Chiral Dirac Superconductors: Second-order and Boundary-obstructed Topology

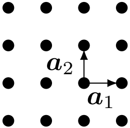
University of Florida, December

Outline

1. Introduction—Topological bands
2. Higher-order topology and boundary-obstructed topologies
3. Chiral Dirac higher-order topological superconductors

Bands structure

Electrons on a lattice can be described by local degrees of freedom,



$$a_i^\dagger(\boldsymbol{R})\,|0\rangle = |\boldsymbol{R}\ i\rangle$$

- $\boldsymbol{R}$ label lattice coordinate.
- i label *internal* degrees of freedom.

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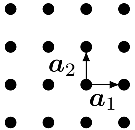

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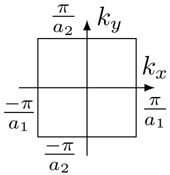
For free electrons,

$$|\boldsymbol{k}\ i\rangle = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\,|\boldsymbol{R}\ i\rangle\,,\quad a^\dagger(\boldsymbol{k})\,|0\rangle = |\boldsymbol{k}\ i\rangle$$

$$H = \int \frac{d\boldsymbol{k}}{(2\pi)^d}\ a_i^\dagger(\boldsymbol{k})\mathcal{H}^{ij}(\boldsymbol{k})a_j(\boldsymbol{k})$$



- Translational symmetry $\rightarrow$ conservation of crystal momentum.
- Diagonalizing the Hamiltonian we end up with a set of bands.
- We will refer to $\mathcal{H}(\boldsymbol{k})$ as the Hamiltonian.
- We are interested in gapped systems (insulators).

Topology of the occupied bands

Suppose we are studying systems with some symmetry group.
Define an equivalence between $\mathcal{H}^0(\boldsymbol{k})$ and $\mathcal{H}^1(\boldsymbol{k})$:

$$\mathcal{H}^0(\boldsymbol{k}) \approx \mathcal{H}^1(\boldsymbol{k}) \text{ iff } \exists$$

- $\mathcal{H}(\boldsymbol{k}, t)$; $\mathcal{H}(\boldsymbol{k}, 0) = \mathcal{H}^0(\boldsymbol{k})$, $\mathcal{H}(\boldsymbol{k}, 1) = \mathcal{H}^1(\boldsymbol{k})$,
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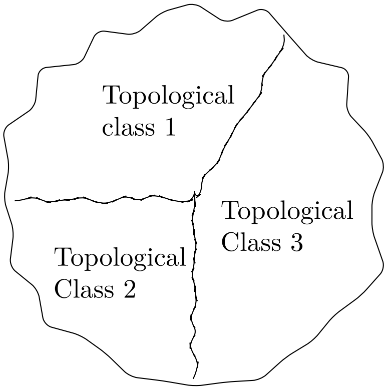
- This can be thought as deforming the occupied (and empty bands) bands from those of $\mathcal{H}^0(\boldsymbol{k})$ to those of $\mathcal{H}^1(\boldsymbol{k})$.
- If this deformation is possible, then the occupied bands of $\mathcal{H}^0(\boldsymbol{k})$ and $\mathcal{H}^1(\boldsymbol{k})$ are topologically equivalent.

Topological classification

- Topological classification require a survey of all possible gapped Hamiltonian and grouping them into equivalence classes under the restrictions of some symmetry group.

Space of Hamiltonians with some symmetry



- Find topological invariants that differentiate one class from the other.

Superconductors

The Bogoliubov-de Gennes (BdG) form for superconducting Hamiltonian,

$$H = \frac{1}{2}\int \frac{d\boldsymbol{k}}{(2\pi)^d} \begin{bmatrix}\Psi^\dagger(\boldsymbol{k})\Psi^T(-\boldsymbol{k})\end{bmatrix} \begin{bmatrix}\mathcal{H}_n(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta^\dagger(\boldsymbol{k}) & -\mathcal{H}_n^*(-\boldsymbol{k})\end{bmatrix} \begin{bmatrix}\Psi(\boldsymbol{k}) \\ \Psi^*(-\boldsymbol{k})\end{bmatrix}$$

- $\Psi^\dagger(\boldsymbol{k}) = (a_1^\dagger(\boldsymbol{k}), \dots, a_N^\dagger(\boldsymbol{k}))$.
- $\mathcal{H}_n(\boldsymbol{k})$ is the normal state Hamiltonian.
- $\Delta(\boldsymbol{k})$ is the superconducting order parameter.
- The BdG Hamiltonian $\mathcal{H}(\boldsymbol{k}) = \begin{bmatrix}\mathcal{H}_n(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta^\dagger(\boldsymbol{k}) & -\mathcal{H}_n^*(-\boldsymbol{k})\end{bmatrix}$ allows us to study the topology of superconductors within the same framework as insulating Hamiltonians.
- BdG Hamiltonians has an *intrinsic* particle-hole symmetry.

Internal symmetries

Internal symmetries are those that do not change the positions of the particles: $\boldsymbol{R} \to \boldsymbol{R}$.

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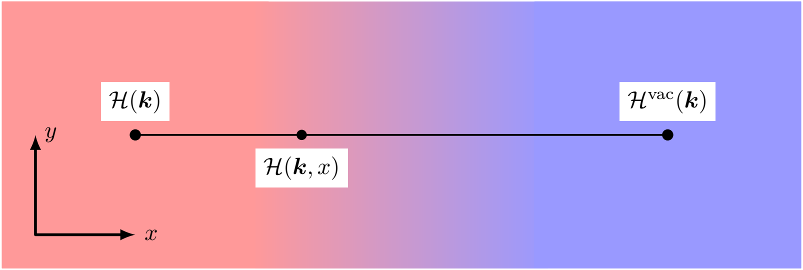
Three important internal symmetries:

- Time-reversal symmetry ($\mathcal{T}$)
- Particle-hole symmetry ($\mathcal{P}$)
- Chiral symmetry ($\mathcal{C} = \mathcal{PT}$)

Complete topological classification exists for the 10 Altland-Zirnbauer (AZ) classes. Teo and Kane (2010)

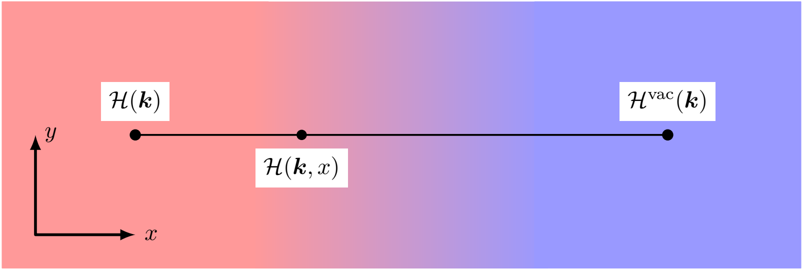
AZ	$\mathcal{T}^2$	$\mathcal{P}^2$	$\mathcal{C}^2$
A	0	0	0
AIII	0	0	1
AI	1	0	0
BDI	1	1	1
D	0	1	0
DIII	-1	1	1
AII	-1	0	0
CII	-1	-1	1
C	0	-1	0
CI	1	-1	1

Gapless boundaries



- A boundary interpolates between a topological system and the vacuum.
- Internal symmetries are not broken on the boundary.

Gapless boundaries

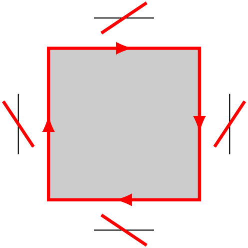


- A boundary interpolates between a topological system and the vacuum.
- Internal symmetries are not broken on the boundary.

> Topological systems protected by internal symmetries *only* will in general have gapless boundaries.

Examples

In 2D:
Chern insulators.
Protecting symmetries: None.
Topological invariant: Chern number.



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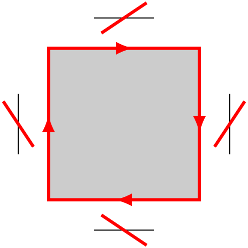

<u>In $1D$:</u>
SSH chain.
Protecting symmetry: Chiral symmetry
Topological invariant: Polarization

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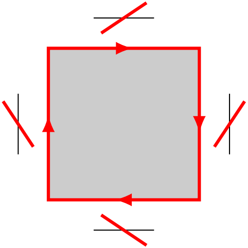
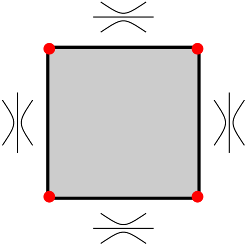
Higher-order topology

Can we find topological systems systems with gapped boundaries?



First-order topology; gapless mode on boundaries of co-dimension 1.



Second-order topology; gapless mode on boundaries of co-dimension 2.

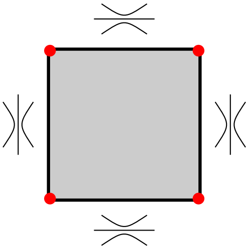
The protecting symmetry must be broken on the boundary.
Internal symmetries are not enough.

Spatial symmetries

Spatial symmetries are those that change the position of the particles. $\boldsymbol{R} \to \boldsymbol{R}'$.

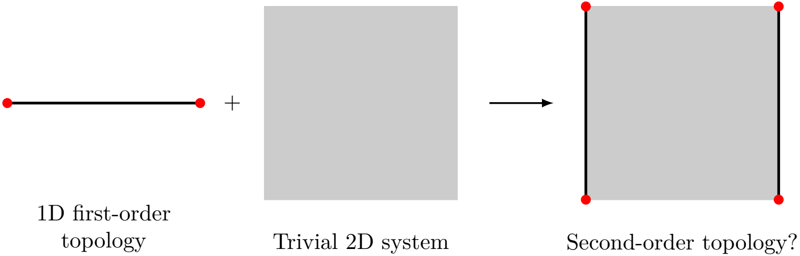
Examples of spacial symmetries:

$$C_4 : (R_x, R_y) \to (-R_y, R_x) \qquad C_2 : (R_x, R_y) \to (-R_x, -R_y)$$



C_4 and C_2 are broken on the boundaries.

A cheap way to get corner modes



- These corner zero modes are not protected by a bulk gap.

Higher-order and boundary-obstructed topologies

Second-order topology

Boundary-obstructed topology

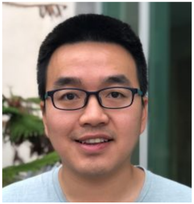
- What kinds of system would show such surface signature?
- What kinds of topological invariants we can find?

Summary

- Topological band systems are those that cannot be deformed to the vacuum without:
  1. Closing a gap
  2. Breaking the symmetry
- Topologies protected by internal symmetries alone lead to first-order topology (gapless boundaries).
- Including spatial symmetries can lead to a much richer topological structure.
- Higher-order topologies have gapless modes on boundaries with co-dimension higher than one.
- Boundary-obstructed topologies are only protected by a boundary gap closing.

Outline

Apoorv Tiwari
University of Zurich

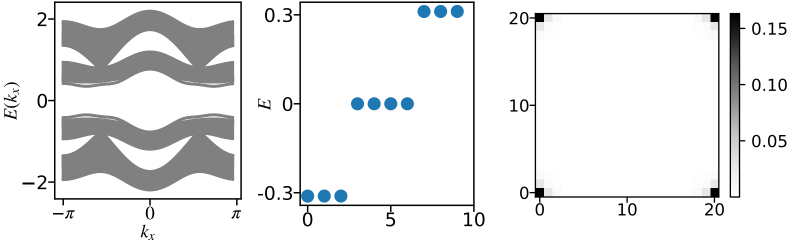


Yuxuan Wang
University of Florida

A concrete model

$$\mathcal{H}(\boldsymbol{k}) = [\gamma_x + \cos(k_x)]\,\sigma_x\tau_z + [\gamma_y + \cos(k_y)]\,\sigma_z\tau_z - \mu\tau_z + \Delta\sin(k_x)\tau_y + \Delta\sin(k_y)\tau_x$$

4 Majorana corner zero modes. Wang, Lin, and Hughes (2018)



$$\gamma_x = \gamma_y = 0.2,\ \Delta = 0.4,\ \mu = 0.5$$

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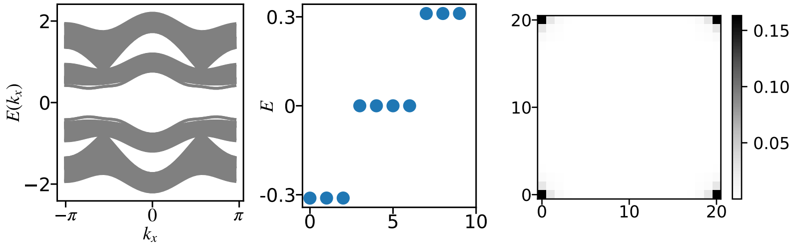
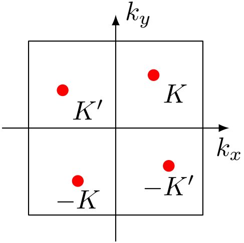


$$\gamma_x = \gamma_y = 0.2,\ \Delta = 0.4,\ \mu = 0.5$$

Can we abstract a sufficient condition that would guarantee the existence of the Majorana zero modes?

A more general model—a sufficient condition

$$\mathcal{H}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x\tau_z + f_2(\boldsymbol{k})\sigma_z\tau_z - \mu\tau_z \qquad +\Delta_1(\boldsymbol{k})\tau_y + \Delta_2(\boldsymbol{k})\tau_x$$



$p + ip$ order parameter.

$$f_{1,2}(\pm\boldsymbol{K}) = f_{1,2}(\pm\boldsymbol{K}') = 0$$

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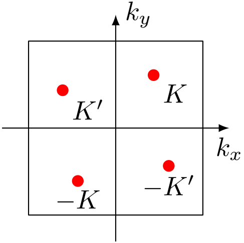

$p + ip$ order parameter.

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- With C_4 symmetry the model has a second-order topological phase with corner Majorana zero modes.
- With only C_2 symmetry the model has a boundary-obstructed phase with corner Majorana zero modes.

Fourfold rotation symmetry

$$\mathcal{H}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x\tau_z + f_2(\boldsymbol{k})\sigma_z\tau_z - \mu\tau_z + \Delta_1(\boldsymbol{k})\tau_y + \Delta_2(\boldsymbol{k})\tau_x$$

$$\begin{aligned} \mathcal{P}\mathcal{H}(\boldsymbol{k})\mathcal{P}^{-1} &= -\mathcal{H}(-\boldsymbol{k}), \qquad && \mathcal{P} = \tau_x K \\ C_4\mathcal{H}(k_x, k_y)C_4^{-1} &= \mathcal{H}(-k_y, k_x), \qquad && C_4 = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_y)e^{-i\frac{\pi}{4}\tau_z} \end{aligned}$$

Symmetry constraints:

$$f_1(k_x, k_y) = f_2(-k_y, k_x)$$
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High-symmetry points:

- $C_4 : \{(0,0),\ (\pi,\pi)\} \to \{(0,0),\ (\pi,\pi)\}$
- $C_2 : \{(0,\pi),\ (\pi,0)\} \to \{(0,\pi),\ (\pi,0)\}$

Define:

$f_\Gamma \equiv f_1(0,0) = f_2(0,0), \quad f_M \equiv f_1(\pi,\pi) = f_2(\pi,\pi)$

Symmetry indicators

Easy topological invariants to calculate

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We first ignore that we are dealing with a BdG Hamiltonian and treat it as an insulating system (two occupied bands). We reinterpret the results for the BdG Hamiltonian in the end.

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- $[\mathcal{H}(0,0), C_4] = 0$
  $[\mathcal{H}(\pi,\pi), C_4] = 0$
- $[\mathcal{H}(0,\pi), C_2] = 0$
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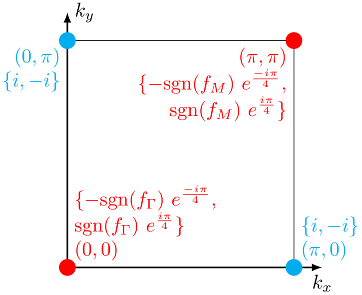
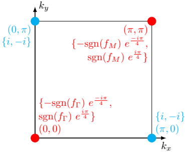
Symmetry operators eigenvalues at the high-symmetry points are topological invariants.

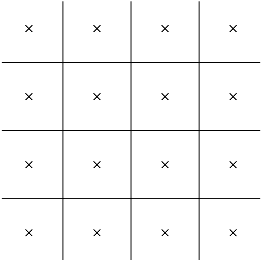


Wannier centers

Wannier centers must:

- Respect the C_4 symmetry.
- Be consistent with the symmetry eigenvalues at the high-symmetry points.





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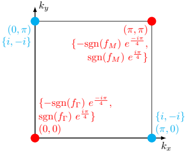

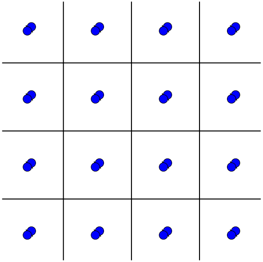

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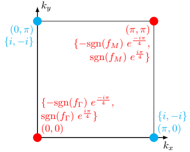

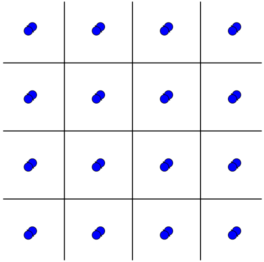

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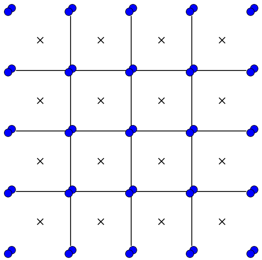

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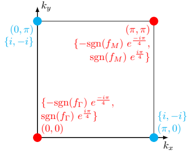

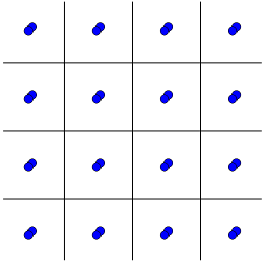

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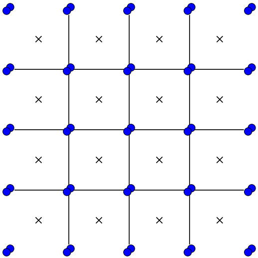


$\mathrm{sgn}(f_\Gamma)\,\mathrm{sgn}(f_M) = -1$

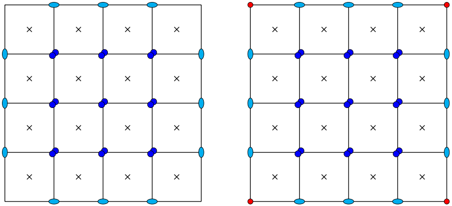
- These are two topologically distinct phases.

Filling anomaly—Majorana corner modes

Filling anomaly means the system cannot be:

1. Neutral
2. Gapped
3. C_4 symmetric

Khalaf, Benalcazar, Hughes, and Queiroz (2019)



One orbital at each corner that can be either empty, or filled.

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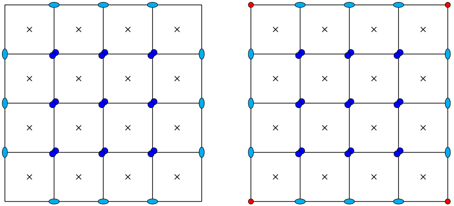


One orbital at each corner that can be either empty, or filled.

What does the filling anomaly mean for the BdG Hamiltonian?

- Filling anomaly means one state localized at each corner.
- Particle-hole symmetry is a local symmetry.
- If $|\Psi\rangle$ is localized on one corner, so is $|\mathcal{P}\Psi\rangle$.
- It must be that $|\mathcal{P}\Psi\rangle \propto |\Psi\rangle$; A Majorana zero mode.

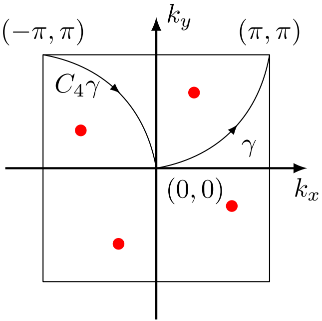
Is the system in the topological phase?

The condition for the topological phase is $\mathrm{sgn}(f_\Gamma)\,\mathrm{sgn}(f_M) = -1$.
Is it true for our system?

$$\mathcal{H}_n(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x + f_2(\boldsymbol{k})\sigma_z$$

- The Dirac point is a source of *magnetic* field.
- Berry phase gained when moving around the loop is π.

$$\hat{\boldsymbol{n}}(\boldsymbol{k}) \equiv \frac{f_1(\boldsymbol{k})e_x + f_2(\boldsymbol{k})e_z}{\sqrt{f_1^2(\boldsymbol{k}) + f_2^2(\boldsymbol{k})}}$$



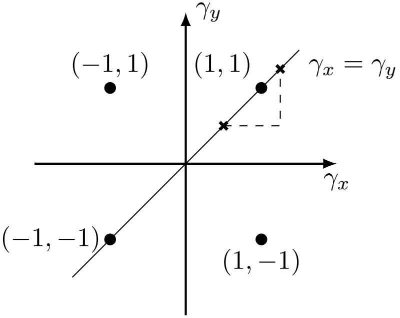
$$N_{\mathsf{w}}(\gamma \circ C_4\gamma) = 2N_{\mathsf{w}}(\gamma) = 1$$
$$\hat{\boldsymbol{n}}(0,0) = -\hat{\boldsymbol{n}}(\pi,\pi)$$

Now we break C_4 down to C_2.

Boundary-obstruction

Going back to

$$\mathcal{H}(\boldsymbol{k}) = [\gamma_x + \cos(k_x)]\,\sigma_x\tau_z + [\gamma_y + \cos(k_y)]\,\sigma_z\tau_z - \mu\tau_z \\ + \Delta\sin(k_x)\tau_y + \Delta\sin(k_y)\tau_x$$



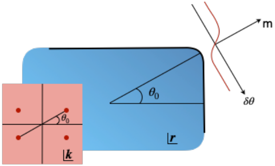
- It can at best be boundary obstructed.

Edge defect approach

When C_4 is broken down to C_2 we no longer have a phase protected by bulk gap.

Our approach:

1. Solve for the edge theory at each *point* on a rounded corner, using knowledge of the low energy properties of the model.
2. Show that the boundary properties, as derived from the bulk, lead to a Majorana corner zero mode.



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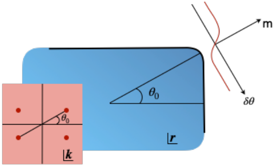


$$h(q_{||}, \delta\theta) = \alpha q_{||} s_1 + m\delta\theta s_2$$

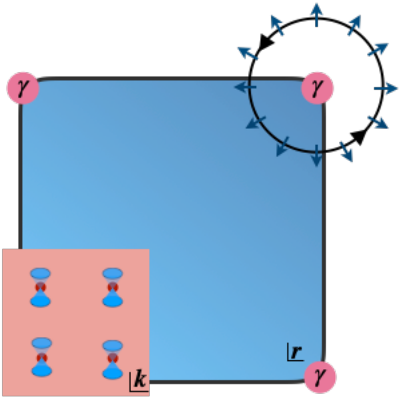
- Looks like a $1D$ Dirac equation with a mass domain wall, which we know host a zero mode at the domain wall. Jackiw and Rebbi (1976)

Conclusions

We find low energy criteria that guarantee the existence of the corner modes.

In $2\mathrm{D}$

- Dirac points in the normal state.
- A $p + ip$ superconducting order parameter gapping the Dirac points.
- With C_4 symmetry $\rightarrow$ second-order topology
- With C_2 symmetry $\rightarrow$ boundary-obstructed topology.



Future work

3D Higher-order topological superconductors:

- A natural extension to the Dirac $+ p + ip$ project in 2D is to look for higher-order topology in 3D.
- Starting from Weyl points in the normal state and adding $p + ip$ order-parameter.

An example of such Hamiltonian:

$$\mathcal{H}(\boldsymbol{k}) = [\gamma_x - 1 + \cos(k_x) + \cos(k_z)]\, \sigma_x \tau_z - \mu \tau_z \\ + [\gamma_y - 1 + \cos(k_y) + \cos(k_z)]\, \sigma_z \tau_z + \sin(k_x)\tau_y + \sin(k_y)\tau_x .$$

- Despite having a very similar look to the 2D Hamiltonian, it turned out to have a lot of features that deserve a closer look.

Future work

Applications in quantum computing?

- Majorana zero mode can be used to implement a fault-tolerant quantum computer. Kitaev (2003)
- Usual platforms for obtaining the Majorana zero modes are the ends of 1D topological superconductors or on the vortices of a 2D topological superconductors.
- The method proposed to manipulate these Majorana modes are not easily implemented experimentally.
- The Majorana zero modes at the corners of a higher-order topological superconductor offers a new platform, for which we can try and look for easier ways of manipulating the Majorana modes.

R. Jackiw and C. Rebbi. Solitons with fermion number ½. *Physical Review D*, 13(12):3398–3409, Jun 1976. ISSN 0556-2821. doi: 10.1103/PhysRevD.13.3398.

Eslam Khalaf, Wladimir A. Benalcazar, Taylor L. Hughes, and Raquel Queiroz. Boundary-obstructed topological phases. *arXiv:1908.00011 [cond-mat]*, Jul 2019. URL `http://arxiv.org/abs/1908.00011`. arXiv: 1908.00011.

A.Yu. Kitaev. Fault-tolerant quantum computation by anyons. *Annals of Physics*, 303(1):2–30, Jan 2003. ISSN 00034916. doi: 10.1016/S0003-4916(02)00018-0.

Jeffrey C. Y. Teo and C. L. Kane. Topological defects and gapless modes in insulators and superconductors. *Physical Review B*, 82 (11):115120, Sep 2010. ISSN 1098-0121, 1550-235X. doi: 10.1103/PhysRevB.82.115120.

Yuxuan Wang, Mao Lin, and Taylor L. Hughes. Weak-pairing higher order topological superconductors. *Physical Review B*, 98 (16):165144, Oct 2018. ISSN 2469-9950, 2469-9969. doi: 10.1103/PhysRevB.98.165144.