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

University of Florida, May 2020

Recap of last time

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

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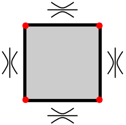
- In the topological phase the model looks like: 

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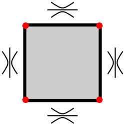
- In the topological phase the model looks like: 
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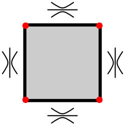
- In the topological phase the model looks like: 
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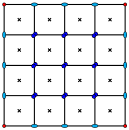
- With C_4 symmetry (had we thought of the system as an insulator): $\mathcal{H}(\boldsymbol{k}) \approx$ 

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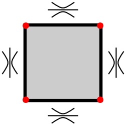
- In the topological phase the model looks like: 
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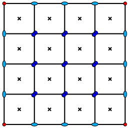
- With C_4 symmetry (had we thought of the system as an insulator): $\mathcal{H}(\boldsymbol{k}) \approx$ 
- Particle-hole symmetry implies that the corner charges of the obstructed atomic phase can be interpreted as Majorana zero modes for our BdG system.

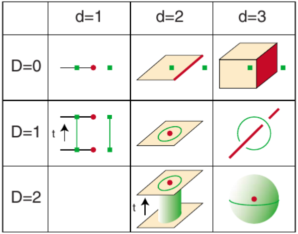
Outline

Model	With C_4	With C_2
With PH	HOTSC_2; corner Majorana	BOTSC_2; corner Majorana
Without PH	HOTI_2; filling anomaly	Trivial

- Understanding the corner mode from defect classification.
- Discuss the second column of the table.

Defect classification

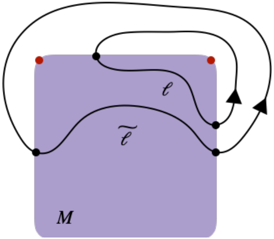
- Teo-Kane classification of defect Hamiltonians, $\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})$.
- d is dimension of $\boldsymbol{k}$. D is the dimension of $\boldsymbol{r}$.
- Depends on the symmetry class and the dimension of the defect.



	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

- The basic idea is to treat the corner of the sample as a defect, $\mathcal{H}(\boldsymbol{k}, \Phi)$.
- For class BDI the topological invariant corresponds to the number of Majorana modes bound to the corner.



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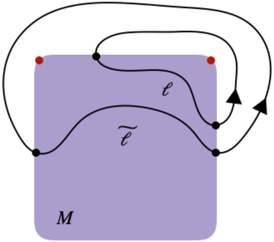
Define $\boldsymbol{q}$ to be a small momentum deviation from the Γ point. The defect Hamiltonian near the Γ point (for $\mu = 0$):

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

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

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



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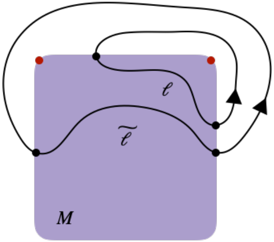
With C_4 symmetry it can be shown:

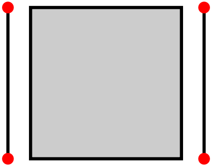
$$\mathsf{N_w} := \frac{1}{2\pi}\oint_\ell \mathrm{d}\Phi = (2n+1).$$

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



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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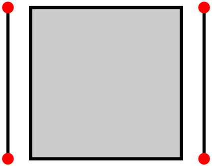

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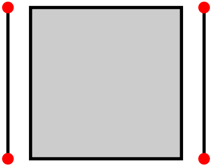

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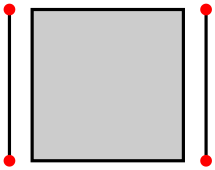

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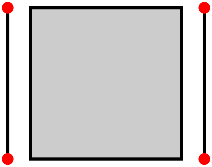

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Such topological phases protected by an edge gap closing are called boundary obstructed topological phases.

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 \\
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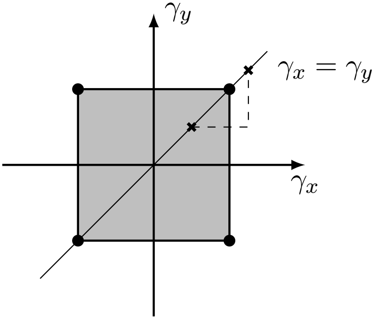
Topological phase can be deformed into trivial phase without closing the bulk gap.

Phase diagram for $\mu = 0$:



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Need to study the edges carefully.

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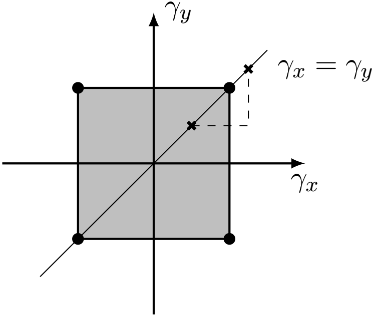
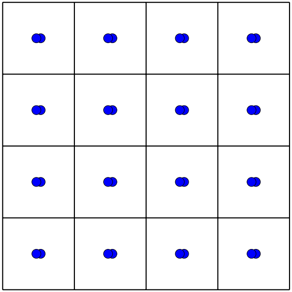


Boundary obstructed atomic phases.

Boundary obstruction protected by mirror symmetry:



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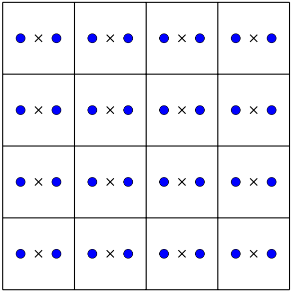

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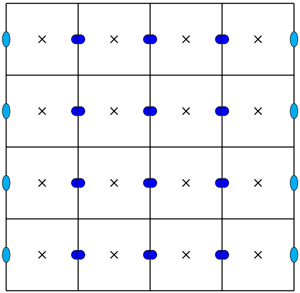

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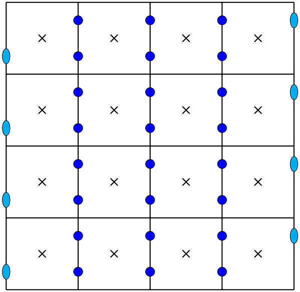

Mirror symmetry broken on the boundaries.

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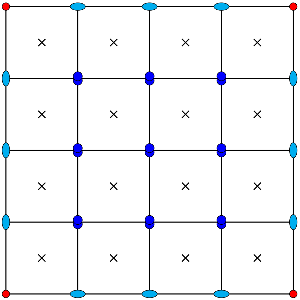

Filling anomaly

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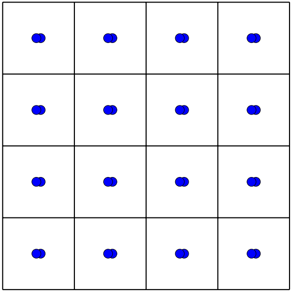

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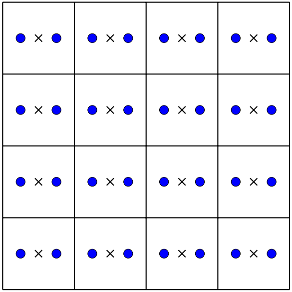

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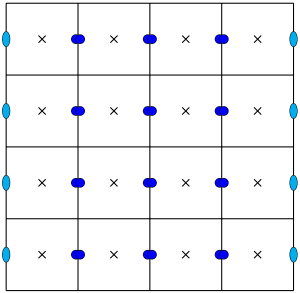

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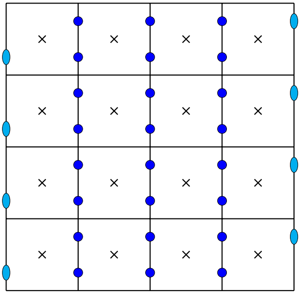

C_2 symmetry is NOT broken on the boundaries.

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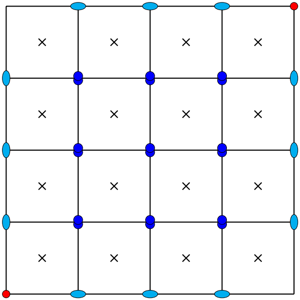

No filling anomaly

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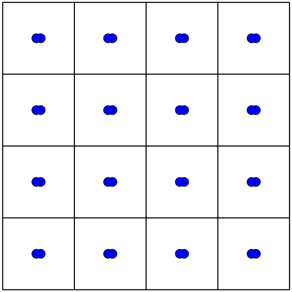
Boundary obstruction protected by C_2 and $\mathcal{P}$ symmetry:



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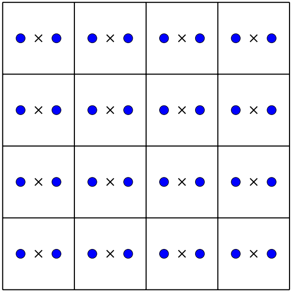

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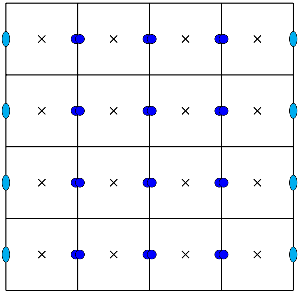

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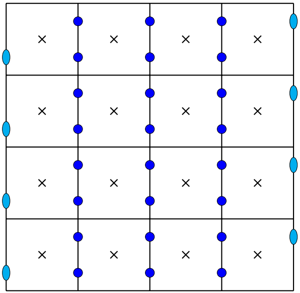

$\mathcal{P}$ is broken on the boundaries.

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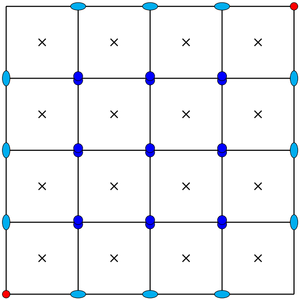

Majorana zero modes

Boundary obstructed atomic phases.

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- Atomic phases show the importance of particle-hole symmetry to protect the boundary obstructed phase.
- Next we show explicitly that our 'Dirac $+$ $(p + ip)$' model with C_2 symmetry is indeed boundary obstructed, by studying its edge theory.

Interlude: The Wannier bands

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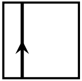

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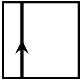

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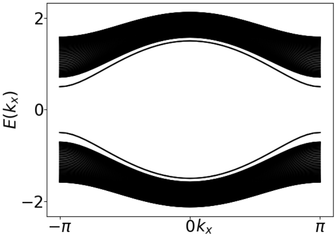
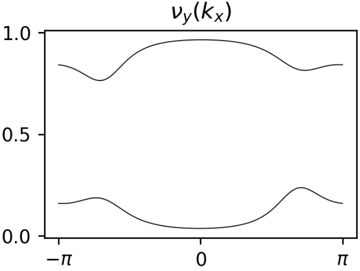
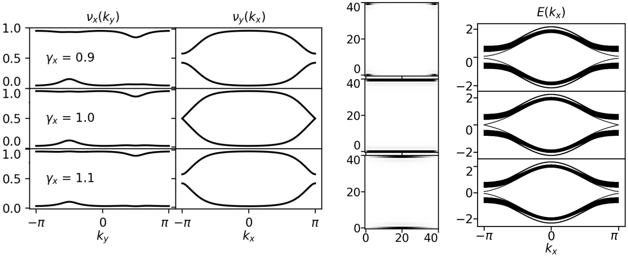




Wannier bands detect boundary gap closing.

A relative bulk topological invariant

$$H = (\cos k_x + \gamma_x)\sigma_x\tau_z + \cos k_y \sigma_z\tau_z - 0.2\tau_z + 0.4\sin k_x\tau_x + 0.4\sin k_y\tau_y$$



- That the Wannier bands gap closing, being a property of the bulk, can be used to define some bulk topological invariant.However the exact form of that invariant may be complicated.

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}_{\mathrm{occ}}(\boldsymbol{k}) \operatorname{sgn}(\hat{\nu}_y) \pm \hat{P}_{\mathrm{emp}}(\boldsymbol{k}) \operatorname{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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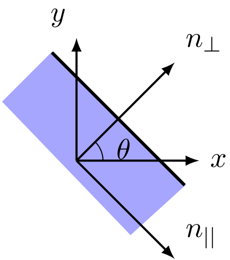
We use $H_{P^\pm}(k_x = 0, \pi)$ as a zero dimensional subsystems.

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	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

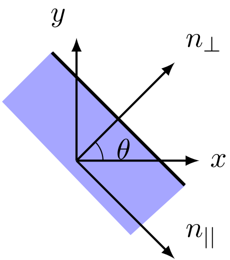
A recipie for getting edge Hamiltonian

1. Choose a direction, θ, to put the edge.



A recipie for getting edge Hamiltonian

1. Choose a direction, θ, to put the edge.
2. Choose how you model empty space. (Different choices will lead to different boundary conditions but doesn't change the physics of the boundary.)
   $\mathcal{H}(\boldsymbol{k}) \rightarrow \mathcal{H}(\partial_{x_\perp}, k_{||}, x_\perp)$



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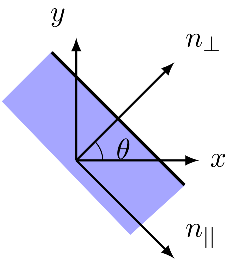
3. Solve for the localized edge states.
   $\Psi_\alpha^{\text{edge}}(x_\perp, k_{||}) = e^{ik_{||}x_{||}}\chi_\alpha(k_{||})\phi(x_\perp)$, such that, $\mathcal{H}\Psi_\alpha^{\text{edge}} = \epsilon^\alpha(k_{||})\Psi_\alpha^{\text{edge}}$



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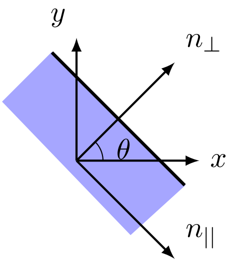
4. The edge Hamiltonian is then, $h^{\text{edge}}(k_{||}) = \sum_\alpha |\chi_\alpha(k_{||})\rangle\, \epsilon^\alpha(k_{||})\, \langle\chi_\alpha(k_{||})|$



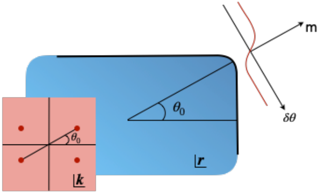
Majorana zero modes as a defect of the edge

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

$$k_x(\theta) = k_\perp \cos\theta - k_\parallel \sin\theta$$

$$k_y(\theta) = k_\perp \sin\theta + k_\parallel \cos\theta$$

$$H \to \tilde{H} = UHU^\dagger$$



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

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