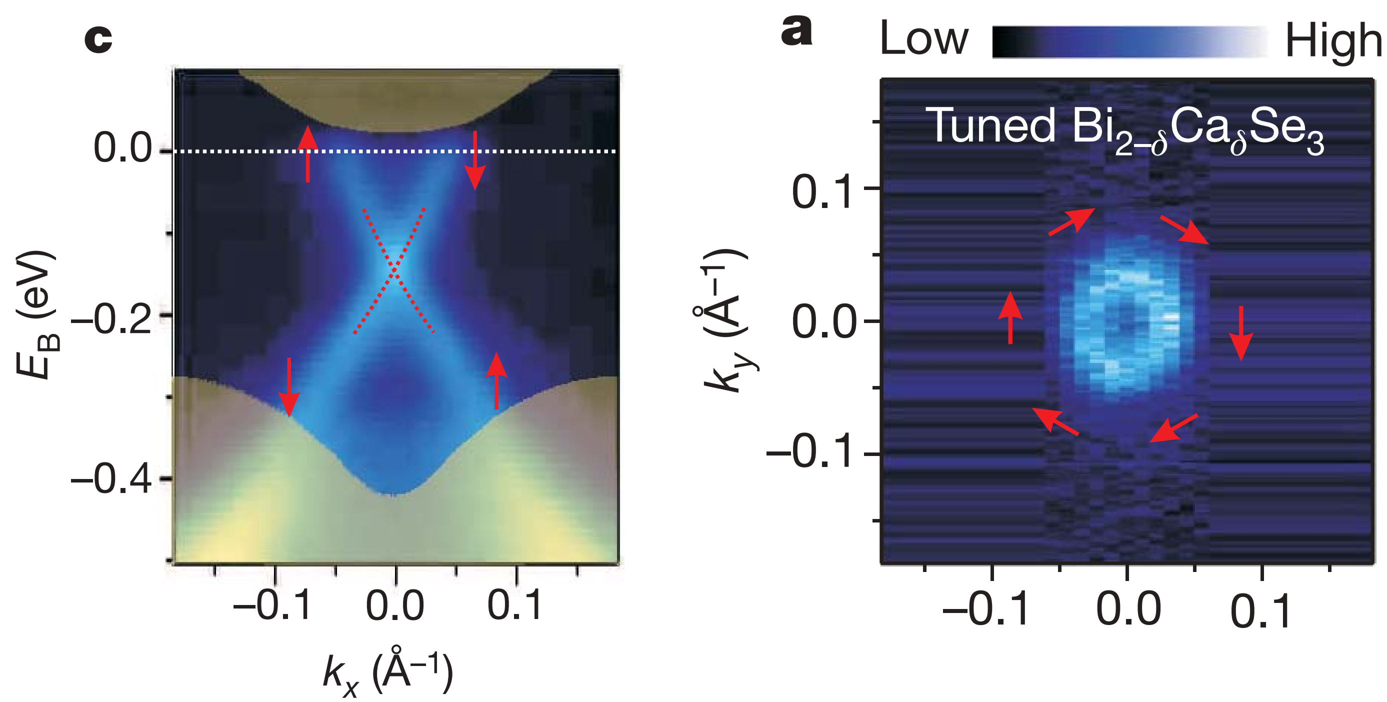
five surface state bands cross E_F between TRI momenta $\bar{\Gamma}$ and $\bar{\mathrm{M}}$

$\Rightarrow$ strong topological insulator

Experimental detection of 3D topological insulators

- $Bi_2\ Se_3$:

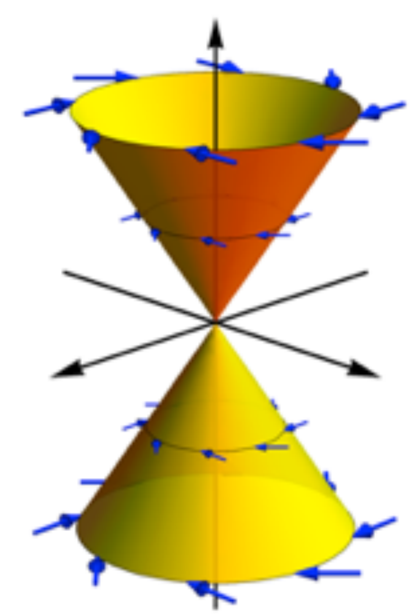
spin resolved and momentum resolved photoemission (ARPES)



[H. Zhang et al., Nat Phys 2009]

[Hsieh, Hasan et al, Nature 2009]

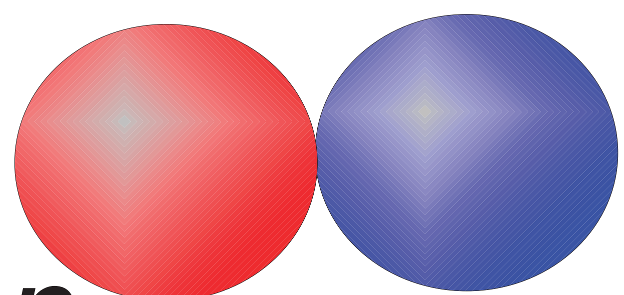
simple surface state structure, similar to graphene



Unique properties of helical surface states:

- spin and momentum are locked
- half of an ordinary 2DEG, "1/4 of graphene"
- robust to disorder, impossible to localize

Topological Superconductors



p

Sr_2RuO_4

Bogoliubov-de Gennes theory for superconductors

Superconductor = Cooper pairs (boson) + Bogoliubov quasiparticles (fermions)

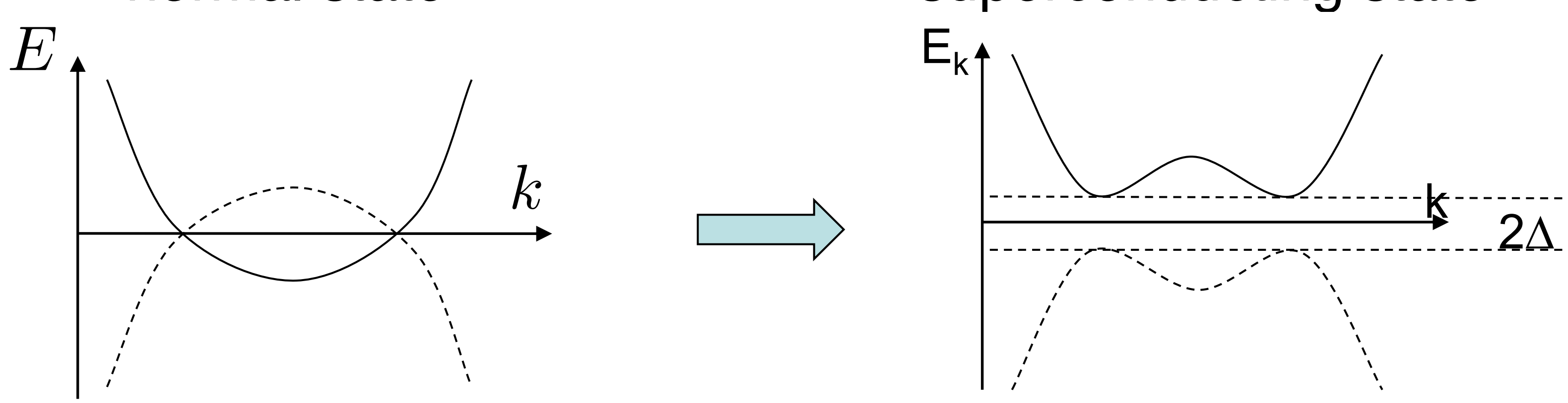
BCS mean field theory: $c^\dagger c\, c^\dagger c \quad \Rightarrow \quad \langle c^\dagger c^\dagger \rangle c\, c = \Delta^* c\, c$

$$H = \frac{1}{2} \sum_{\boldsymbol{k}} \begin{pmatrix} c^\dagger & c \end{pmatrix} H_{\mathrm{BdG}} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

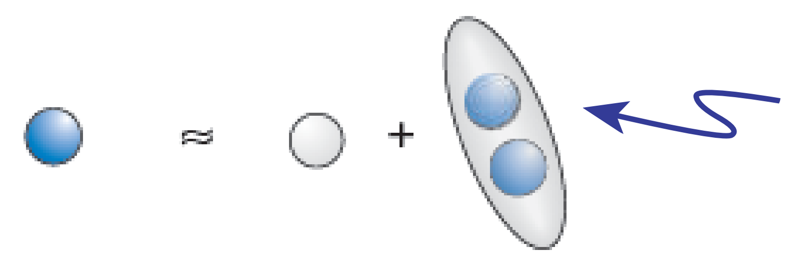
Bogoliubov-de Gennes Hamiltonian

$$H_{\mathrm{BdG}} = \begin{pmatrix} h_0 & \Delta \\ \Delta^\dagger & -h_0^T \end{pmatrix}$$

normal state superconducting state



Built-in anti-unitary particle-hole symmetry:



Cooper pair

$$\boxed{C\mathcal{H}_{\mathrm{BdG}}(\mathbf{k})C^{-1} = -\mathcal{H}_{\mathrm{BdG}}(-\mathbf{k})} \qquad C = \tau_x \mathcal{K} \qquad C^2 = +1 \qquad \tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(for triplet pairing)

Particle-hole symmetry: $C\psi_{+\mathbf{k},+E} = \tau_x \psi^*_{-\mathbf{k},-E} \quad \Rightarrow \quad \gamma^\dagger_{\boldsymbol{k},E} = \gamma_{-\boldsymbol{k},-E}$

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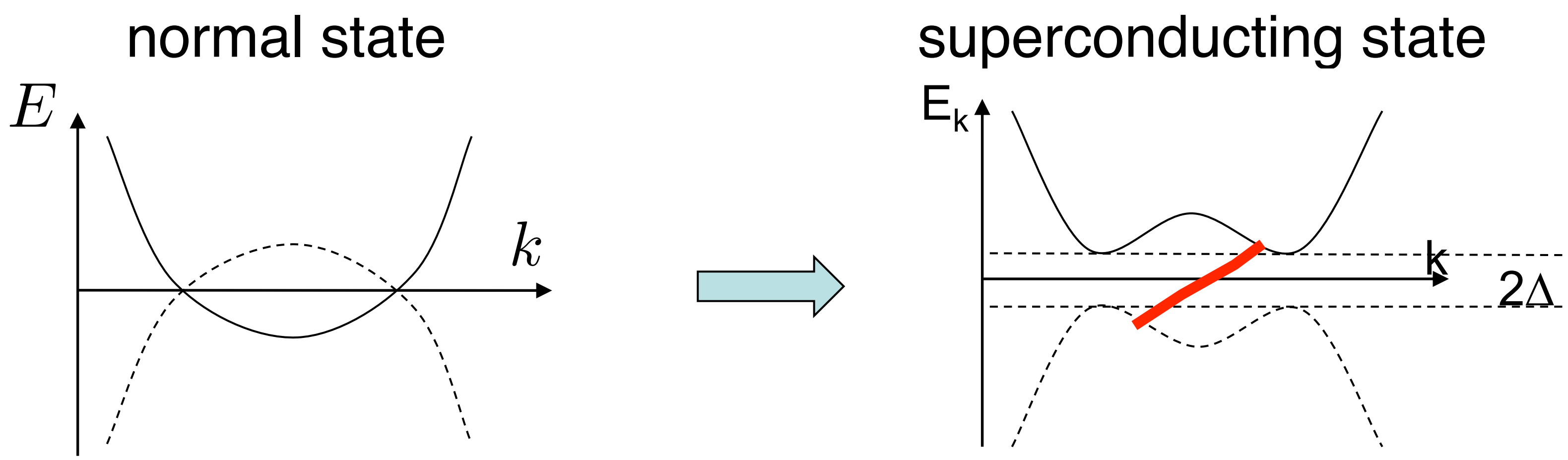

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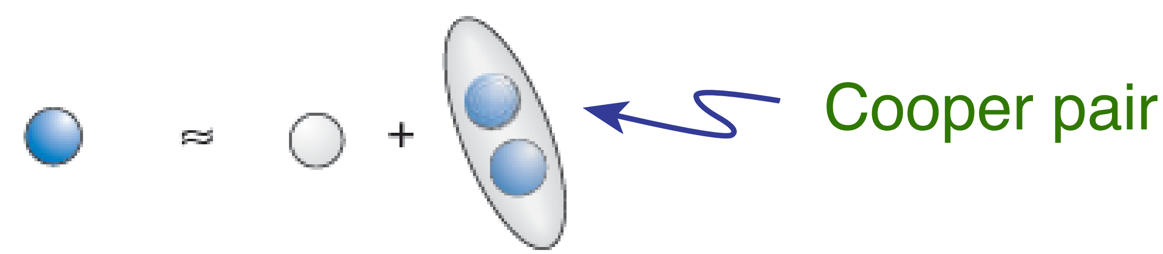


$$\boxed{C\mathcal{H}_{\mathrm{BdG}}(\mathbf{k})C^{-1} = -\mathcal{H}_{\mathrm{BdG}}(-\mathbf{k})}$$

$C = \tau_x \mathcal{K}$ $\qquad C^2 = +1$ (for triplet pairing) $\qquad \tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Particle-hole symmetry + bulk-boundary correspondence:

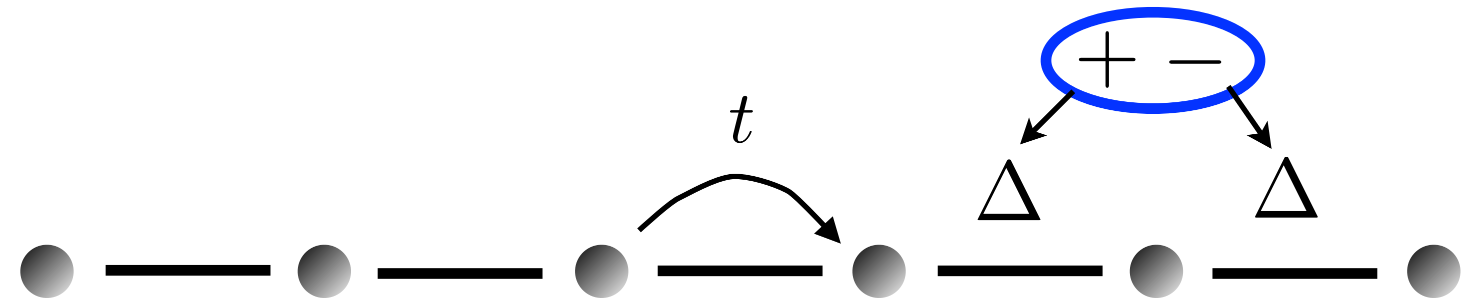
→ Majorana edge state at zero energy

1D topological superconductor: Majorana chain

[Kitaev 2000]

One-dimensional spinless p-wave superconductor: Majorana chain

Experiments:
InSb-nanowire-heterostructures



Hamiltonian: $$\mathcal{H} = \sum_j \left[t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j - \mu c_j^\dagger c_j + \Delta(c_{j+1}^\dagger c_j^\dagger + c_j c_{j+1}) \right]$$

in momentum space: $$\mathcal{H} = \frac{1}{2} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_{\mathrm{BdG}}(k) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}$$

$$\mathcal{H}_{\mathrm{BdG}}(k) = \mathbf{d}(k) \cdot \vec{\tau}$$

$$d_x(k) = 2i\Delta \sin k \quad d_y(k) = 0$$

$$d_z(k) = 2t \cos k - \mu$$

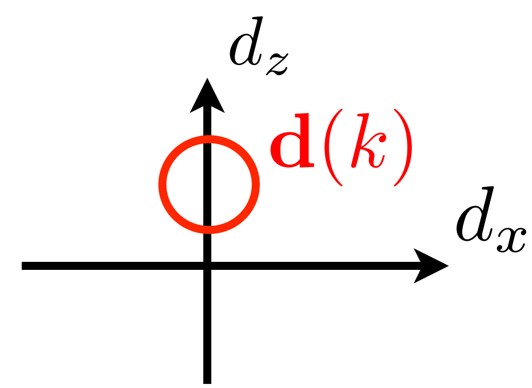
Particle-hole symmetry:

$$\tau_x \mathcal{H}_{\mathrm{BdG}}^*(k) \tau_x = -\mathcal{H}_{\mathrm{BdG}}(-k)$$

Time-reversal symmetry:

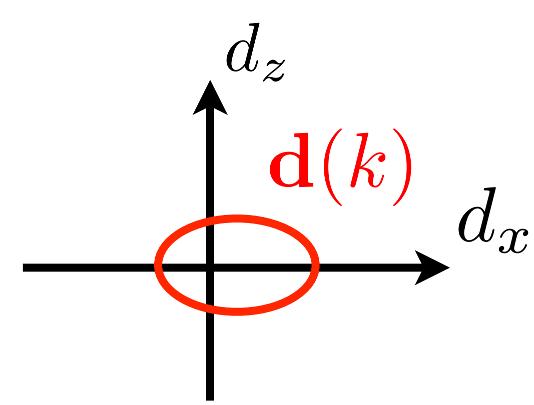
$$\tau_z \mathcal{H}_{\mathrm{BdG}}^*(k) \tau_z = +\mathcal{H}_{\mathrm{BdG}}(-k)$$

energy spectrum: $E_\pm = \pm |\mathbf{d}(k)|$



$|\mu| > 2t$:

trivial super-
conductor



$|\mu| < 2t$:

topological
superconductor

1D topological superconductor: Majorana chain

[Kitaev 2000]

To reveal zero-energy edge states, consider different viewpoint: **Majorana representation**

Majorana fermion:
Particle = Antiparticle

$$c_j = \frac{1}{2}\left(\gamma_{1j} + i\gamma_{2j}\right) \qquad c_j^\dagger = \frac{1}{2}\left(\gamma_{1j} - i\gamma_{2j}\right)$$

Anti-commutation relations: $\left\{\gamma_{lj}, \gamma_{l'j'}\right\} = 2\delta_{ll'}\delta_{jj'} \qquad \left(\gamma_{lj}\right)^2 = 1$

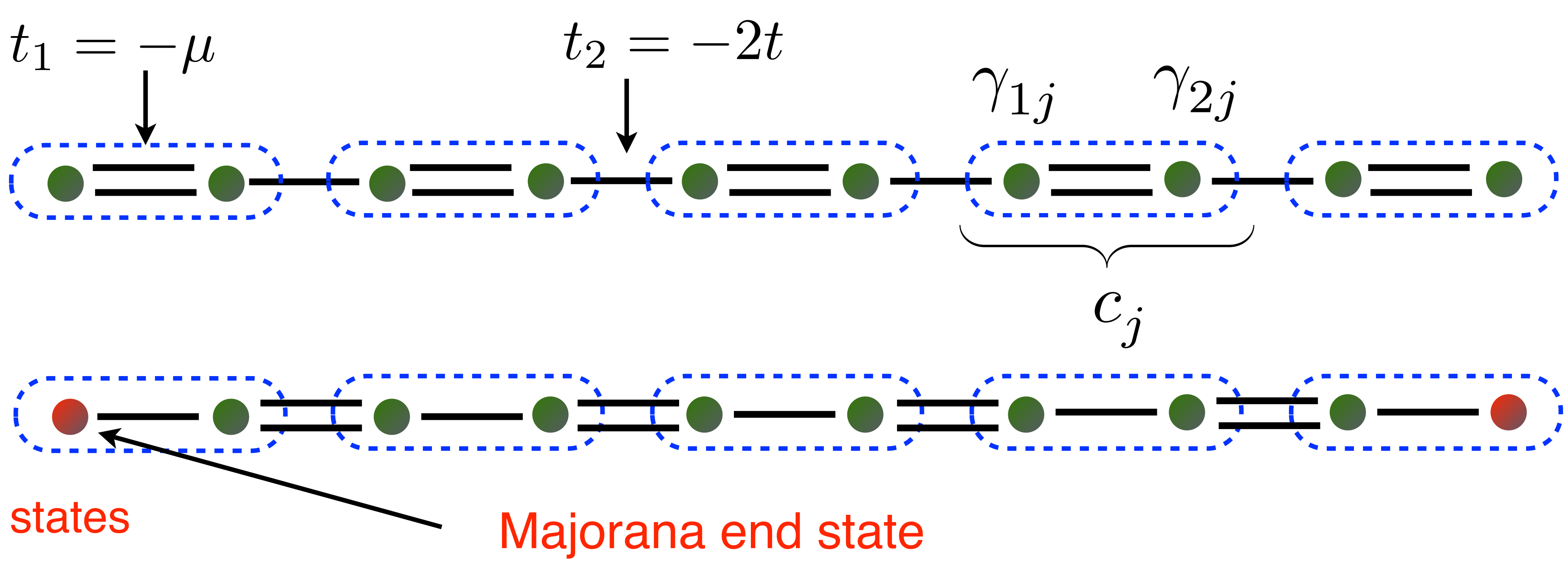
$\Longrightarrow$ Majorana chain for spinless fermions

$$H = \frac{i}{2}\sum_j \left[-\mu\gamma_{1j}\gamma_{2j} + (\Delta - t)\gamma_{2j}\gamma_{1j+1} + (\Delta + t)\gamma_{1j}\gamma_{2j+1}\right]$$

for $\Delta = -t$: nearest neighbor Majorana chain

$t_1 > t_2$:
trivial superconductor

$t_1 < t_2$:
topological superconductor

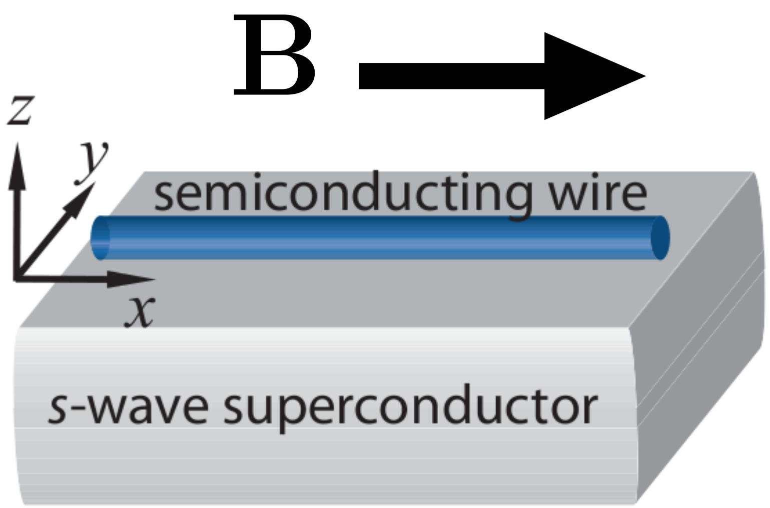


— zero-energy Majorana end states

Experimental detection of 1D spinless topological SC

1D spinless chiral p-wave superconductor is likely (?) realized in InSb-nanowire-heterostructures

magnetic field B

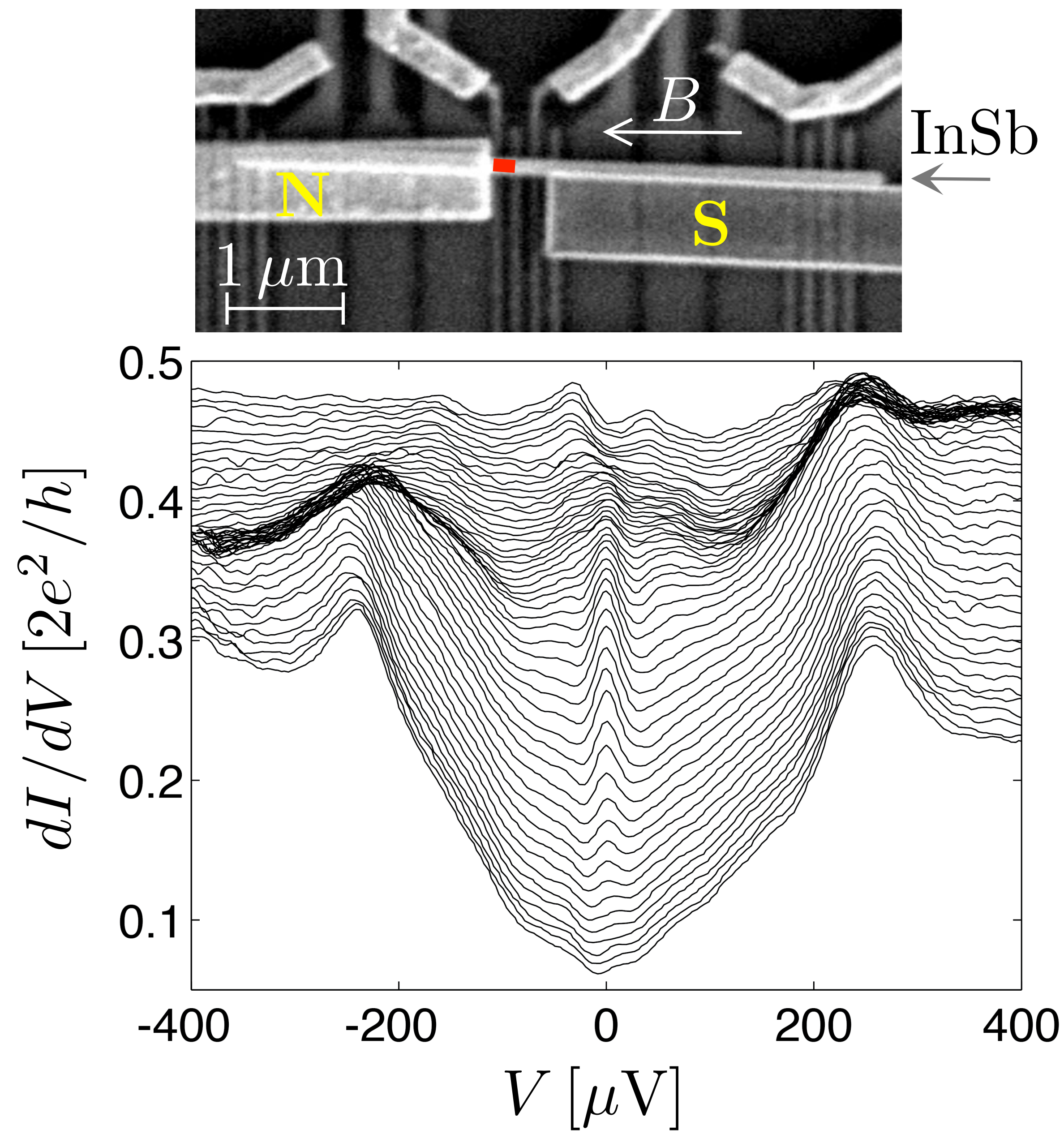


- Condition for topological phase:

$$B \propto E_{\text{Zeeman}} > \sqrt{\Delta^2 - \mu^2}$$

[Sau, Lutchyn, Tewari, das Sarma, et al 2009]
[Oreg, von Oppen, et al 2010]

[after Alicea, Rep. Prog. Phys. 2012]



Differential tunneling conductance as a function of magnetic field B

[Mourik, Kouwenhoven et al, Science 2012]

Two-dimensional spinless chiral p-wave SC

[Read & Green 00]

Lattice BdG model: $H_{\mathrm{BdG}} = \frac{1}{2}\sum_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}} \quad c_{-\mathbf{k}} \right) \mathcal{H}_{\mathrm{BdG}} \begin{pmatrix} c_{\mathbf{k}} \\ c^\dagger_{-\mathbf{k}} \end{pmatrix}$ $\quad \mathcal{H}_{\mathrm{BdG}} = \mathbf{m}(\mathbf{k}) \cdot \vec{\tau}$

(on square lattice)

$$m_x(\mathbf{k}) = \Delta_0 \sin k_x \qquad m_y(\mathbf{k}) = \Delta_0 \sin k_y \qquad m_z(\mathbf{k}) = 2t\left[\cos k_x + \cos k_y\right] - \mu$$

Particle-hole symmetry: $\tau_x \mathcal{H}^*_{\mathrm{BdG}}(\mathbf{k})\tau_x = -\mathcal{H}_{\mathrm{BdG}}(-\mathbf{k})$

$(\tau_x)^2 = 1 \quad \Rightarrow \quad \text{class D}$

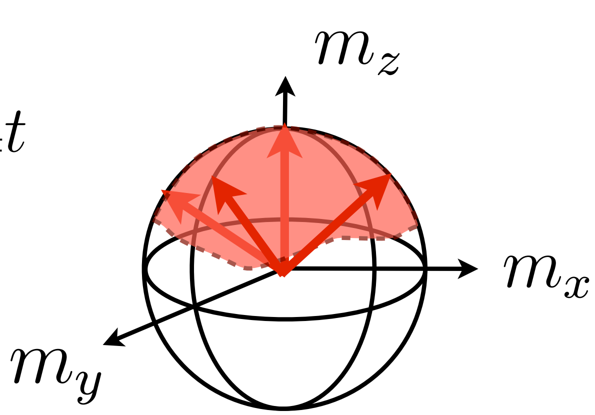
$$E = \pm\left|\boldsymbol{m}(\boldsymbol{k})\right|$$

Spectrum flattening: $\hat{\boldsymbol{m}}(\boldsymbol{k}) = \dfrac{\boldsymbol{m}(\boldsymbol{k})}{|\boldsymbol{m}(\boldsymbol{k})|}$

trivial phase

$|\mu| > 4t$

$n = 0$

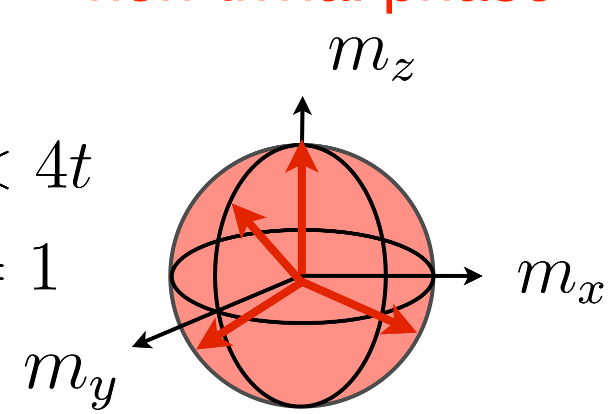


no edge state

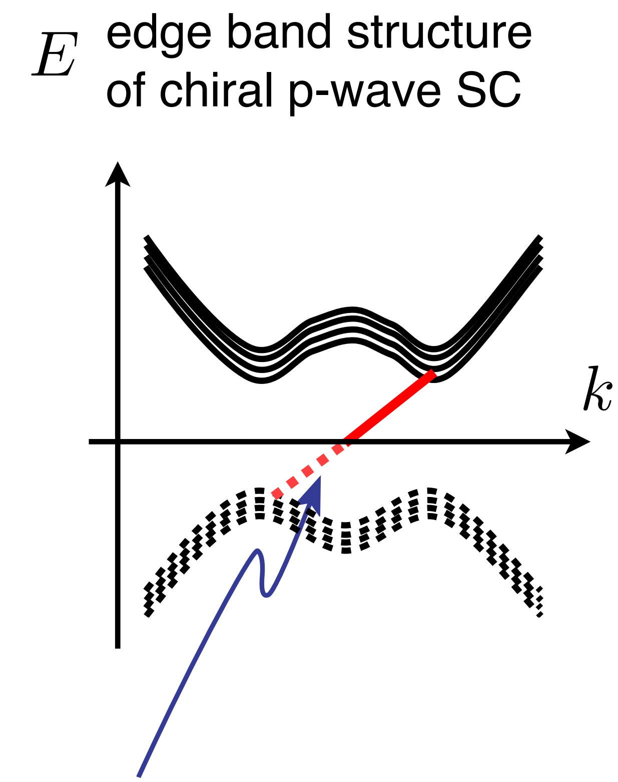
non-trivial phase

$|\mu| < 4t$

$n = 1$



chiral Majorana edge state



classified by Chern number: (winding number)

$$n = \frac{1}{8\pi}\int_{\mathrm{BZ}} d^2\mathbf{k}\,\epsilon^{\mu\nu}\hat{\mathbf{m}} \cdot \left[\partial_{k_\mu}\hat{\mathbf{m}} \times \partial_{k_\nu}\hat{\mathbf{m}}\right]$$

Sr_2RuO_4 (n=2)

Mapping $\quad \hat{\boldsymbol{m}}(\boldsymbol{k})$: Brillouin zone $\longmapsto \hat{\boldsymbol{m}}(\boldsymbol{k}) \in S^2 \qquad$ "$\pi_2(S^2) = \mathbb{Z}$"

Majorana fermions in chiral p-wave superconductor

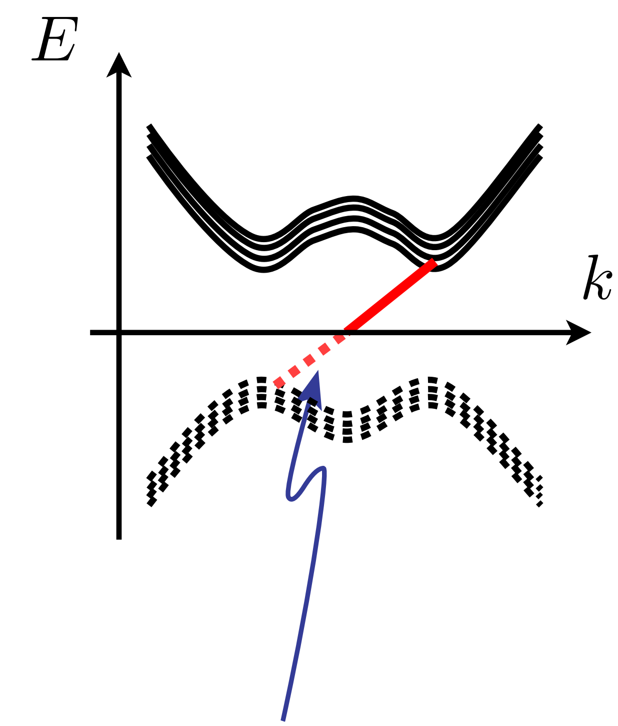
▶ Bulk-boundary correspondence: $n = \#$ Majorana edge modes

Majorana edge states are perfect heat conductor

⟹ Quantized thermal Hall conductance

$$\frac{\kappa_{xy}}{T} = \frac{\pi k_B^2}{48h} \int_{\mathrm{BZ}} d^2\mathbf{k}\, \epsilon^{\mu\nu} \hat{\mathbf{m}} \cdot \left[\partial_{k_\mu} \hat{\mathbf{m}} \times \partial_{k_\nu} \hat{\mathbf{m}}\right]$$

edge band structure of chiral p-wave SC

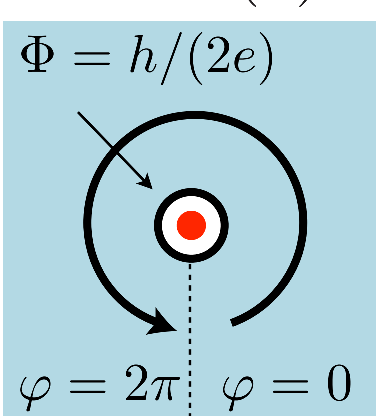


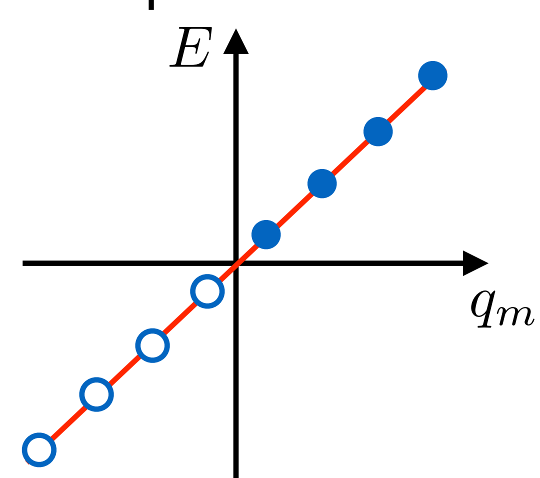
Majorana state

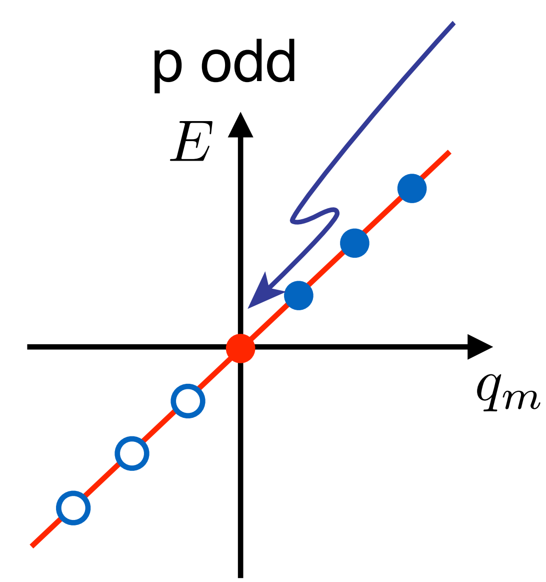
▶ Majorana zero mode at a vortex:

- vortex: small hole with edge states
- Majorana zero mode for $\Phi = p\frac{h}{2e}$ with p odd
(periodic vs. anti-periodic BC)

$$\Delta = \Delta(r) e^{i\varphi}$$



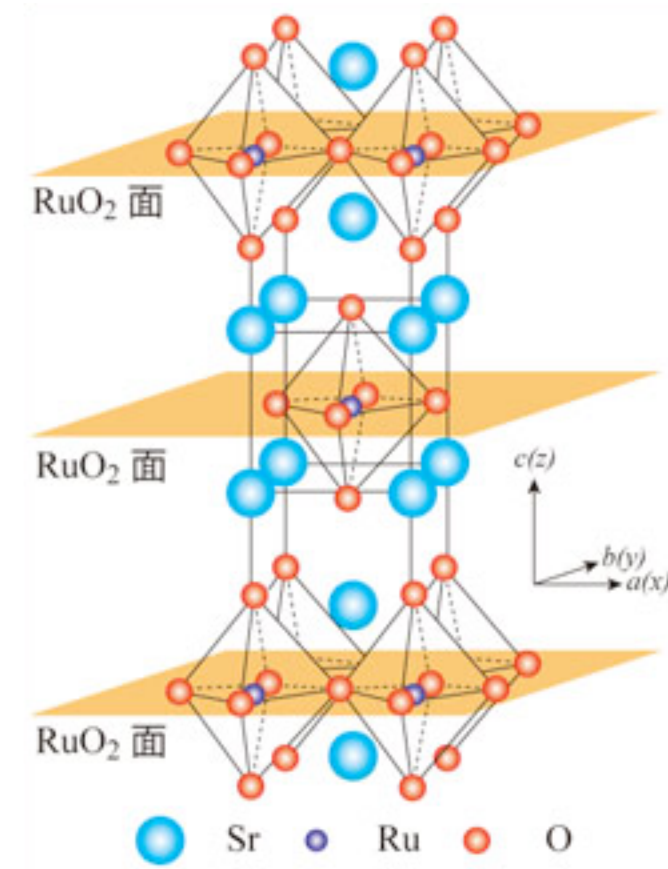




[Caroli, de Gennes, Matricon '64]

Experimental detection of spinful chiral p-wave SC

The transition-metal-oxide Sr_2RuO_4 is likely (?) a *spinful* chiral p-wave superconductor with Chern number n=2 (per layer)



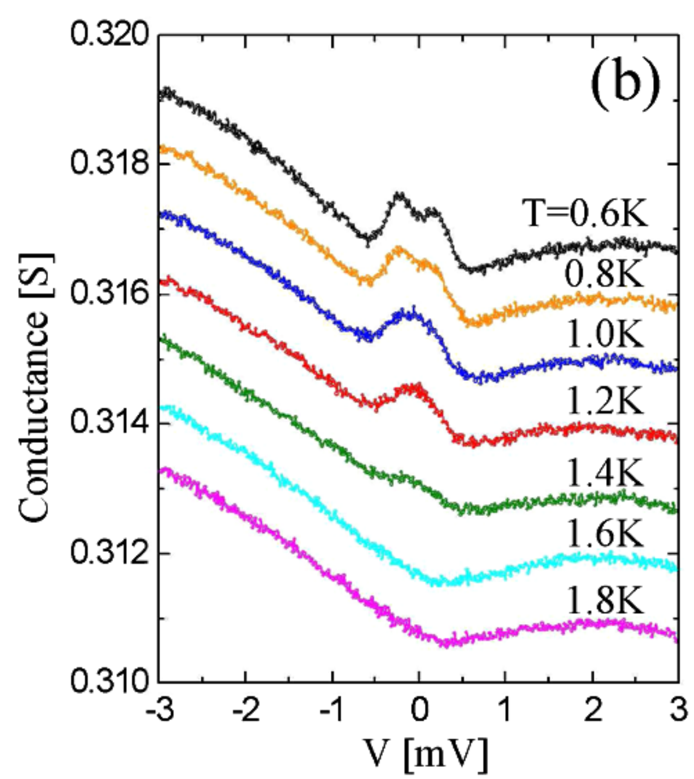
— Ru t_{2g}-orbitals ($4d^4$-electrons) hybridized with O p-oribitals form quasi-two-dimensional Fermi surfaces

— transition temperature T_C = 1.5K

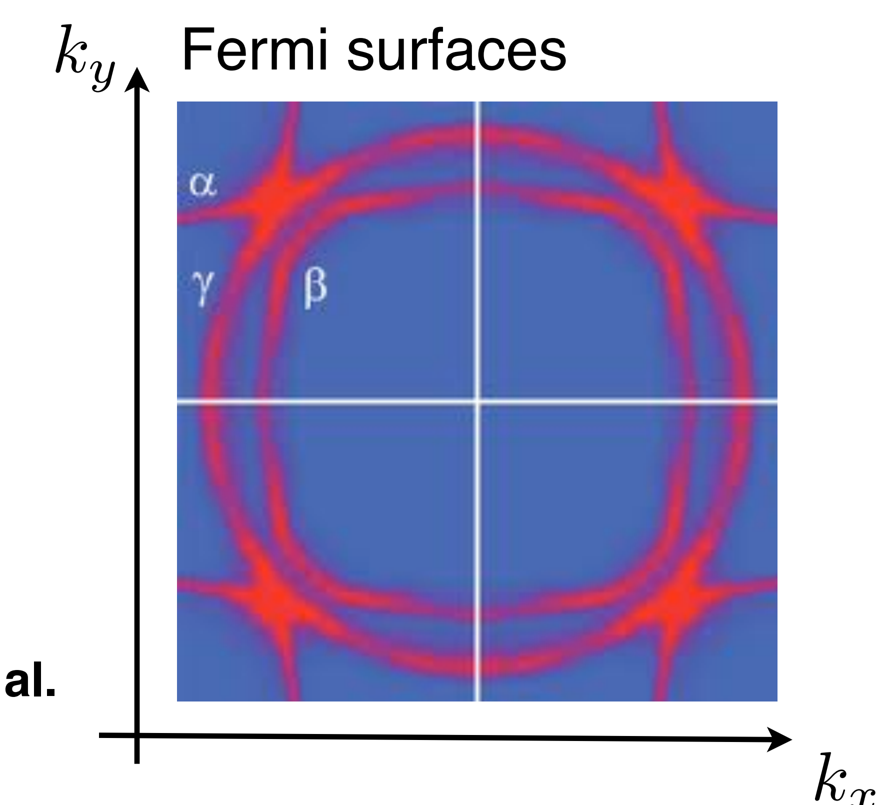
— strong anisotropies in spin dependent responses (NMR and Knight shift)

— signatures of edge states in tunneling conductance

tunneling conductance



Fermi surfaces



[Maeno et al. JPSJ 81, 011009]

[Kashiwaya et al. PRL 2011]

[Damascelli et al. PRL 2000]