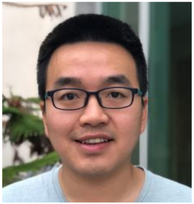
Chiral Dirac Superconductors: Second-order and Boundary-obstructed Topology

University of Florida, May 2020

Apoorv Tiwari
University of Zurich



Yuxuan Wang
University of Florida

Introduction

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Quick answer (the goal of this talk is to explain this quick answer):

Model	With C_4	With C_2
With PH	HOTSC$_2$; corner Majorana	BOTSC$_2$; corner Majorana
Without PH	HOTI$_2$; filling anomaly	Trivial

HOTI = Higher Order Topological Insulator
HOTSC = Higher Order Topological Superconductor
BOTSC = Boundary Obstructed Topological Superconductor

Outline

1. The model
   Dirac + $(p + ip)$

2. Second-order topology
   Dirac + $(p + ip)$ with C_4 symmetry

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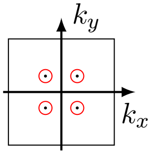
The normal state

We take 4 Dirac points in the normal state as a given. In general a Dirac semi-metal in 2D can be modeled by,

$$\mathcal{H}^{\mathsf{normal}}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x + f_2(\boldsymbol{k})\sigma_z - \mu$$



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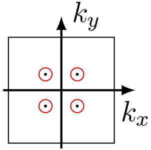

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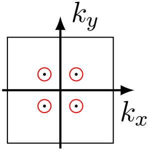

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$$\hat{C}_4 = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$$

$$\hat{C}_2 = \hat{C}_4^2 = \mathbb{1}$$

$$\boxed{\hat{C}_4(\sigma_z, \sigma_x)\hat{C}_4^{-1} = (\sigma_x, \sigma_z)}$$

$$\hat{C}_{4/2}\mathcal{H}^{\text{normal}}(\boldsymbol{k})\hat{C}_{4/2}^{-1} = \mathcal{H}^{\text{normal}}(C_{4/2}\boldsymbol{k})$$

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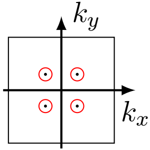

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Adding pairing terms

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$$\mathcal{P}\mathcal{H}(\boldsymbol{k})\mathcal{P}^{-1} = -\mathcal{H}(-\boldsymbol{k}), \qquad \mathcal{P} = \tau_x K$$

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For $\mu = 0$ the model has a chiral symmetry,

$$\mathsf{S}\mathcal{H}(\boldsymbol{k})\mathsf{S}^{-1} = -\mathcal{H}(\boldsymbol{k}), \qquad \mathsf{S} = \sigma_y\tau_z$$

C_4 and C_2 symmetries for the BdG Hamiltonian

$$\hat{C}_4 = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)e^{\frac{i\pi}{4}\tau_z}$$

$$\hat{C}_2 = \hat{C}_4^2 = e^{\frac{i2\pi}{4}\tau_z}$$

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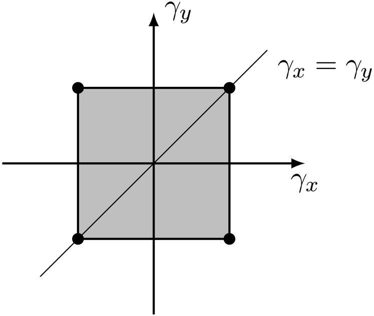
A prototypical example:

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

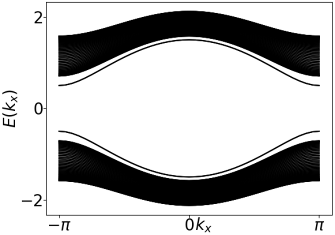
Phase diagram for $\mu = 0$:



Edge spectrum and Majorana zero modes

For $\gamma_x = \gamma_y = 0.5$, $\Delta = 0.4$, and $\mu = 0.2$.

On a cylindrical:



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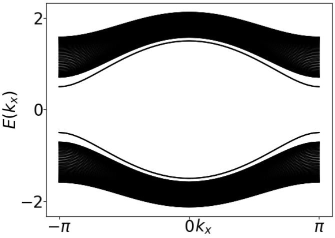
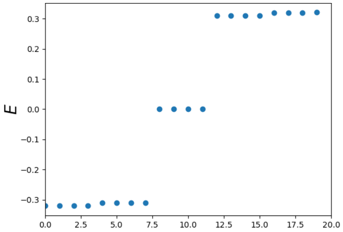


With open boundaries:



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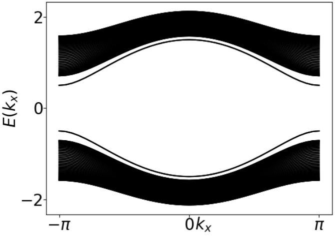

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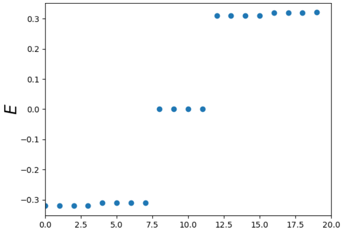
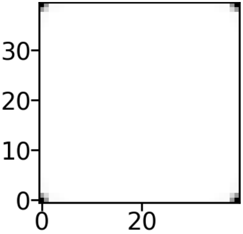


Zero modes:



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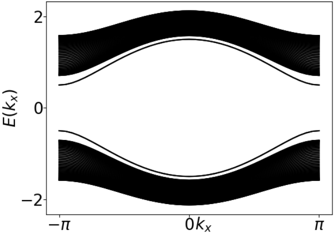

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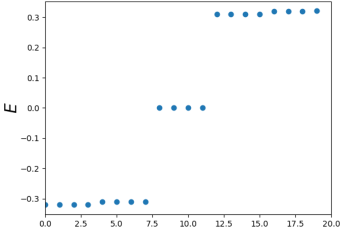

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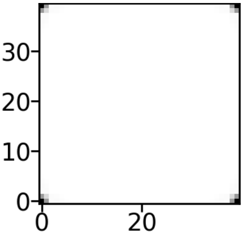
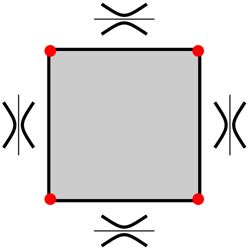




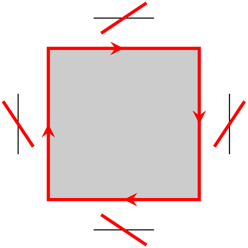
Outline

1. The model
   Dirac + $(p + ip)$

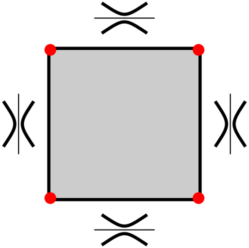
2. Second-order topology
   Dirac + $(p + ip)$ with C_4 symmetry

First-order topology vs second-order topology (I)

In contrast to first-order topology, second-order topology has gapped boundaries in addition to it's gapped bulk, but supports non-trivial gapless modes on the boundary of the boundary.



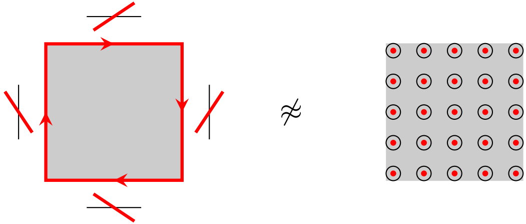
Non-trivial modes
co-dimension = 1



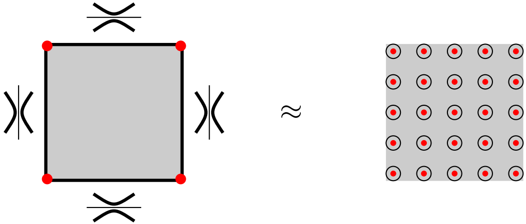
Non-trivial modes
co-dimension = 2

This definition will be refined later on.

First-order topology vs second-order topology (II)



Atomic description cannot be found for first-order topology



Atomic description can be found for second-order topology

Different kinds of atomic phases

Obstructed atomic phases need crystalline symmetries to protect them.

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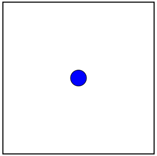
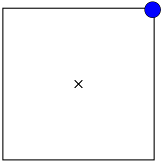
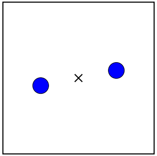


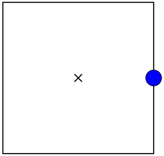
$\{(0,0)\}$
Multiplicty $= 1$



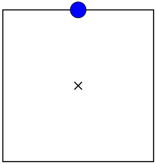
$\{(1/2,1/2)\}$
Multiplicty $= 1$



$\{C_2^n(x,y)\}$
Multiplicty $= 2$



$\{(1/2,0)\}$
Multiplicty $= 1$



$\{(0,1/2)\}$
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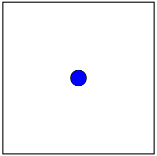
Different kinds of atomic phases

Obstructed atomic phases need crystalline symmetries to protect them.

With C_4 atomic orbitals have to be put in on of the following Wyckoff positions relative to the center of the unit cell (corresponding to different representations of the symmetry group):



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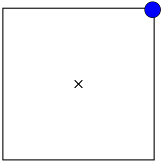
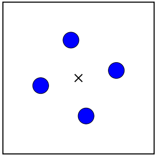
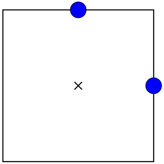


$\{(1/2,1/2)\}$
Multiplicty $= 1$



$\{C_4^n(x,y)\}$
Multiplicty $= 4$



$\{(1/2,0),(0,1/2)\}$
Multiplicty $= 2$

Different kinds of atomic phases

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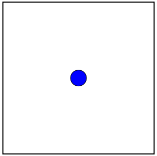
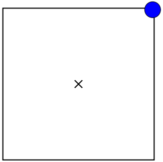
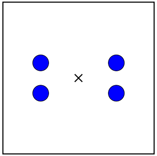
With M_x and M_y atomic orbitals have to be put in on of the following Wyckoff positions relative to the center of the unit cell (corresponding to different representations of the symmetry group):



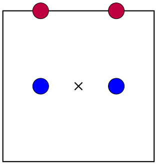
$\{(0,0)\}$
Multiplicty $= 1$



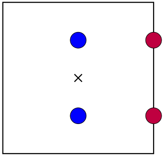
$\{(1/2,1/2)\}$
Multiplicty $= 1$



$\{(\pm x, \pm y)\}$
Multiplicty $= 4$



$\{(\pm x, 0)\}$
$\{(\pm x, 1/2)\}$
Multiplicty $= 2$



$\{(0, \pm y)\}$
$\{(1/2, \pm y)\}$
Multiplicty $= 1$

Symmetry of Block wavefunctions

Bloch wavefunctions can be written as:

$$|\psi_{\boldsymbol{k}}^{\alpha}\rangle = \sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} \left|\phi^{\alpha}_{\boldsymbol{R}_i+\boldsymbol{r}_\alpha}\right\rangle, \quad \langle \boldsymbol{r}|\phi^{\alpha}_{\boldsymbol{R}_i+\boldsymbol{r}_\alpha}\rangle = \phi^{\alpha}(\boldsymbol{r}-(\boldsymbol{R}_i+\boldsymbol{r}_\alpha)).$$

$\boldsymbol{r}_\alpha$ is defined relative to the the unit cell centers R_i. $\phi^{\alpha}(\boldsymbol{r})$ is localized around $\boldsymbol{r}=0$.

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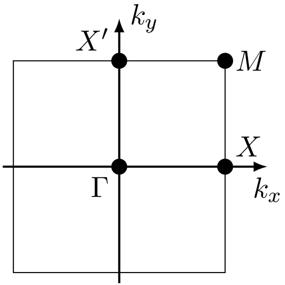
For C_4 symmetry:

$\boldsymbol{k}_* = (0,0)$ & (π,π) are C_4 symmetric

$\boldsymbol{k}_* = (0,\pi)$ & $(\pi,0)$ are C_2 symmetric

$$\boxed{\hat{C}_n |\psi_{\boldsymbol{k}_*}^{\alpha}\rangle = e^{i\theta_\alpha(\boldsymbol{k}_*)} |\psi_{\boldsymbol{k}_*}^{\alpha}\rangle}$$



$e^{i\theta_\alpha(\boldsymbol{k}_*)}$ at each $\boldsymbol{k}_*$ depend on:
(i) Angular momentum of ϕ^α.
(ii) The position $\boldsymbol{r}_\alpha$.

Symmetry indicators as a topological invariant

For one or more orbitals per unit cell, the 4 (one for each $\boldsymbol{k}_*$) sets $\{e^{i\theta_\alpha(\boldsymbol{k}_*)}\}$ are called the symmetry indicators.

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Take the case with one s-orbit per unit cell:

	$\hat{C}_{4,2}$ eigenvalues	
$\boldsymbol{k}_*$	$\boldsymbol{r}_\alpha = (0,0)$	$\boldsymbol{r}_\alpha = (1/2,1/2)$
$\Gamma = (0,0)$	1	1
$X' = (0,\pi)$	1	-1
$X = (\pi,0)$	1	-1
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- The different phases have different symmetry indicators.
- Phases with different symmetry indicators are distinct and cannot be deformed into one another.
- Symmetry indicators can be used as a topological invariant.

Obstructed atomic phases and the filling anomaly

- Corner charges can appear on these obstructed atomic phases.
- The key idea is that, on a sample with open boundaries, sometimes it's impossible to achieve charge neutrality while preserving the crystalline symmetry.

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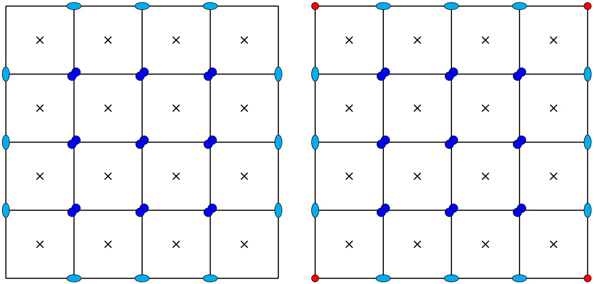


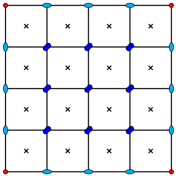
C_4 symmetric lattice with two electrons per unit cell, both at the Wyckoff position $\boldsymbol{r} = (1/2, 1/2)$. With open boundaries, both possible way of fillings give a net total charge to the system, and corner charges.

Symmetry indicators as a topological invariant

We ask with C_4 symmetry, and thinking of the BdG system as an insulator at half filling:

$$\mathcal{H}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x\tau_z + f_2(\boldsymbol{k})\sigma_z\tau_z + \Delta g_1(\boldsymbol{k})\tau_x + \Delta g_2(\boldsymbol{k})\tau_y - \mu\tau_z$$

$\approx$?



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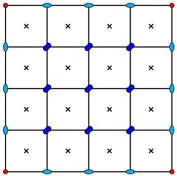

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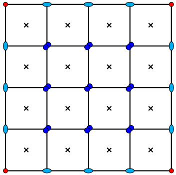

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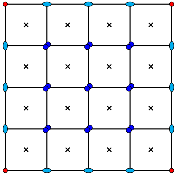

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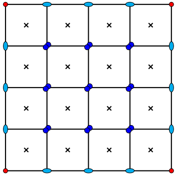

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$\boldsymbol{k}_*$	$C_{4,2}$ eigenvalues of $\mathcal{H}(k_*)$
$\Gamma = (0,0)$	$\{-\operatorname{sgn}(f_\Gamma)\ e^{\frac{i\pi}{4}},\ \operatorname{sgn}(f_\Gamma)\ e^{-\frac{i\pi}{4}}\}$
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$\operatorname{sgn}(f_\Gamma)$	$\operatorname{sgn}(f_M)$	orbitals and Wyckoff position
$+$	$+$	$j=7/2, j=5/2$ @ $\boldsymbol{r}=(0,0)$
$+$	$-$	$j=7/2, j=5/2$ @ $\boldsymbol{r}=(1/2,1/2)$
$-$	$+$	$j=3/2, j=1/2$ @ $\boldsymbol{r}=(1/2,1/2)$
$-$	$-$	$j=3/2, j=1/2$ @ $\boldsymbol{r}=(0,0)$

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- The symmetry indicators depend on the pairing terms only indirectly.
- The condition to be in the non-trivial obstructed phase is $\operatorname{sgn}(f_\Gamma)\operatorname{sgn}(f_M) = -1$.

Topology with C_4: HOTSC$_2$ with Majorana zero modes

The condition $\mathrm{sgn}(f_\Gamma)\,\mathrm{sgn}(f_M) = -1$ is guaranteed by the Dirac points in the normal state and C_4 symmetry.

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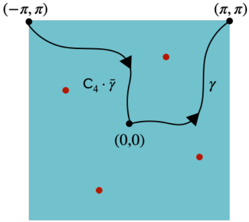
$$\mathcal{H}^{\text{normal}}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x + f_2(\boldsymbol{k})\sigma_z$$
$$=: ||f(\boldsymbol{k})||\hat{\boldsymbol{n}}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$$
$$\hat{\boldsymbol{n}}(\boldsymbol{k}_* = \Gamma, M) = 1/\sqrt{2}(e_x + e_z)$$

$\mathrm{N_w}$ (a path) $=$ winding of $\hat{\boldsymbol{n}}(\boldsymbol{k})$

Because of the the Dirac point:

$$\mathrm{N_w}\left(\gamma \circ (C_4 \cdot \bar{\gamma})\right) = 1$$
$$\mathrm{N_w}\left(\gamma \circ (C_4 \cdot \bar{\gamma})\right) = 2\mathrm{N_w}(\gamma)$$
$$\mathrm{N_w}(\gamma) = 1/2$$



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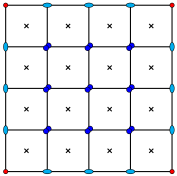

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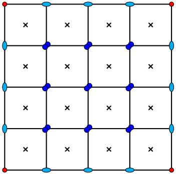

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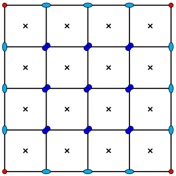

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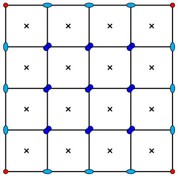

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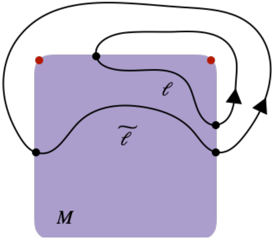
- Particle-hole symmetry is a local symmetry $\rightarrow$ doesn't mix different corners $\rightarrow$ corner states must be Majorana zero modes.

Real space picture of the topological invariant

The basic idea is to treat the corner of the sample as a defect, then use the Teo-Kane defect classification to detect the Majorana zero mode.



		Symmetry			$\delta = d - D$							
s	AZ	Θ^2	Ξ^2	Π^2	0	1	2	3	4	5	6	7
0	A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
1	AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
0	AI	1	0	0	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
1	BDI	1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
2	D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
3	DIII	−1	1	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
4	AII	−1	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
5	CII	−1	−1	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
6	C	0	−1	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
7	CI	1	−1	1	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

Real space picture of the topological invariant

Model the outside by:

$$\mathcal{H}_{\mathsf{triv}}(\boldsymbol{k}) = -f_0(\sigma_x\tau_z + \sigma_z\tau_z) + \Delta\sin(k_x)\tau_x + \Delta\sin(k_y)\tau_y - \mu\tau_z$$

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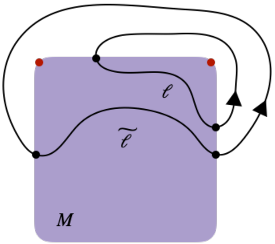
Define $\boldsymbol{q}$ to be a small momentum deviation from the Γ point. The defect Hamiltonian near the Γ point (for $\mu = 0$):

$$\begin{aligned}\mathcal{H}(\boldsymbol{q}) &= \Delta q_x\tau_x + \Delta q_y\tau_y \\ &\quad + f_0\left[\cos(\Phi)\sigma_x\tau_z + \sin(\Phi)\sigma_z\tau_z\right]\end{aligned}$$

$\Phi = \pi/4 \rightarrow$ inside material

$\Phi = 5\pi/4 \rightarrow$ outside material



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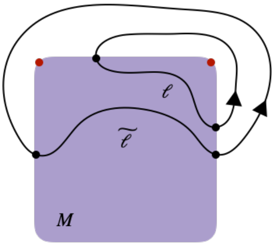
With C_4 symmetry it can be shown:

$$\mathrm{N_w} := \frac{1}{2\pi}\oint_{\ell} \mathrm{d}\Phi = (2n+1).$$

Adding the Chemical potential reduces the Z topological invariant to a Z_2.



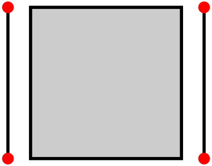
Summary

Model	With C_4	With C_2
With PH	HOTSC$_2$; corner Majorana	BOTSC$_2$; corner Majorana
Without PH	HOTI$_2$; filling anomaly	Trivial

- Today we looked at the first column of this table.
- Next time we discuss the second column.

A sneak peak: A cheap way of getting Majorana zero modes

Consider the following cheap way of getting Majorana zero modes on the corners:



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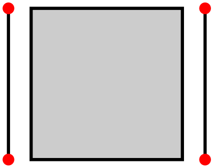

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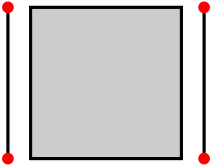

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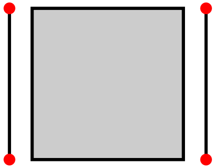

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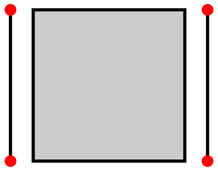

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Such topological phases protected by an edge gap closing are called boundary obstructed topological phases.