Title: Inversion-protected higher-order topological superconductivity in monolayer WTe2

Speakers: Yi-Ting Hsu

Series: Condensed Matter

Date: September 10, 2019 - 3:30 PM

URL: http://pirsa.org/19090064

Abstract: Monolayer WTe2, an inversion-symmetric transition metal dichalcogenide, has recently been established as a quantum spin Hall insulator and found superconducting upon gating. Here we show that generally a superconducting inversion-symmetric quantum spin Hall material whose normal state is ``effectively gapped", such as gated monolayer WTe2, can be an inversion-protected topological crystalline superconductor featuring ``higher-order topology" if the superconductivity is parity-odd. We explicitly demonstrate how the bulk-boundary correspondence naturally emerges in such type of superconductors within a two-dimensional minimal model. We then study the pairing symmetry of superconducting WTe2 with a microscopic model, and find two types of self-consistently obtained exotic pairings. First is an odd-parity pairing that possesses a nontrivial bulk symmetry indicator and hosts two Majorana Kramers pairs localizing at opposite corners. Even when the conventional pairing is energetically favored, we find that an intermediate in-plane field exceeding the Pauli limit stabilizes an equal-spin pairing aligning with the field. Our findings suggest gated monolayer WTe2 is a playground for exotic odd-parity superconductivity, and possibly the first material realization for inversion-protected Majorana corner modes without utilizing proximity effect.

Inversion-protected higher-order topological superconductivity in monolayer WTe_2

Yi-Ting Hsu

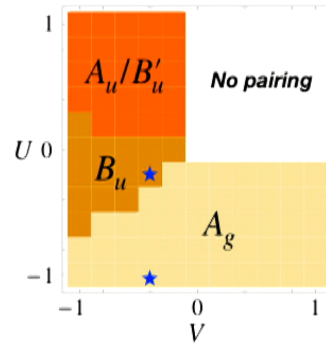
University of Maryland

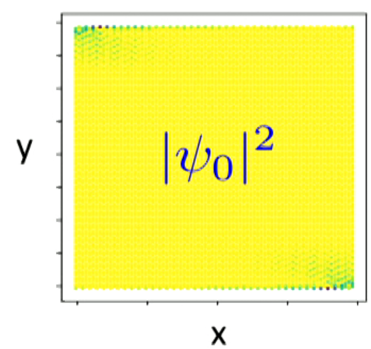
CMTC

YTH, Will Cole, Ruixing Zhang, Jay Sau arxiv: 1904.06361 (2019)

Perimeter Institute

09/10/19

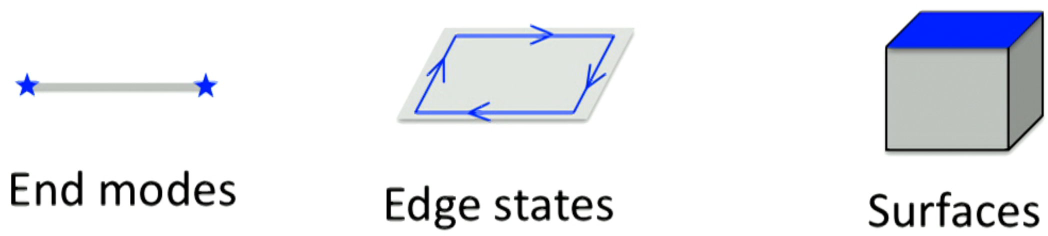




Higher-order topological phases

❖ Signature of traditional topo phases in d dimension:

- Boundary modes in (d-1)-dimension



How to achieve HOT phases?

- Extrinsic

  Protected by **surface gap in (d-1)** dimension

  No bulk symmetries are involved

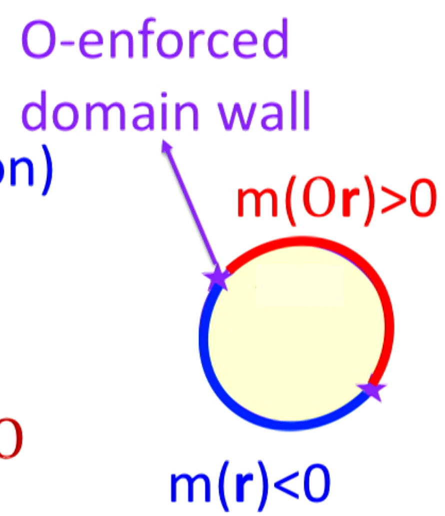
- Intrinsic

  Protected by bulk **symmetries**

  bulk gap (in d dimension)

  Q: What kind of symmetries?

  A: Some **non-local** bulk symmetries O



How to achieve HOT phases?

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  Protected by surface gap in (d-1) dimension

  No bulk symmetries are involved

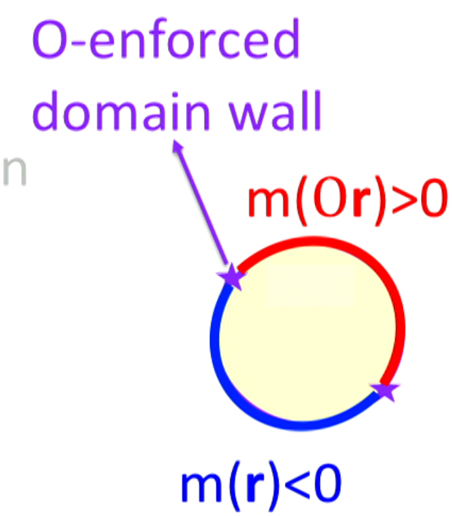
- Intrinsic

  Protected by bulk **symmetries**

  bulk gap in d dimension

Q: What kind of symmetries?

A: Some **crystalline** symmetries O



Crystalline symmetries vs Band topology

Q: Effects of crystalline symmetries on SPTs?

1. Allow inference of topology from symmetry eigenvalues:

E.g. Fu-Kane criteria:

For 3D time-reversal TIs with inversion symmetry,

Z_2 index is given by parity eigenvalues of the occupied bands

Such topological indices => **symmetry indicators**

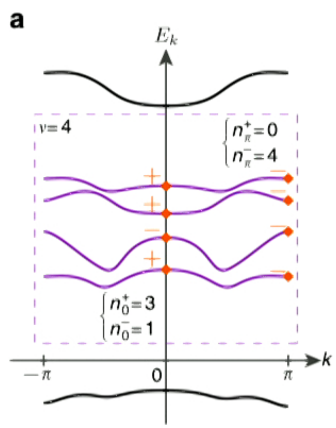
Classify TR insulators under all space groups

Q: Effects of crystalline symmetries on SPTs?

2. Change the topological classification

Consider 3D time-reversal insulators (class AII)

+ 230 space groups (SGs):



$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}\,.$$

$$= X_{\mathrm{BS}}^{(w)} \times X_{\mathrm{BS}}^{(s)}$$

Po, Vishwanath, Watanabe, Ncomm (2017)

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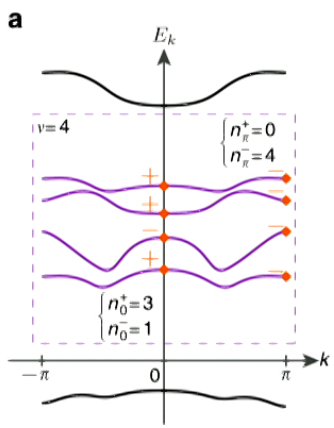

$$X_{\rm BS} \equiv \frac{\{\rm BS\}}{\{\rm AI\}}.$$

$$= X_{\rm BS}^{(w)} \times X_{\rm BS}^{(s)}$$

- Compatible with weak TI indices, weak mirror Chern numbers

Po, Vishwanath, Watanabe, Ncomm (2017)

Classify TR insulators under all space groups

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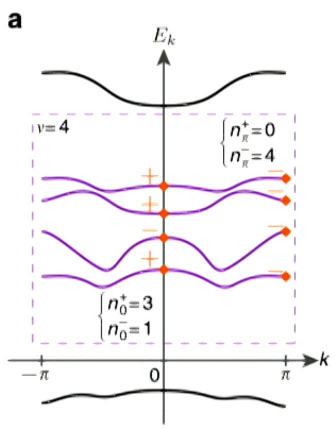

$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}} .$$

$$= X_{\mathrm{BS}}^{(w)} \times X_{\mathrm{BS}}^{(s)}$$

- **NOT** compatible with known indices

- **Band topology changes** for SGs with certain crystalline symmetries

Po, Vishwanath, Watanabe, Ncomm (2017)

Classify TR insulators under all space groups

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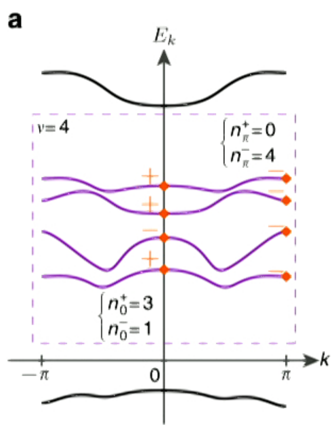

$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}\,.$$

$$= X_{\mathrm{BS}}^{(w)} \times X_{\mathrm{BS}}^{(s)}$$

E.g. SGs with **inversion** symmetry:

$\mathbf{Z_4}$ instead of Z_2 (strong TI index)

Po, Vishwanath, Watanabe, Ncomm (2017)

Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Classify TR insulators under all space groups

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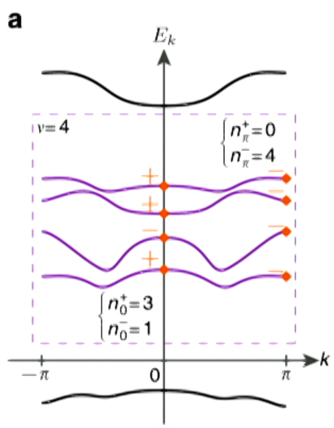


$$X_{\rm BS} \equiv \frac{\{\rm BS\}}{\{\rm AI\}} .$$
$$= X_{\rm BS}^{(w)} \times X_{\rm BS}^{(s)}$$

E.g. SGs with **inversion** symmetry: Z_4

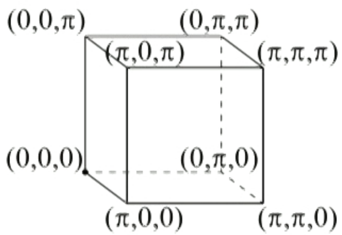
Q: How to see it's Z_4?

Po, Vishwanath, Watanabe, Ncomm (2017)   Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Inversion-protected TCI in 3D

❖ Z_4 Symmetry indicator:

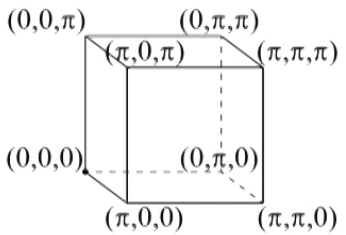
$$\kappa_N \equiv \frac{1}{4} \sum_{K \in \mathrm{TRIMs}} (n_K^+ - n_K^-)$$



Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Inversion-protected TCI in 3D

- Z_4 Symmetry indicator:



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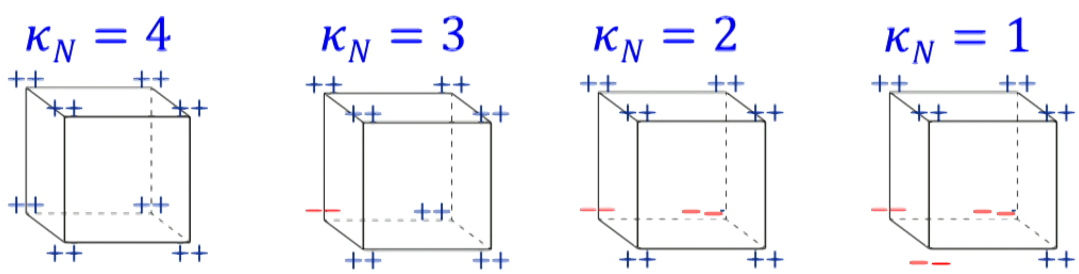

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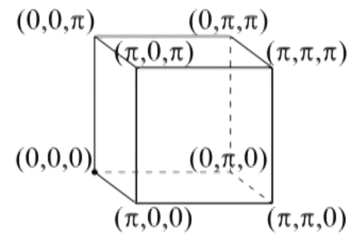
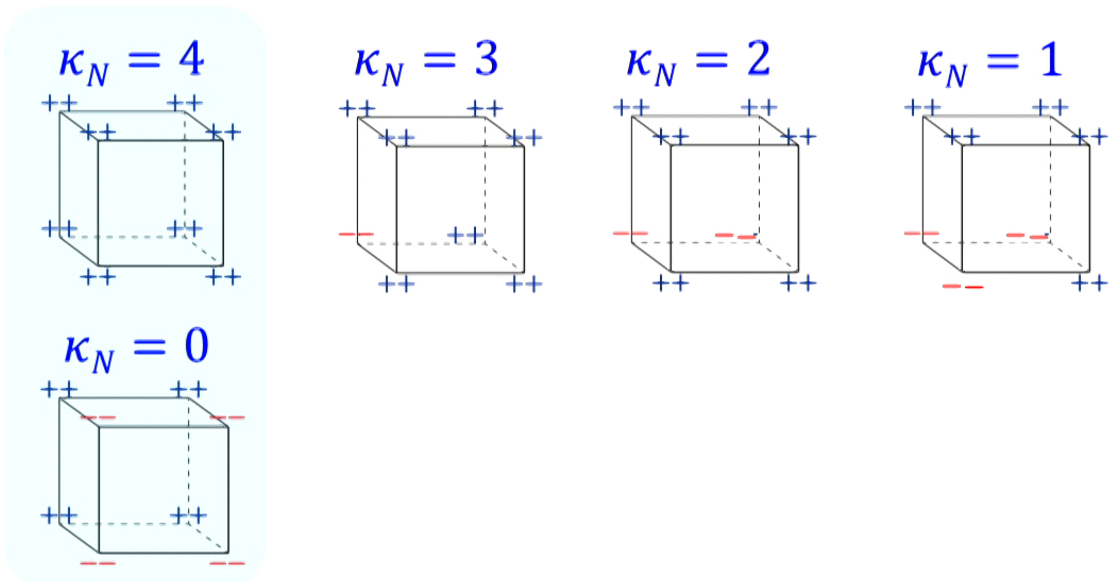




Atomic insulators

Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

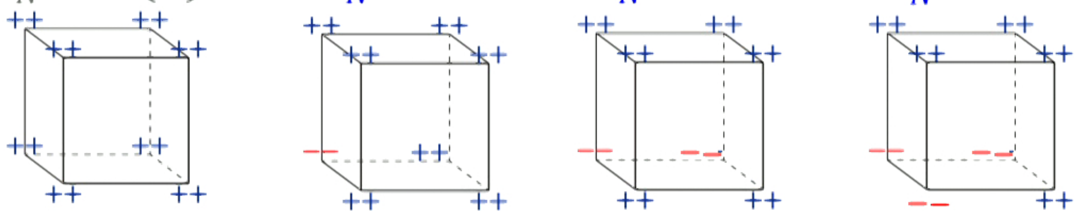
Inversion-protected TCI in 3D

❖ Z_4 Symmetry indicator:

$$\kappa_N \equiv \frac{1}{4} \sum_{K \in \mathrm{TRIMs}} (n_K^+ - n_K^-) \mod 4$$

Z_2 strong index

$$\nu_N = \kappa_N \mod 2$$



	$\kappa_N = 4(0)$	$\kappa_N = 3$	$\kappa_N = 2$	$\kappa_N = 1$
	Trivial (atomic insulator)			
Surface state	x	✓	x	✓

Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Inversion-protected TCI in 3D

- Z_4 Symmetry indicator:

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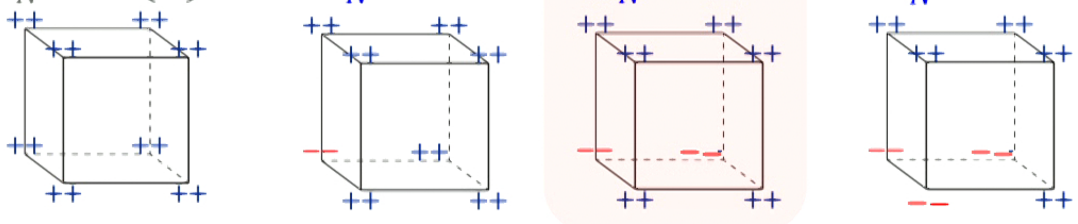

	Trivial (atomic insulator)	Topo	?	Topo
Surface state	x	✓	x	✓

Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Inversion-protected TCI in 3D

- Z_4 Symmetry indicator:

$$\kappa_N \equiv \frac{1}{4} \sum_{K \in \mathrm{TRIMs}} (n_K^+ - n_K^-) \mod 4$$

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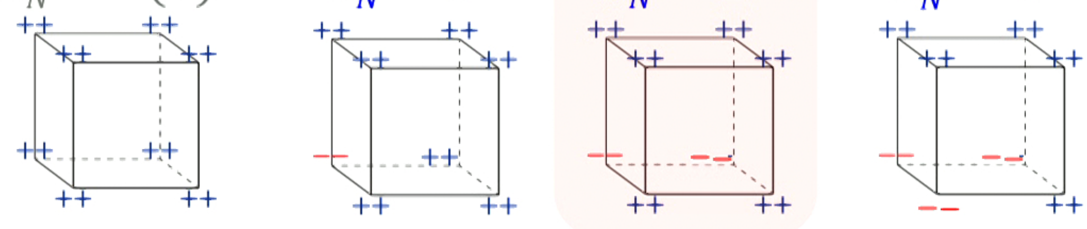
$$\nu_N = \kappa_N \mod 2$$

$\kappa_N = 4(0)$ | $\kappa_N = 3$ | $\kappa_N = 2$ | $\kappa_N = 1$



	Trivial (atomic insulator)	Topo	? (Not atomic insulator)	Topo
Surface state	x	✓	x	✓

Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

Inversion-protected TCI in 3D

❖ Z_4 Symmetry indicator: Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

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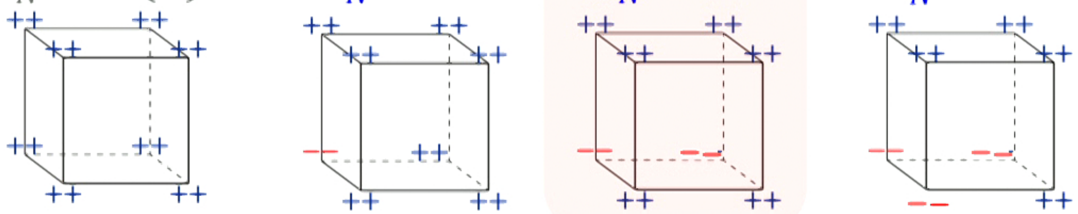


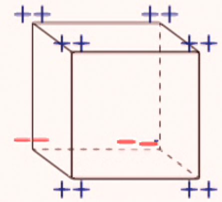
	Trivial	Topo	Higher-order TI (?)	Topo
Surface state	x	✓	Hinge modes (?)	✓

Inversion-protected TCI in 3D

- Z_4 Symmetry indicator: Khalaf, Po, Vishwanath, Watanabe, PRX (2018)

$$\kappa_N \equiv \frac{1}{4} \sum_{K \in \mathrm{TRIMs}} (n_K^+ - n_K^-) \mod 4 \qquad \nu_N = \kappa_N \mod 2$$

$\kappa_N = 2$



Higher-order TI (?)

Bulk-boundary correspondence

in double-TI construction

Q: Is there a **superconductor** analogue?

i.e. **Inversion**-protected TCsc with some $\boldsymbol{\kappa_{BdG}}$**=2**

$\Rightarrow$ Intrinsic **higher-order** topo sc (HOTsc)

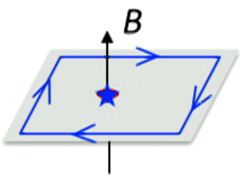
(Majoranas!)

Why higher-order superconductors?

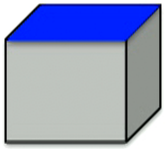
❖ Signature of topo sc:

- Boundary: Majorana modes in (d-1)-dimension

End modes



Edge states
Vortex cores



Surfaces

Higher-order topo sc
(HOTsc)

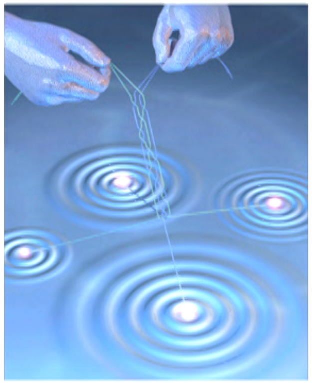
2D case:
*Majorana **corner** modes!*

Why 2D HOTsc?

❖ Majorana zero modes

- **0-dimensional** zero-energy modes

- Qubits for **topological quantum computation**



Scientific American

*How to **realize 2D intrinsic HOTsc**?*

3D inversion-protected HOTsc

- Define analogous symmetry indicator for

$$H_{\boldsymbol{k}}^{\mathrm{BdG}} = \begin{pmatrix} H_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^{\dagger} & -H_{-\boldsymbol{k}}^{*} \end{pmatrix}$$

- Define symmetry operation for H_{BdG}

$$U_{\boldsymbol{k}}^{\mathrm{BdG}}(g) = \begin{pmatrix} U_{\boldsymbol{k}}(g) & 0 \\ 0 & \chi_g U_{-\boldsymbol{k}}(g)^{*} \end{pmatrix}$$

$U_{\boldsymbol{k}}(g)$ → for normal-state H

χ_g=+1: even parity pairing

χ_g=-1: odd parity pairing

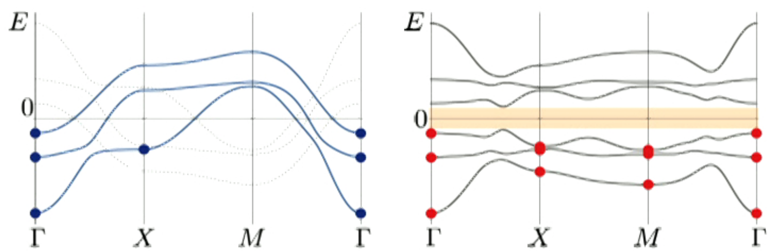
such that H_{BdG} is invariant under U_k^{BdG}

Ono, Yanase, Watanabe, PR Research (2019)

3D inversion-protected HOTsc

❖ Define **inversion** symmetry indicator for $H_{\boldsymbol{k}}^{\mathrm{BdG}}$

Normal bands BdG bands



Inversion $P_{\mathrm{BdG}} = \begin{pmatrix} P & 0 \\ 0 & \pm P \end{pmatrix}$

$$\kappa_{BdG} \equiv \frac{1}{4} \sum_{\boldsymbol{k} \in \text{3D TRIMs}} \sum_{\alpha=\pm 1} \alpha (n_{\boldsymbol{k}}^{\alpha})^{\mathrm{BdG}} \pmod 4$$

Metal (FS circle TRIMs)

- Even-parity pairing: κ_{BdG} is always 0
- Odd-parity pairing: κ_{BdG} is Z_4 (Z_8?)

Ono et al. PR research (2019)

Skurativska, Titus, Fischer (2019)

Goal:* *Realize* *inversion-protected HOTsc in* *2D

1. Find a **recipe** => construct **minimal model**

2. Demonstrate **bulk- boundary correspondence**

3. Prediction for **material**

Hard: few candidates for even traditional topo sc ☹

- Making prediction for unconventional sc is hard
- Challenging: **Topology** + **symmetry** + **interaction**

Beyond band structure calculation

Z_4 Symmetry indicator for 2D TCsc

❖ Conjecture Z_4 symmetry indicator for a 2D time-reversal superconductor (DIII) with inversion:

- $$\kappa = \frac{1}{4} \sum_{\mathbf{k} \in \mathrm{TRIM}} \sum_{n} \xi_{\mathbf{k}n} \mod 4$$

  $\xi_{\mathbf{k}n}$: parity of the occupied BdG band n

  Inversion: $P_{\mathrm{BdG}} = \begin{pmatrix} P & 0 \\ 0 & -P \end{pmatrix}$ for **odd-parity** pairing

- $\nu = \kappa$ mod 2

  Z_2 index for DIII

YTH et. al. arxiv: 1904.06361 (2019)

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- $\nu = \kappa$ mod 2

κ=0: No edge modes κ=1,3: Majorana edge modes

κ=2: No edge modes

YTH et. al. arxiv: 1904.06361 (2019)

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- $\nu = \kappa$ mod 2

κ=0: No edge modes κ=1,3: Majorana edge modes

κ=2: No edge modes, possible **Majorana corner** modes!

YTH et. al. arxiv: 1904.06361 (2019)

Recipe *for* ***2D*** inversion-protected TCsc with κ=2

What kind of **normal state** $\mathbf{H_0}$ **(metallic)**

What kind of **pairing** Δ

(Predictable)

Band topology $\mathbf{k} \longrightarrow H_0(\mathbf{k})$ $\Longleftrightarrow$ (?) $\mathbf{k} \longrightarrow H_{BdG}(\mathbf{k})$

This is what we want
to understand

Recipe for κ=2 TCsc in 2D

- For 2D **insulators** with time-reversal & inversion:

Step1: Relate 2D TI index with indicator for 2D Inversion-protected TCI

$$\nu_N = \kappa_N$$

Z_2 still Z_2

- *For **metallic** systems (Fermi surface **circle TRIM**):*

κ_N can be half integers => not Z_2 anymore

YTH et. al. arxiv: 1904.06361 (2019)

Recipe for κ=2 TCsc in 2D

❖ For 2D systems with time-reversal & inversion:

Step1: Relate 2D TI index with
indicator for 2D Inversion-protected TCI

$$\nu_N = \kappa_N$$

Z_2 still Z_2

✓ *For **metallic** systems (Fermi surface **away from TRIM**):*

"Effectively gapped" topological metal

YTH et. al. arxiv: 1904.06361 (2019)

Recipe for κ=2 TCsc in 2D

❖ For 2D systems with time-reversal & inversion:

Step1: Relate indices for **metallic** H_0 **(effectively gapped)**

$$\nu_N = \kappa_N$$

1 1

(Z$_2$) (Z$_4$)

Step2: Relate symmetry indicators for H_0 and H_{BdG}

$$\kappa = 2\,\kappa_N \text{ mod } 4$$

for weak odd-parity sc

2 1

=> TCsc with κ =2!

YTH et. al. arxiv: 1904.06361 (2019)

Recipe for inversion-protected TCsc

Normal state:

***Centrosymmetric quantum spin Hall** material*

- Gated QSH insulator
- Fermi surface away from TRIMs

Pairing:

Odd-parity sc *e.g. p-wave*

⇨ *Topo crystalline sc with* $\kappa=2$

YTH et. al. arxiv: 1904.06361 (2019)

Recipe for κ=2 TCsc in 2D

- For 2D systems with time-reversal & inversion:

Step1: Relate indices for **metallic** H_0 **(effectively gapped)**

$$\nu_N = \kappa_N$$

1 1

(Z$_2$) (Z$_4$)

Step2: Relate symmetry indicators for H_0 and H_{BdG}

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YTH et. al. arxiv: 1904.06361 (2019)

Recipe for inversion-protected TCsc

Normal state:

Centrosymmetric ***quantum spin Hall*** *material*

- Gated QSH insulator
- Fermi surface away from TRIMs

Pairing:

Odd-parity sc *e.g. p-wave*

⇨ *Topo crystalline sc with* κ*=2*

Higher-order?  *Show bulk-boundary correspondence!*

YTH et. al. arxiv: 1904.06361 (2019)

Bulk-boundary correspondence

❖ What kind of boundary modes: $\kappa = 2$ | $\kappa = 4$ (vacuum)

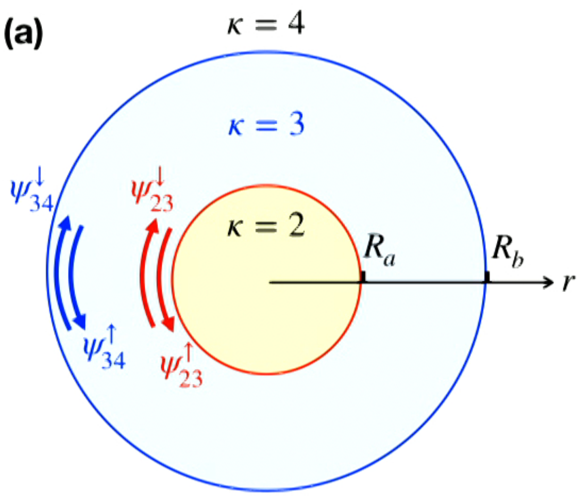
1. Minimal model: BHZ model + odd-parity pairing
   (Gated) $\kappa = 4 \dashrightarrow 3 \dashrightarrow 2$

2. Three-regime geometry

Solve for the two pairs of helical edge modes from $\kappa = 3$

Shrink $\kappa = 3$ regime ---> 0

(a)

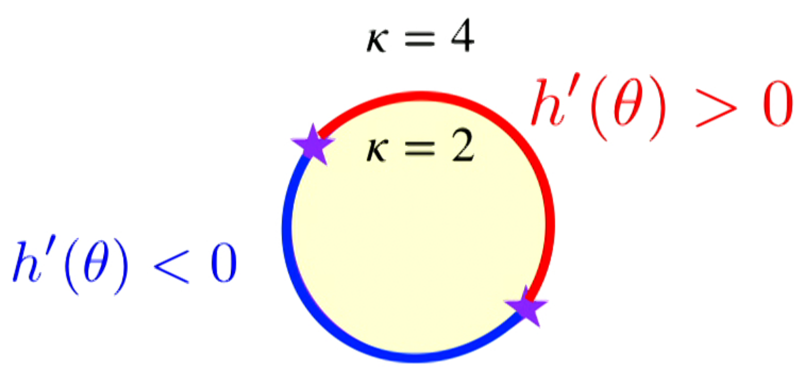


Bulk-boundary correspondence

❖ What kind of boundary modes: $\kappa = 2$ | $\kappa = 4$ (vacuum)

3. Effective edge theory for edge modes $\psi_{23}^{\uparrow/\downarrow}$ and $\psi_{34}^{\uparrow/\downarrow}$:

=> Lowest-order back-scattering term $h'(\theta) \propto \alpha \cos\theta + \beta \sin\theta$



At least two zero-dim Majorana modes ★

=> *Higher order topology!*

$(\kappa=2)$

Recipe *for inv-protected **higher-order** sc:*

1. **Centrosymmetric**
2. **Quantum spin Hall** (FS away from TRIMs)
3. **Odd-parity pairing**

Go look for the material!

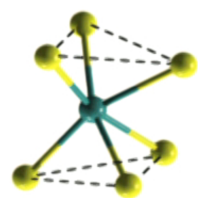
Monolayer WTe_2

- Van der Waal material

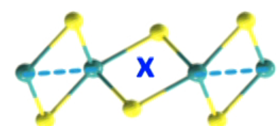
Monolayer from scotch tape

- **Centrosymmetric**

Unit cell



Side view

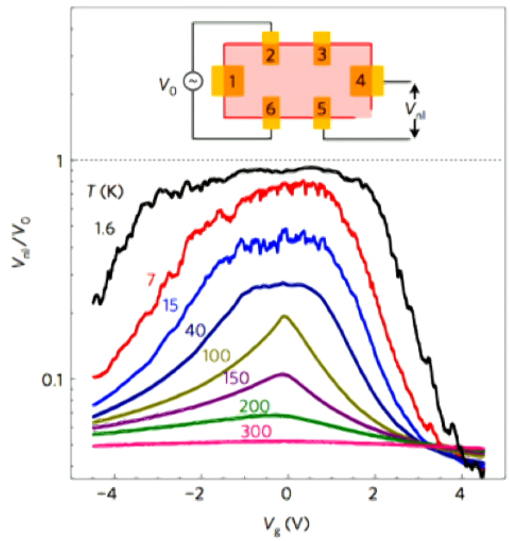


Inversion center

As-grown WTe_2: Quantum Spin Hall Insulator

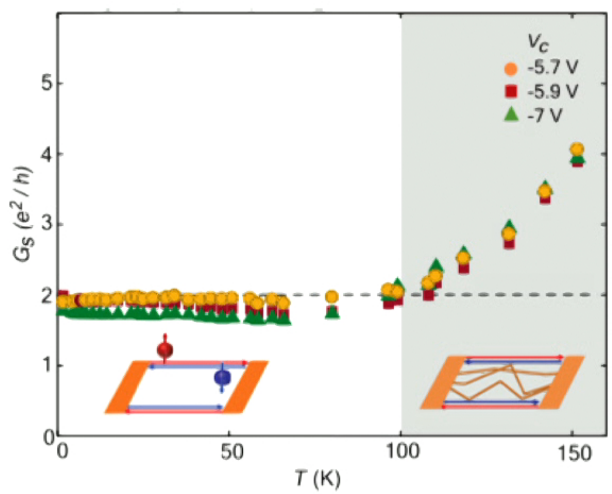
- ❖ Prediction: Qian et. al. Science (2014)
  Zheng et. al. Adv. Mat. (2016)
- ❖ Exp:

Edge conductance



Fei et. al. Nat. Phys. (2017)

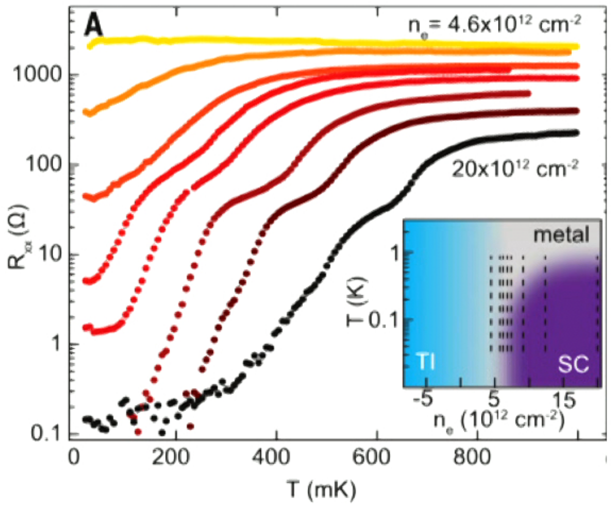
Quantized conductance



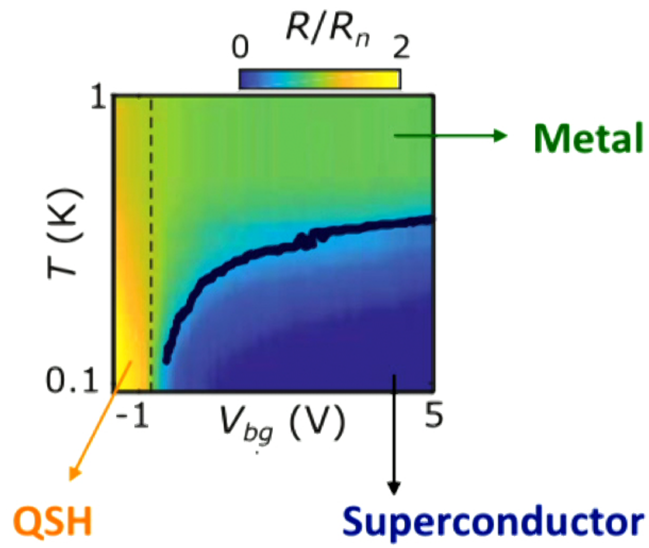
Wu et. al. Science (2018)

ARPES: Tang et. al. Nat Phys (2018)

Gated WTe_2: Superconductor



Sajadi et. al. Science (2018)



Fatemi et. al. Science (2018)

s-wave? non s-wave?

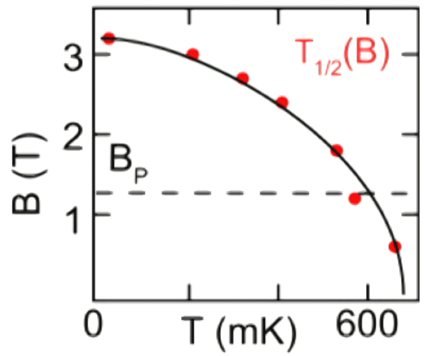
Can it be ***odd-parity*** *sc?*

Hints for unconventional sc

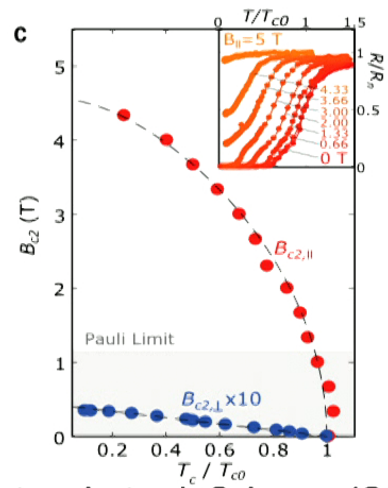
- Low carrier density (small gate voltage)

- Electronic correlation is important (PBE v.s. ARPES)

- In-plane Hc_2 higher than Pauli limit



Sajadi et. al. Science (2018)



Fatemi et. al. Science (2018)

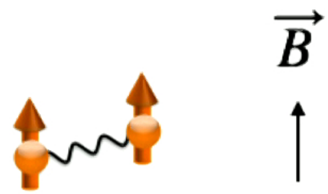
What can cause high Hc_2?

Possible origins for high Hc_2

- Higher spin-orbit scattering rate

- g factor not 2

- Equal-spin pairing



Spin-triplet: ↑↑, ↓↓, ↑↓ + ↓↑

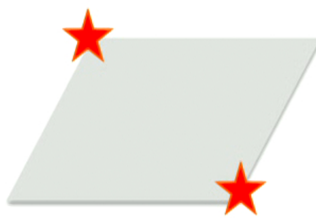
Parity-odd *required by fermionic statistics (e.g.* ***p-wave****)*

Gated monolayer WTe_2

✓ 1. Centrosymmetric

✓ 2. Quantum spin Hall

? 3. Odd-parity pairing

=>  ?

Gated monolayer WTe_2

(=> Inversion-protected HOTsc)

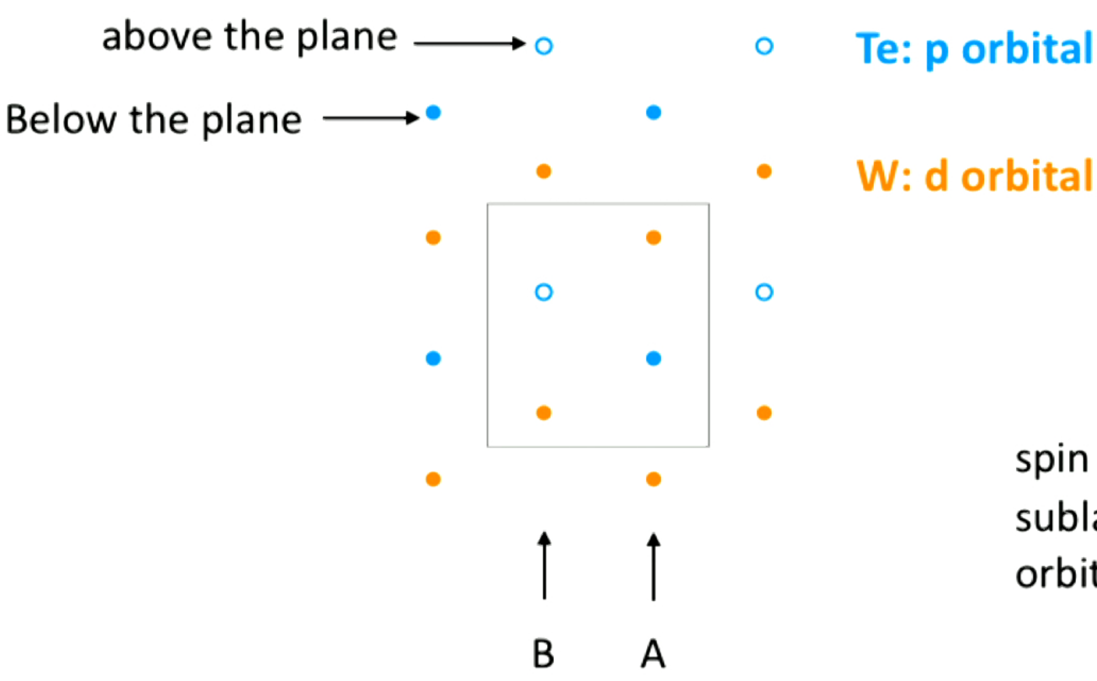
Study pairing symmetry at $H_{in\text{-}plane}$=0, >0

&

topo properties (κ, boundary modes)

Lattice symmetries

❖ 1T'- lattice of WTe_2: (low-energy Wannier centers)



spin s (up/down)
sublattice σ (A/B)
orbital l (d/p)

Muechler et. al. PRX (2016)

Lattice symmetries

❖ Two nonsymmorphic symmetries: extra half translations

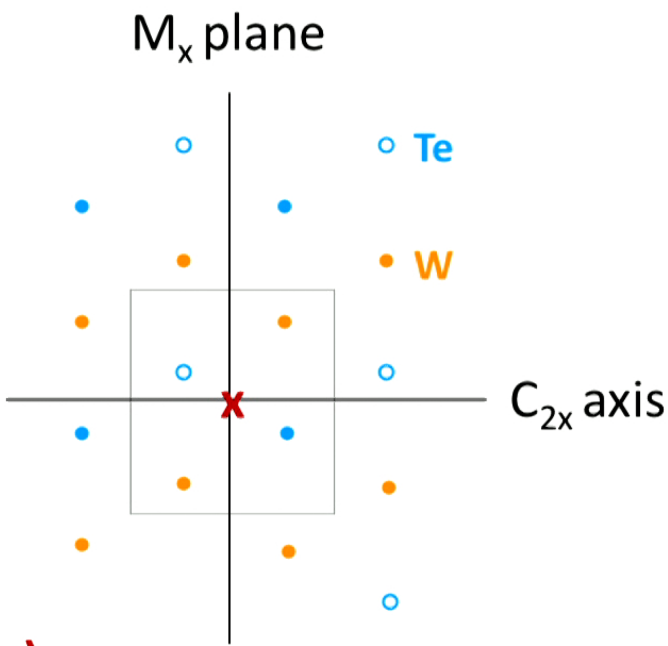
- Glide mirror symmetry M_x

- C_{2x} screw rotational symmetry

⇩

Inversion P= M_x C_{2x}

(Parity is a good quantum number)



Pairing symmetries

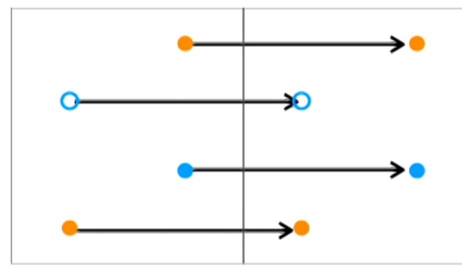
❖ Classify possible pairing symmetries using C_{2x} and M_x

4 irreducible representations

	C_{2x}	M_x
A_g	+	+
B_g	-	-
A_u	+	-
B_u	-	+

Parity-even: A_g, B_g — Spin-singlet — e.g. Ag: on-site pairing

Parity-odd: A_u, B_u — Spin-triplet — e.g. Bu: $\Delta_{\uparrow\downarrow+\downarrow\uparrow}$



Which irrep is energetically favorable?

YTH et. al. arxiv: 1904.06361 (2019)

Mean-field calculation

❖ Solve linearized gap equations

$$\Delta_{\alpha'\beta'}(\mathbf{k}') = -\sum_{\mathbf{k}''\mathbf{k}} V_{\alpha'\beta',\beta''\alpha''}(\mathbf{k}',\mathbf{k}'')\ \chi_{\beta''\alpha'',\alpha\beta}(\mathbf{k}'',\mathbf{k},T)\Delta_{\alpha\beta}(\mathbf{k})$$

Gap functions — Pairing interaction — Noninteracting pairing susceptibility

α, β : spin, sublattice, orbital

$\mathbf{k}$: incoming, outgoing momenta

T : temperature

Mean-field calculation

❖ Solve linearized gap equations

$$\underbrace{\Delta_{\alpha'\beta'}(\mathbf{k}')}_{\text{Gap functions}} = -\sum_{\mathbf{k}''\mathbf{k}} \underbrace{V_{\alpha'\beta',\beta''\alpha''}(\mathbf{k}',\mathbf{k}'')}_{\text{Pairing interaction}} \; \underbrace{\chi_{\beta''\alpha'',\alpha\beta}(\mathbf{k}'',\mathbf{k},T)}_{\text{Noninteracting pairing susceptibility}} \underbrace{\Delta_{\alpha\beta}(\mathbf{k})}_{\text{Gap functions}}$$

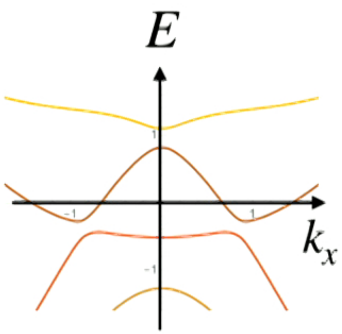
Gap functions **Pairing interaction** **Noninteracting pairing susceptibility**

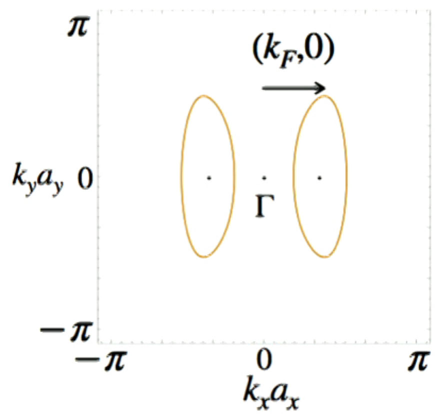
- Input: **Fermi surface, interactions V**
- Output: **Pairing symmetry** of the dominant gap function (Ag, Bu etc.)

Model: H_0

❖ **Kinetic terms:** tight-binding model of Wannier orbitals from DFT

+ finite chemical potential (gating)





Muechler et. al. PRX (2016)

Ok et. al. 1811.00551 (2018)

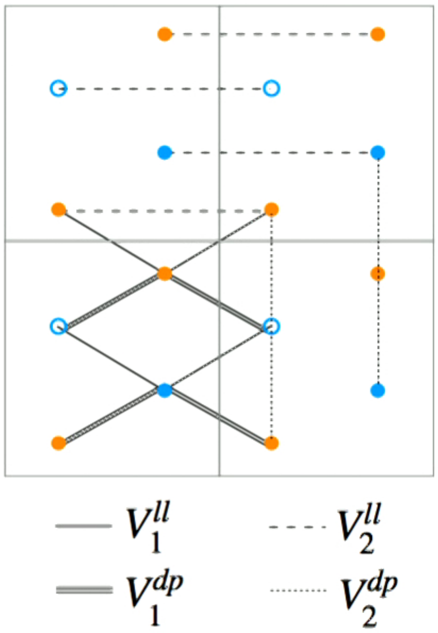
- Include both W and Te orbitals, SOC
- Inversion + Time-reversal => 2-fold degeneracy
- SOC breaks SU(2), but preserves Sz

Model: H_{int}

❖ **Microscopic density-density interactions:**

U: **On-site** interactions

V: **Short-range** interactions up to **nearest neighbor unit cells**



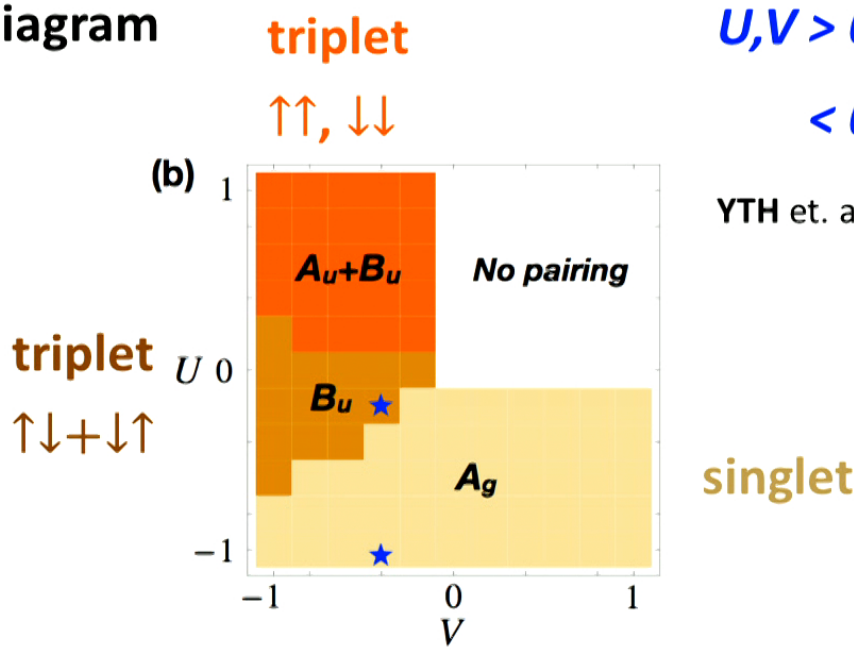
Result: pairing symmetry

❖ **Phase diagram**

U,V > 0: repulsion

< 0: attraction

YTH et. al. arxiv: 1904.06361

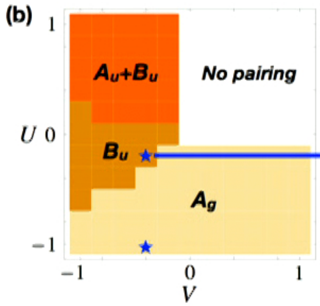


Q1: Z_4 indicator κ =?

Q2: Edge modes? Corner modes?

Q3: How does in-plane field affect pairing?

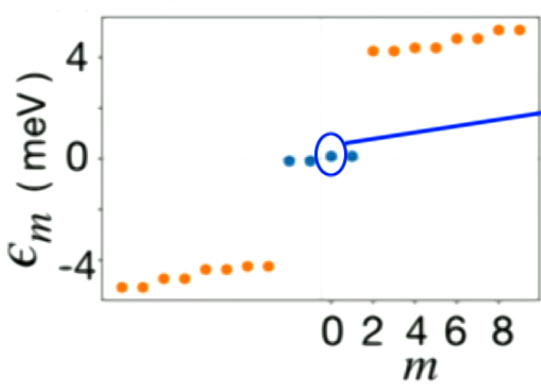
Topological properties

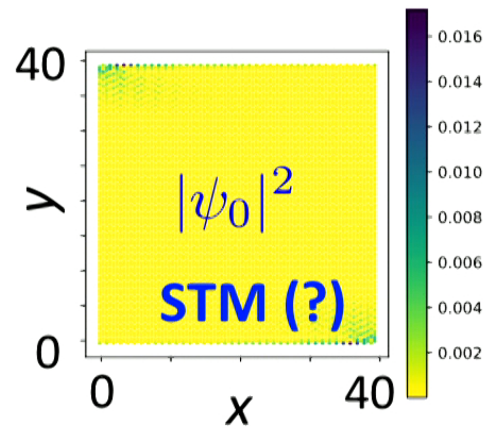


κ=2

Inversion-protected HOT sc !

H_{BdG} *spectrum*



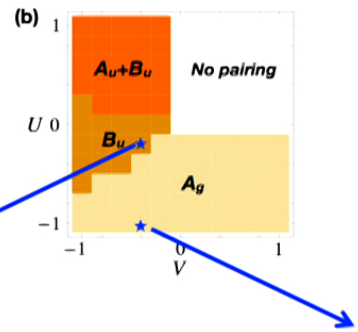


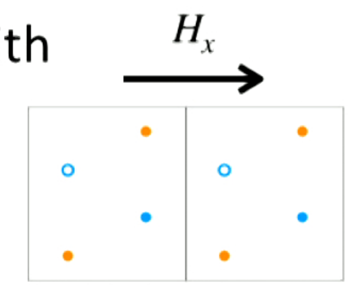
*Majorana Kramer's pairs at **corners***

YTH et. al. arxiv: 1904.06361

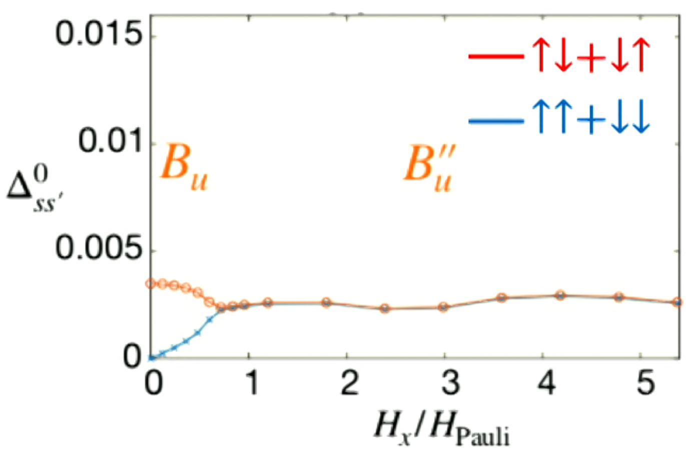
How does in-plane field affect pairing?

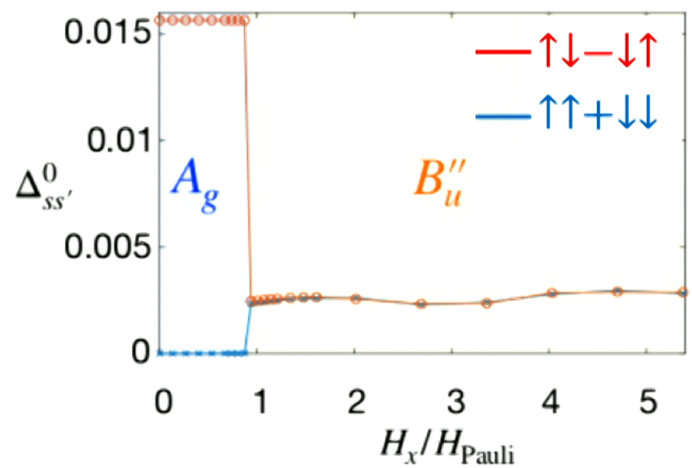
❖ Self-consistent gap equation in real space with in-plane magnetic field:





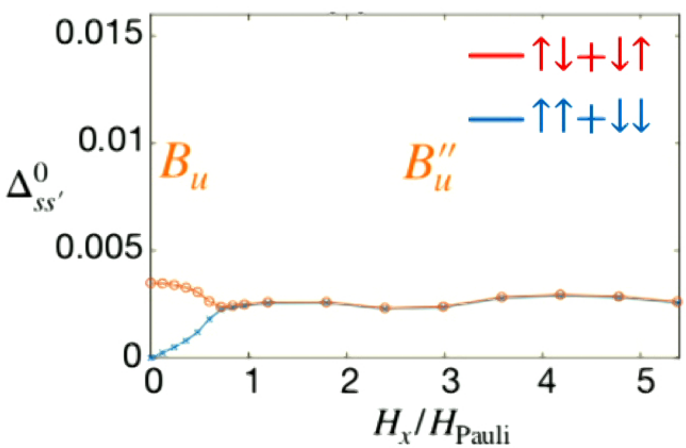
(breaks inversion)

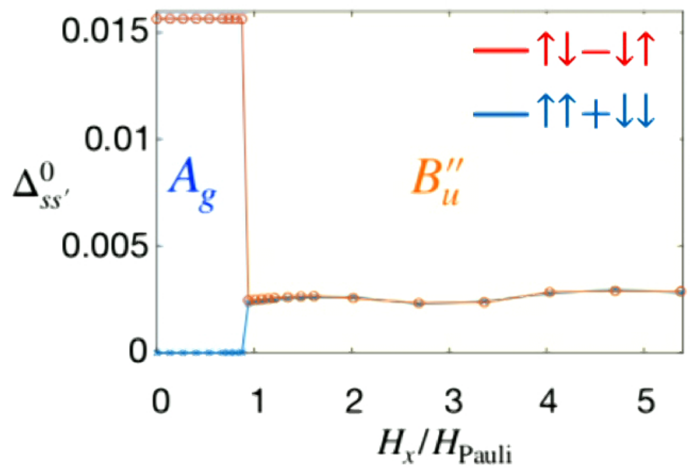




YTH et. al. arxiv: 1904.06361

With in-plane magnetic field Hx





- ***Crossover:*** *s_x=1*
  Spin rotates ↑↓+↓↑ ⇨ → →
  Symmetry unchanged

- ***First-order transition:***
  singlet ⇨ *triplet* → →
  C_{2x} even ⇨ *odd*

***Bu'': Extrinsic** higher-order topo sc*
(if bulk gap is not closed)

YTH et. al. arxiv: 1904.06361

Summary: Inversion-protected HOTsc

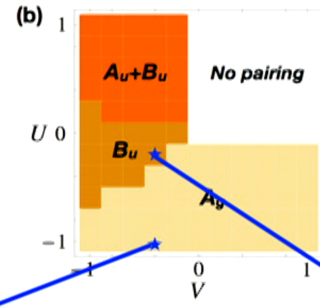
General Recipe

1. Centrosymmetric

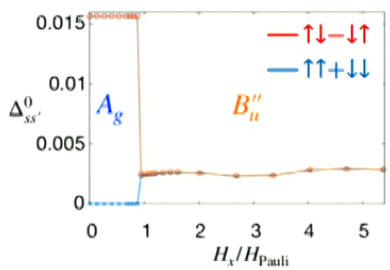
2. H_0 = Quantum spin Hall

3. Odd-parity pairing

WTe_2 superconductivity

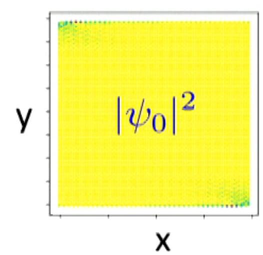


Field-induced triplet sc



*(**Extrinsic** higher-order topo sc)*

__Intrinsic__ higher-order topological sc



YTH et. al. arxiv: 1904.06361 (2019)