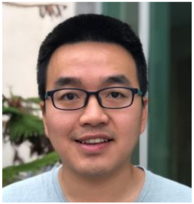
Chiral Dirac Superconductors: Second-order and Boundary-obstructed Topology

University of Florida, May 2020

Apoorv Tiwari
University of Zurich



Yuxuan Wang
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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

3. Boundary-obstructed topology
   Dirac + $(p+ip)$ with C_2 symmetry

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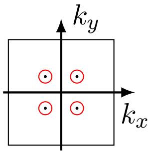
The normal state

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

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



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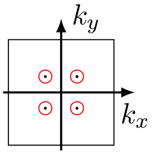

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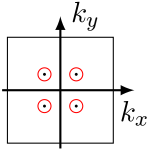

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$$\hat{C}_4 = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$$

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

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

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

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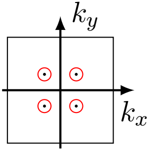

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$$\boxed{f_1(\boldsymbol{k}) = f_1(-\boldsymbol{k}),\ \text{and}\ f_2(\boldsymbol{k}) = f_2(-\boldsymbol{k})}$$

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

where τ_i act on the Nambu space.

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

$$\boxed{g_1(\boldsymbol{k}) = -g_1(-\boldsymbol{k}), \text{ and } g_2(\boldsymbol{k}) = -g_2(-\boldsymbol{k})}$$

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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

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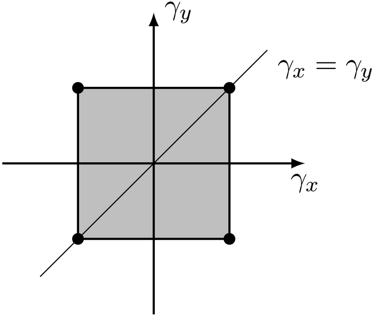
A prototypical example:

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

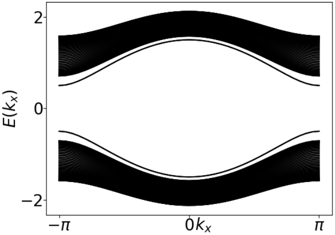
Phase diagram for $\mu = 0$:



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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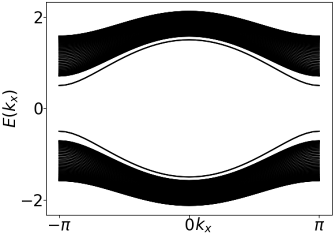
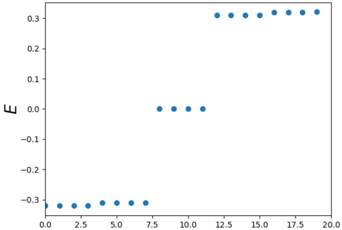


With open boundaries:



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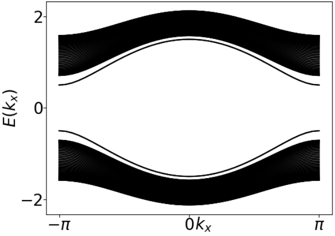

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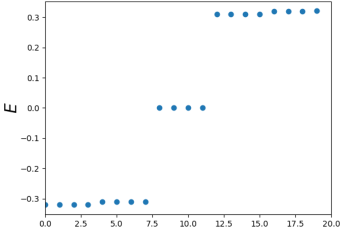
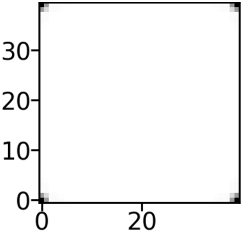


Zero modes:



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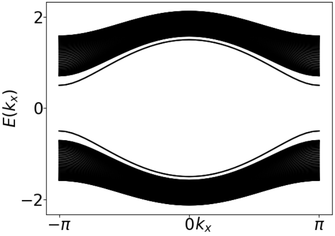

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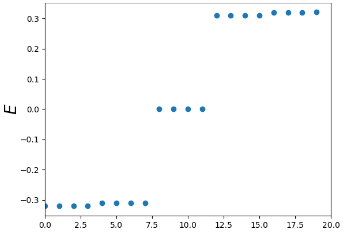

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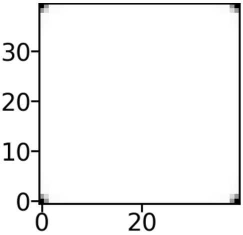

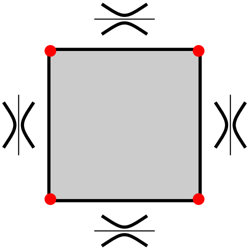

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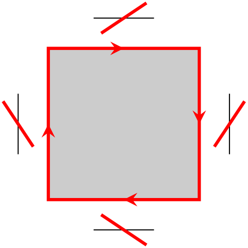
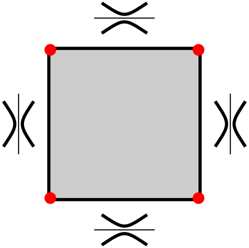
First-order topology vs second-order topology (I)

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.



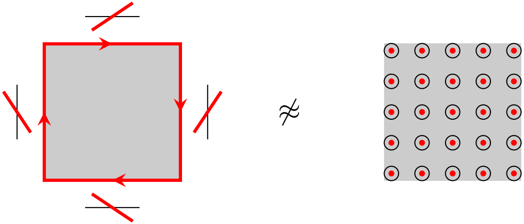
Non-trivial modes
co-dimension = 1



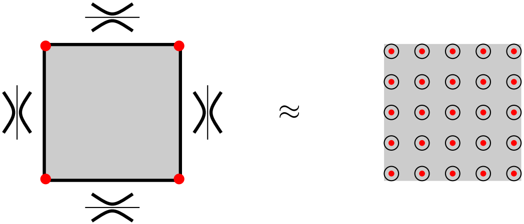
Non-trivial modes
co-dimension = 2

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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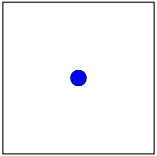
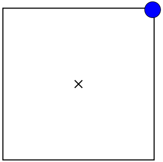
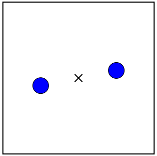


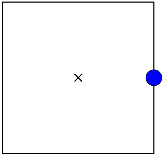
$\{(0,0)\}$
Multiplicty $= 1$



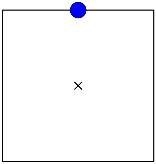
$\{(1/2,1/2)\}$
Multiplicty $= 1$



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



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



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

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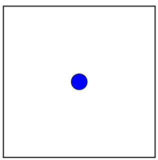
With C_4 atomic orbitals have to be put in on of the following Wyckoff positions relative to the center of the unit cell (corresponding to different representations of the symmetry group):



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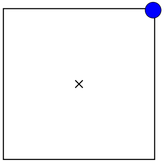
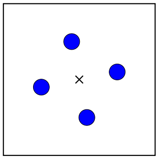
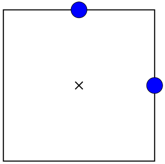


$\{(1/2,1/2)\}$
Multiplicty $= 1$



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



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

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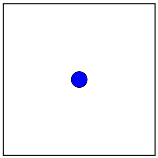
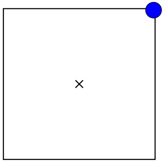
With M_x and M_y atomic orbitals have to be put in on of the following Wyckoff positions relative to the center of the unit cell (corresponding to different representations of the symmetry group):



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



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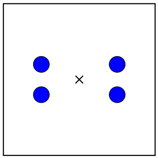
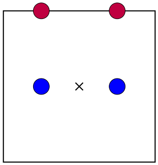
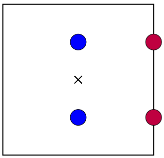


$\{(\pm x,\pm y)\}$
Multiplicty $= 4$



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



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

Symmetry of Block wavefunctions

Bloch wavefunctions can be written as:

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

$\boldsymbol{r}_\alpha$ 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

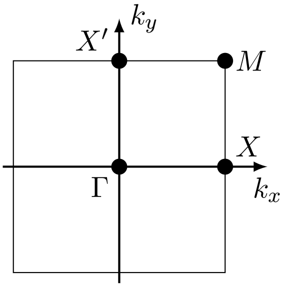
$\boldsymbol{k}_* = (0,\pi)$ & $(\pi,0)$ are C_2 symmetric

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

$e^{i\theta_\alpha(\boldsymbol{k}_*)}$ 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
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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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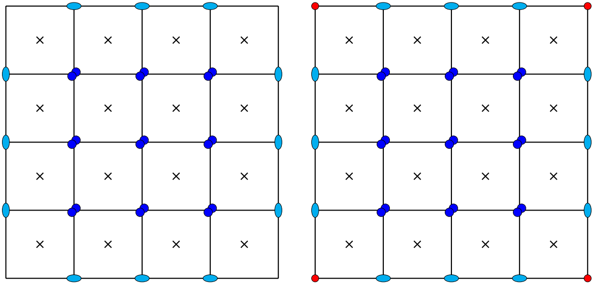

C_4 symmetric lattice with two electrons per unit cell, both at the Wyckoff position $\boldsymbol{r} = (1/2, 1/2)$. With open boundaries, both possible way of fillings give a net total charge to the system, and corner charges.

Symmetry indicators as a topological invariant

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

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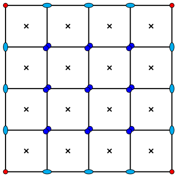

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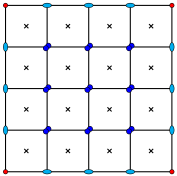

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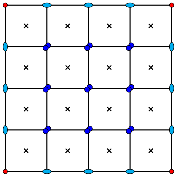

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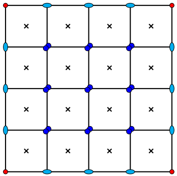

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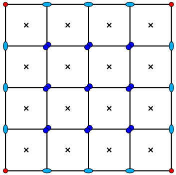

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$\boldsymbol{k}_*$	$C_{4,2}$ eigenvalues of $\mathcal{H}(k_*)$
$\Gamma = (0,0)$	$\{-\,\mathrm{sgn}(f_\Gamma)\; e^{\frac{i\pi}{4}},\; \mathrm{sgn}(f_\Gamma)\; e^{-\frac{i\pi}{4}}\}$
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$\mathrm{sgn}(f_\Gamma)$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

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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$$\mathcal{H}^{\text{normal}}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x + f_2(\boldsymbol{k})\sigma_z$$
$$=: ||f(\boldsymbol{k})||\hat{\boldsymbol{n}}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$$

$\hat{\boldsymbol{n}}(\boldsymbol{k}_* = \Gamma, M) = 1/\sqrt{2}(e_x + e_z)$

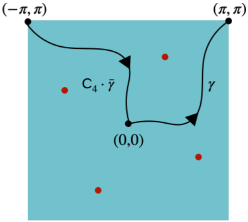
$\mathsf{N_w}$ (a path) $=$ winding of $\hat{\boldsymbol{n}}(\boldsymbol{k})$

Because of the the Dirac point:

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

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

$\mathsf{N_w}(\gamma) = 1/2$



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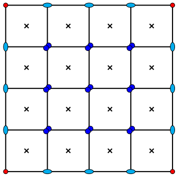

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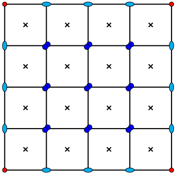

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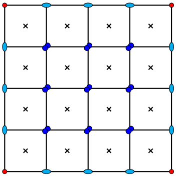

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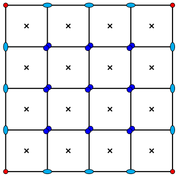

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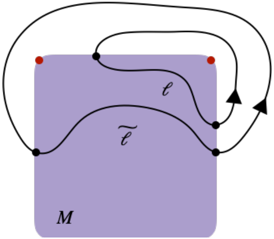
- Particle-hole symmetry is a local symmetry $\rightarrow$ doesn't mix different corners $\rightarrow$ corner states must be Majorana zero modes.

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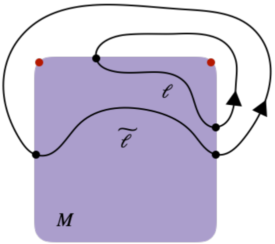
Define $\boldsymbol{q}$ to be a small momentum deviation from the Γ point. The defect Hamiltonian near the Γ point (for $\mu = 0$):

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

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

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



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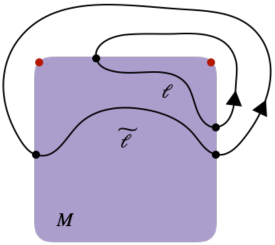
With C_4 symmetry it can be shown:

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

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



Outline

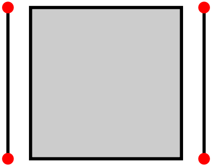
1. The model
   Dirac + $(p + ip)$

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

3. Boundary-obstructed topology
   Dirac + $(p + ip)$ with C_2 symmetry

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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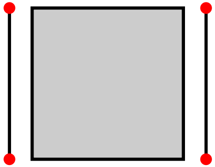

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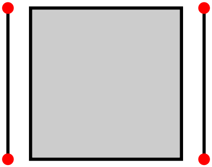

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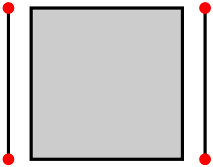

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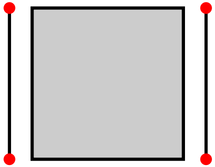

- Not C_4 symmetric, relax C_4 to C_2.
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Such topological phases protected by an edge gap closing are called boundary obstructed topological phases.

The prototypical Hamiltonian as an example of BOTSC$_2$

Our prototypical model with only C_2 symmetry can at best be boundary obstructed.

$$
\begin{aligned}
\mathcal{H}(\boldsymbol{k}) = &(\gamma_x + \cos(k_x))\tau_z \\
&+ (\gamma_y + \cos(k_y))\sigma_z\tau_z \\
&+ \Delta \sin(k_x)\tau_x \\
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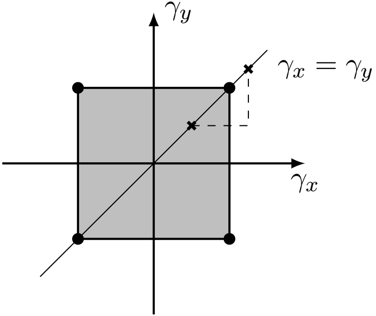
Topological phase can be deformed into trivial phase without closing the bulk gap.

Phase diagram for $\mu = 0$:



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Need to study the edges carefully.

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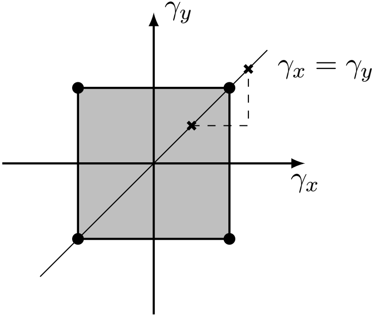
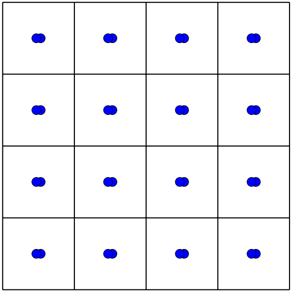


Boundary obstructed atomic phases.

Boundary obstruction protected by mirror symmetry:



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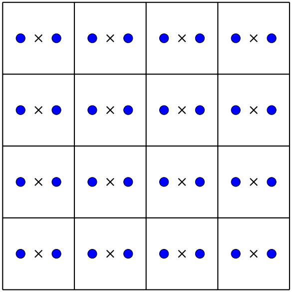

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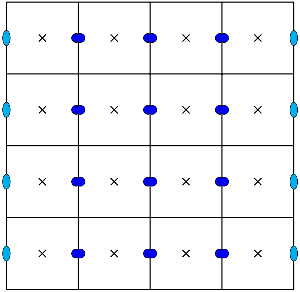

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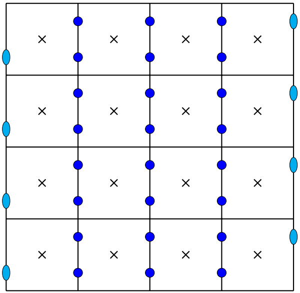

Mirror symmetry broken on the boundaries.

Boundary obstructed atomic phases.

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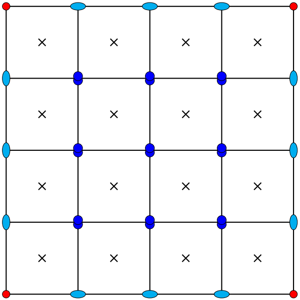

Filling anomaly

Boundary obstructed atomic phases.

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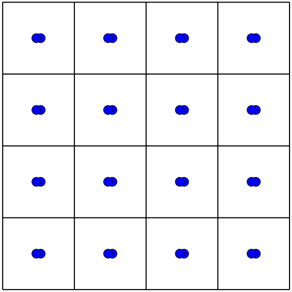

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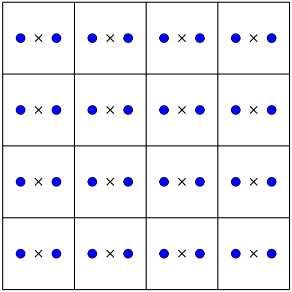

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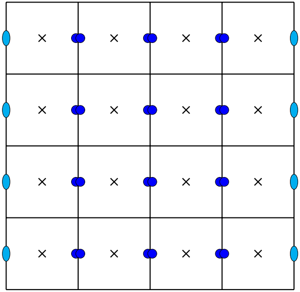

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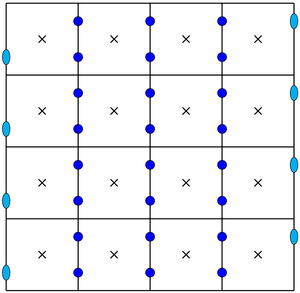

C_2 symmetry is NOT broken on the boundaries.

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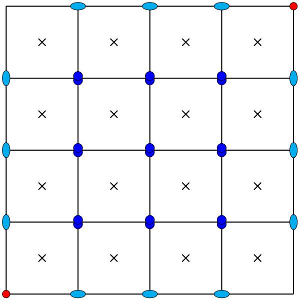

No filling anomaly

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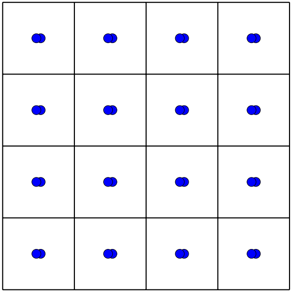
Boundary obstruction protected by C_2 and $\mathcal{P}$ symmetry:



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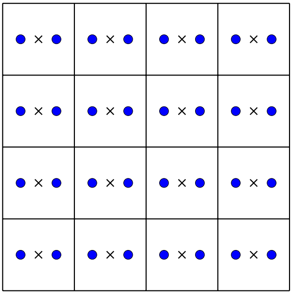

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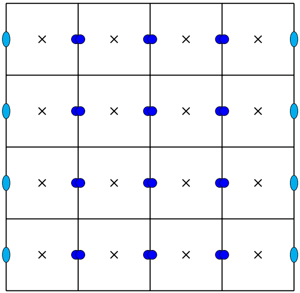

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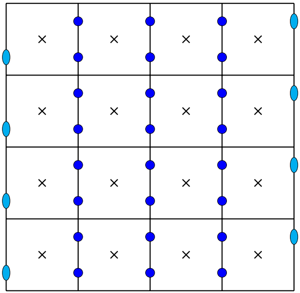

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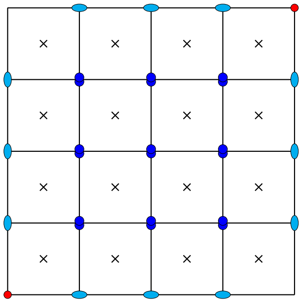

Majorana zero modes

Interlude: The Wannier bands

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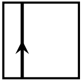

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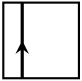

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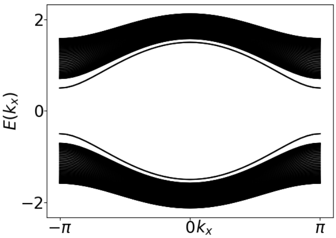
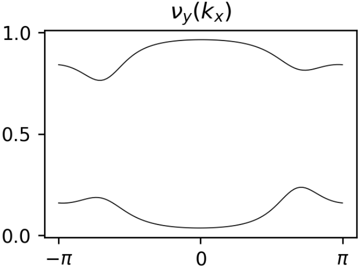
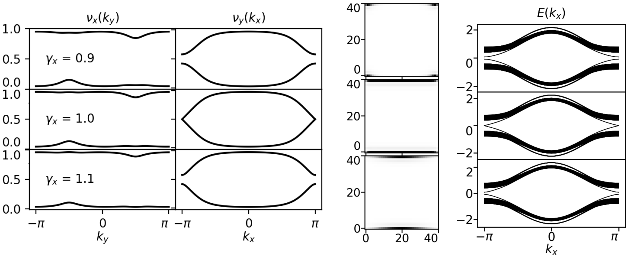




Wannier bands detect boundary gap closing.

A relative bulk topological invariant

$$
\begin{aligned}
H = &(\cos k_x + \gamma_x)\sigma_x\tau_z + \cos k_y \sigma_z\tau_z - 0.2\tau_z \\
&+ 0.4\sin k_x \tau_x + 0.4 \sin k_y \tau_y
\end{aligned}
$$



That the Wannier bands close a gap can be used to define some bulk topological invariant.

Wannier-projected Hamiltonian

$$
\begin{aligned}
H_{P^\pm}(k_x) =& P^\pm(k_x) H P^\pm(k_x), \text{where} \\
P^\pm(k_x) \equiv& \frac{1 \pm \hat{P}_{\text{occ}}(\boldsymbol{k})\,\mathrm{sgn}(\hat{\nu}_y) \pm \hat{P}_{\text{emp}}(\boldsymbol{k})\,\mathrm{sgn}(\hat{\nu}'_y)}{2} \\
\tilde{\mathcal{P}}(k_x) K =& P^\pm(k_x) \mathcal{P} \left[P^\pm(-k_x) \right]^* K \\
H_{P^\pm}(k_x) =& -\tilde{\mathcal{P}}(k_x) H^*_{P^\pm}(-k_x) \tilde{\mathcal{P}}^\dagger(k_x)
\end{aligned}
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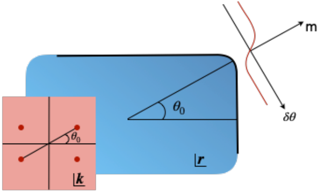
\end{aligned}
$$

We use $H_{P^{\pm}}(k_x = 0, \pi)$ as a zero dimensional subsystems.

		Symmetry			δ=$d-D$							
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	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

Majorana zero modes as a defect of the edge

$$\mathcal{H}(\boldsymbol{k}) = f_1(\boldsymbol{k})\sigma_x\tau_z + f_2(\boldsymbol{k})\sigma_z\tau_z$$
$$+ \epsilon g_1(\boldsymbol{k})\tau_x + \epsilon g_2(\boldsymbol{k})\tau_y - \mu\tau_z$$
$$k_x(\theta) = k_\perp \cos\theta - k_\parallel \sin\theta$$
$$k_y(\theta) = k_\perp \sin\theta + k_\parallel \cos\theta$$
$$H \to \tilde{H} = UHU^\dagger$$



$$\tilde{H}(k_\perp, k_\parallel = 0; \theta_0) = \tilde{f}_1(k_\perp)\sigma_x\tau_z + \epsilon\tilde{g}_1(k_\perp)\tau_x - \mu\tau_z$$

Do a perturbative expansion for: (i) Small $k_\parallel$, (ii) Small $\delta\theta$

$$h(k_\parallel, \theta_0 + \delta\theta) = \alpha k_\parallel s_x + \beta\delta\theta s_y.$$

This looks like a kitaev chain with a domain wall, hence it host a Majorana zero mode.

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