The classification of Surface states of topological superconductors

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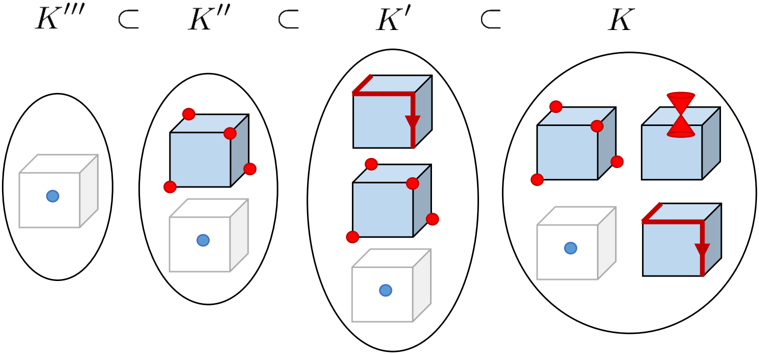
Main result

- We want to know the existence/absence of stable gapless surface states on the boundary of the 3-ball for given magnetic point group symmetry.
- No translation symmetry
- The dimensionality of surface states $\rightarrow$ higher-order TIs/TSCS



- In this work, we formulated how to compute the quotient group K/K''', the classification of surface states, and computed the classification for all 122 magnetic point groups in TIs and TSCs.

Plan

- Compute K
  - Cornfeld-Chapman trick
  - Periodic table
- Compute K'''
  - $0d$ state $= 3d$ Dirac Hamiltonian with a hedgehog mass potential
  - Compute the homomorphism $K''' \to K$

Dirac Hamiltonian with point group symmetry

- Dirac Hamiltonian in d space dimensions ($\boldsymbol{k} = -i\boldsymbol{\partial}$) with a uniform mass

$$H(\boldsymbol{k}) = -i\sum_{j=1}^{d} \gamma_j \partial_j + M, \qquad \{\gamma_i, \gamma_j\} = 2\delta_{ij}, \qquad \{\gamma_i, M\} = 0.$$

- Let G be a point group, i.e., G acts on the real-space coordinate $\boldsymbol{x}$ as a discrete subgroup of $O(d)$.

$$g : \boldsymbol{x} \mapsto O_g \boldsymbol{x}, \qquad g \in G.$$

- We denote the operator acting on the one-particle Hilbert space by $\hat{g}$.
- As usual, symmetry operators form a projective representation with a factor system

$$\hat{g}\hat{h} = z_{g,h}\widehat{gh}, \qquad g, h \in G,$$

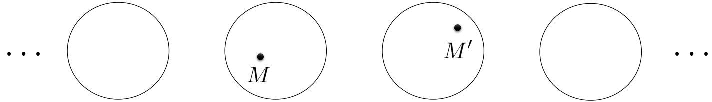
  where $z_{g,h} \in U(1)$ is called the factor system.
- $\hat{g}$ can be antiunitary. We specify if $\hat{g}$ is unitary or not by $\phi_g \in \{\pm 1\}$.
- $\hat{g}$ can flip the Hamiltonian $H(\boldsymbol{k})$, which specified by $c_g \in \{\pm 1\}$.
- In sum,

$$\hat{g}H(\boldsymbol{k})\hat{g}^{-1} = c_g H(\phi_g O_g \boldsymbol{k}), \qquad \hat{g}i\hat{g}^{-1} = \phi_g i, \qquad g \in G.$$

- Mass term M obeys the following complicated algebra.

$$\hat{g}\hat{h} = z_{g,h}\widehat{gh}.$$
$$\hat{g}\boldsymbol{\gamma}\hat{g}^{-1} = \phi_g c_g O_g^{-1}\boldsymbol{\gamma}, \qquad \hat{g}M\hat{g}^{-1} = c_g M,$$
$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}, \qquad \{\gamma_i, M\} = 0.$$

- **Question.** How to get the topological classification of the "space" of the mass term M?



Step 1: Cornfeld-Chapman trick

- The gamma matrices γ_j themselves can be used to make $Spin(d)$ rotation operators.
- Let

$$R_\theta = \exp \frac{i}{2}\theta_{ij}L_{ij}, \qquad [L_{ij}]_{kl} = -i(\delta_{ik}\delta_{jl} - \delta_{jk}\delta_{il}),$$

  be an $SO(d)$ rotation.
- The set $\{\theta_{ij} \in [0, 2\pi]\}$ of $SO(d)$ rotation parameters gives us a lift $SO(d) \to Spin(d)$,

$$U_\theta = \exp \frac{i}{2}\theta_{ij}\Sigma_{ij}, \qquad \Sigma_{ij} = \frac{-i}{4}[\gamma_i, \gamma_j].$$

- The key equality:

$$U_\theta \boldsymbol{\gamma} U_\theta^{-1} = R_\theta \boldsymbol{\gamma}.$$

- Therefore, the $SO(d)$ part of $\hat{g}$ can be "onsite".

- For generic $O(d)$ rotations, we write

$$O_g = \begin{cases} R_{\theta_g} & (O_g \in SO(d)), \\ M_1 R_{\theta_g} & (O_g \notin SO(d)), \end{cases}$$

where $M_1 : (x_1, x_2, \dots) \mapsto (-x_1, x_2, \dots)$ is the reflection for the x_1-direction.

- Let

$$p_g := \det O_g \in \{\pm 1\}$$

is the marker for specifying orientation-preserving/reversing elements.

- Per the value of p_g, we introduce the modified operator

$$\tilde{g} := (\gamma_1)^{\frac{1-p_g}{2}} \times U_\theta \times \hat{g}.$$

- We find that $\tilde{g}$ is now an onsite symmetry operator

$$\tilde{g}\boldsymbol{\gamma}\tilde{g}^{-1} = c_g p_g \phi_g \boldsymbol{\gamma}, \qquad \tilde{g} M \tilde{g}^{-1} = c_g p_g M,$$

i.e.,

$$\tilde{g} H(\boldsymbol{k}) \tilde{g}^{-1} = c_g p_g H(\phi_g \boldsymbol{k}).$$

Step 2: The Wigner criteria and the orthogonal test

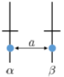
- For onsite symmetry, the classification of the mass term M is straightforward.
- First, we decompose the symmetry group G with respect to whether $\tilde{g}$ is TRS, PHS, or chiral symmetry.

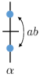
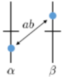
$$
\begin{aligned}
&G = \underbrace{G_0}_{\text{unitary}} \sqcup \underbrace{aG_0}_{\text{TRS}} \sqcup \underbrace{bG_0}_{\text{PHS}} \sqcup \underbrace{abG_0}_{\text{chiral}}, \\
&G_0 = \{g \in G | \phi_g = c_g p_g = 1\}, \\
&a \in G, \qquad \phi_a = -1, \qquad c_a p_a = 1, \\
&b \in G, \qquad \phi_b = -1, \qquad c_b p_b = -1, \\
&ab \in G, \qquad \phi_{ab} = 1, \qquad c_{ab} p_{ab} = -1.
\end{aligned}
$$

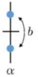
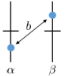
- An "irrep of G" can be seen as an irrep of G_0 with the data of how remaining operators a, b, and ab act on its irrep. $\rightarrow$ 19 patterns.

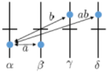
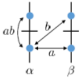
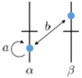
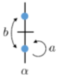
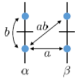
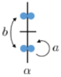
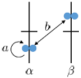
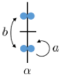
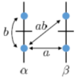
There are 19 patterns of the presences/absences of a, b, ab and the values of the Wigner criteria W_α^T, W_α^C and the orthogonal test $O_{\alpha\alpha}^\Gamma$, which we call the effective AZ (EAZ) classes.

EAZ	Band str.
A	

W_α^T	EAZ	Band str.
1	AI	
−1	AII	
0	A_T	

W_α^Γ	EAZ	Band str.
1	AIII	
0	A_Γ	

W_α^C	EAZ	Band str.
1	D	
−1	C	
0	A_C	

W_α^T	W_α^C	W_α^Γ	EAZ	Band str.
0	0	0	$A_{T,C}$	
0	0	1	$AIII_T$	
1	0	0	AI_C	
1	1	1	BDI	
0	1	0	D_T	
−1	1	1	DIII	
−1	0	0	AII_C	
−1	−1	1	CII	
0	−1	0	C_T	
1	−1	1	CI	

Once the EAZ class of the irrep α is fixed, the classification of the mass term for the irrep α is found by the periodic table.

EAZ class	$d=0$	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	$d=7$
$\mathrm{A}, \mathrm{A}_T, \mathrm{A}_C, \mathrm{A}_\Gamma, \mathrm{A}_{T,C}$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
$\mathrm{AIII}, \mathrm{AIII}_T$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
$\mathrm{AI}, \mathrm{AI}_C$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
D, D_T	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
$\mathrm{AII}, \mathrm{AII}_C$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
C, C_T	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

$3d$ superconductors (SCs) with magnetic point group symmetry

- A subtle point for SCs is that the symmetry algebra depends on what the representation of the gap function is.
- Suppose that the normal part $h(\boldsymbol{k})$ is invariant under a magnetic point group

$$u_g h(\boldsymbol{k}) u_g^{-1} = h(\phi_g O_g \boldsymbol{k}), \qquad u_g u_h = z_{g,h} u_{gh}.$$

- The superconducting gap function $\Delta(\boldsymbol{k}) = \sum_{i=1}^{N} \eta_i \Delta_i(\boldsymbol{k})$ is a rep of G in general.

$$\Delta_i(\phi_g O_g \boldsymbol{k}) = [D_\rho(g)]_{ij} \times u_g \Delta_j(\boldsymbol{k}) u_g^T.$$

- When $\Delta(\boldsymbol{k})$ obeys a nontrivial rep of G, such SCs are said unconventional.
- For unconventional SCs, the superconducting order spontaneously breaks the magnetic point group symmetry.
- By the $U(1)$ phase rotation

$$\hat{U}_{\theta_g/2} \hat{\psi}_{\boldsymbol{x}} \hat{U}_{\theta_g/2}^{-1} = \hat{\psi}_{\boldsymbol{x}} e^{-i\theta_g/2}$$

  of the complex fermion, the gap function changes as $\Delta(\boldsymbol{k}) \mapsto e^{i\theta_g} \Delta(\boldsymbol{k})$.
- This means, for the subgroup $G_* \subset G$ of which the rep is 1-dimensional, the symmetry of the magnetic point group G_* recovers.

- From the above reason, we assume that the gap function obeys a 1-dim irrep of G, which we denote it by $e^{i\theta_g}$.

$$\Delta(\phi_g O_g \boldsymbol{k}) = e^{i\theta_g} \times u_g \Delta(\boldsymbol{k}) u_g^T.$$

- The BdG Hamiltonian

$$H(\boldsymbol{k}) = \begin{pmatrix} h(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta(\boldsymbol{k})^\dagger & -h(-\boldsymbol{k})^T \end{pmatrix}_\tau$$

is invariant under the symmetry group $G \times \mathbb{Z}_2^C$ where $\hat{C} = \tau_x K$ is PHS operator.

- The symmetry operator $\hat{g}$ for $g \in G$ depends on the 1-dim irrep as in

$$\hat{g} = \begin{pmatrix} u_g & \\ & e^{i\theta_g} u_g^* \end{pmatrix}, \qquad \hat{g}\hat{C} = e^{i\theta_g} \hat{C} \hat{g}.$$

- There are 380 inequivalent symmetry classes from 122 magnetic point groups and 1-dim irreps in $3d$.
- The effective AZ classes for spinless and spinful SCs in $3d$ are listed in [KS].
- Spinful systems:

MPG	Ker ϕ	Irrep	EAZ	$K_0^G(\mathbb{R}^3)$	$K_{-1}^G(\mathbb{R}^3)$	$K_{-2}^G(\mathbb{R}^3)$	$\cdots$
1	1	A	{D}	0	0	0	
$11'$	1	A	{DIII}	$\mathbb{Z}$	0	0	
$\bar{1}$	$\bar{1}$	A_g	{BDI}	0	0	$2\mathbb{Z}$	
$\bar{1}$	$\bar{1}$	A_u	{DIII}	$\mathbb{Z}$	0	0	
$\bar{1}1'$	$\bar{1}$	A_g	{D_T}	0	0	0	
$\bar{1}1'$	$\bar{1}$	A_u	{DIII^2}	$\mathbb{Z}^{\times 2}$	0	0	
$\vdots$							
$m\bar{3}m'$	$m\bar{3}$	A_g	{D_T^2,DIII}	$\mathbb{Z}$	0	0	
$m\bar{3}m'$	$m\bar{3}$	E_g	{D_T^2,DIII}	$\mathbb{Z}$	0	0	
$m\bar{3}m'$	$m\bar{3}$	A_u	{DIII^5}	$\mathbb{Z}^{\times 5}$	0	0	
$m\bar{3}m'$	$m\bar{3}$	E_u	{DIII^5}	$\mathbb{Z}^{\times 5}$	0	0	
$m'\bar{3}'m'$	432	A_1	{D^{10}}	0	0	0	
$m'\bar{3}'m'$	432	A_2	{D^2,A_C}	0	$\mathbb{Z}$	0	

Plan

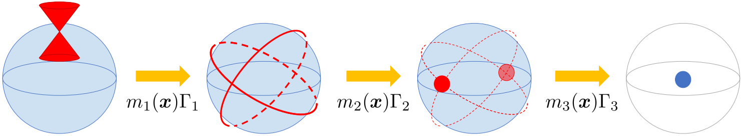
- Compute K
  - Cornfeld-Chapman trick
  - Periodic table
- Compute K'''
  - $0d$ state $= 3d$ Dirac Hamiltonian with a hedgehog mass potential
  - Compute the homomorphism $K''' \to K$

Additional masses

- The effective AZ class provides the classification of Dirac Hamiltonian with a *uniform* mass, which we denote $K = K_n^G(\mathbb{R}^d)$.
- However, the classification of the uniform mass does not imply the classification of the gapless surface states.
- Put differently, not every element in the K-group K obeys the bulk-boundary correspondence.
- This is because for point group symmetry there may be spatially-varying mass terms that induce mass gap to the surface state. [Isobe-Fu '15, ...]

$$H = -i\boldsymbol{\partial} \cdot \boldsymbol{\gamma} + M + m_1(\boldsymbol{x})\Gamma_1 + m_2(\boldsymbol{x})\Gamma_2 + \cdots$$

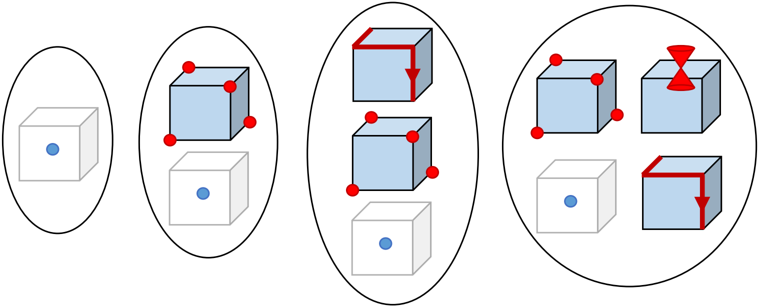
- For 3d:



Higher-order SPT phases [Huang-Song-Huang-Hermele '17, ...]

- This observation leads to the concept of so-called higher-order TIs/TSCs.
- We define $K^{(n)} \subset K$ as the subgroup of Dirac Hamiltonians in the K-group K that admits at least n spatially-varying masses.
- For $3d$:

$$K''' \subset K'' \subset K' \subset K$$

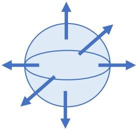


- The quotient group $K^{(n-1)}/K^{(n)}$ is called nth-order TIs/TSCs.

Equivalence between atomic insulators and Dirac Hamiltonians with a hedgehog mass

- One can also canonically compute the group $K^{(d)}$ of dth-order TIs/TSCs, the localized states at the center of the point group.
- To compute $K^{(d)}$, we note the equivalence between the atomic insulators exactly at the point group center and the d-dim Dirac Hamiltonian with hedgehog-mass potential with a unit winding number. This is known as the Jackiw-Rossi bound state.

$$H_{0D} \quad \leftrightarrow \quad H_{dD} = -i\boldsymbol{\partial}\cdot\boldsymbol{\gamma} + \boldsymbol{m}(\boldsymbol{x})\cdot\boldsymbol{\Gamma} + M.$$



$\boldsymbol{m}(\boldsymbol{x})$

- The explicit construction is as follows.
- Let H_{0D} be a $0d$ Hamiltonian. We have the successive isomorphic maps:

$$\begin{aligned}
0d \to 1d: &\qquad H_{1D} = -i\partial_1\sigma_y + x_1\sigma_x + H_{0D}\sigma_z, \\
1d \to 2d: &\qquad H_{2D} = -i\partial_2 s_y + x_2 s_x + H_{1D} s_z, \\
2d \to 3d: &\qquad H_{3D} = -i\partial_3\mu_y + x_3\mu_x + H_{2D}\mu_z, \\
\dots &
\end{aligned}$$

The homomorphism $f : K_{\mathrm{AI}} \to K$

- Let K_{AI} be the abelian group generated by atomic insulators exactly at the point group center.
- Not every $0d$ Hamiltonian H_{0D} in K_{AI} is pinned at the point group center, since some combination of atomic orbitals can go far away without breaking the point group symmetry.
- We define the homomorphism

$$f : K_{\mathrm{AI}} \to K,$$

by neglecting the hedgehog-mass potential $\boldsymbol{m}(\boldsymbol{x}) \cdot \boldsymbol{\Gamma}$ in the dD Hamiltonian H_{dD},

$$H_{dD} = -i\boldsymbol{\partial} \cdot \boldsymbol{\gamma} + \boldsymbol{m}(\boldsymbol{x}) \cdot \boldsymbol{\Gamma} + M \mapsto H'_{dD} = -i\boldsymbol{\partial} \cdot \boldsymbol{\gamma} + H_{0D}\Gamma_0.$$

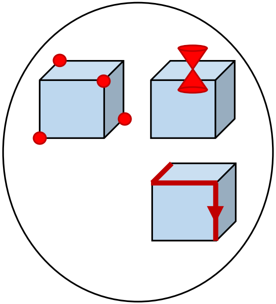
- The image of f has the physical meaning of the Jackiw-Rossi bound state pinned at the point group center, i.e., the dth-order TIs/TSCs. Thus,

$$K^{(d)} = \mathrm{Im}\ f.$$

- It is easy to compute the group K_{AI}, which is just the K-group of reps of the point group G with the data $(\phi_g, c_g, z_{g,h})$.
- Thus, we conclude that the group $K^{(d)}$ of dth-order TIs/TSCs is computed canonically.

- Therefore, one can in principle compute the quotient $K/K^{(d)}$, the group composed of surface gapless states, by the irreducible character.
- For $3d$:

$$K/K'''$$



- The explicit form of the homomorphism f for $3d$ is given in [KS].
- For instance, for an irrep β of $K_{\rm AI}$, the $3d$ winding number detecting a direct summand $\mathbb{Z}$ in K belonging to the irrep α of G_0, is given by

$$w_{3d}|_{\beta\to\alpha} = \frac{1}{|G_0|} \sum_{\substack{g\in G,\\ \phi_g=c_g=-p_g=1}} \tilde{\chi}^{+}_{\alpha}(g)^* \times 2\cos\frac{\theta_g}{2}$$

$$\times \begin{cases} \chi_\beta(g) & \text{for A, AI,} \\ \chi_\beta(g)+\chi_{\underline{a}(\beta)}(g) & \text{for AII, A}_T, \\ \chi_\beta(g)-\chi_{\underline{b}(\beta)}(g) & \text{for D, C, A}_C\text{, AI}_C\text{, BDI, CI,} \\ \chi_\beta(g)-\chi_{\underline{ab}(\beta)}(g) & \text{for AIII, A}_\Gamma, \\ \chi_\beta(g)+\chi_{\underline{a}(\beta)}(g)-\chi_{\underline{b}(\beta)}(g)-\chi_{\underline{ab}(\beta)}(g) & \text{for A}_{T.C}\text{, AIII}_T\text{, D}_T\text{, DIII, AII}_C\text{, CII, C}_T. \end{cases}$$

- See [KS] for the detail.
- What I want to empathize is that the homomorphism f can be computed by the data $(G, O_g, \phi_g, c_g, z_{g,h})$ and the irreducible character.

The classification of spherical surface states

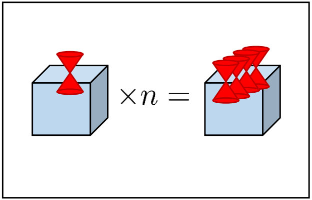
- Along the line of the above thought, one can compute the classification of gapless states on $(d-1)D$ sphere $S^{d-1} = \partial B^d$, the boundary states of dD TIs/TSCs over the d-ball B^d.
- In [KS], I summarized the complete list of the surface states of $3d$ TIs/TSCs for 122 magnetic point group symmetry.
- Ex: SCs in spinful systems.

MPG	Ker ϕ	Irrep	EAZ	$K_0^G(\mathbb{R}^3)$	FreeK/K'''	TorK/K'''
1	1	A	{D}	0	0	$\{\}$
$11'$	1	A	{DIII}	$\mathbb{Z}$	1	$\{\}$
$\bar{1}$	$\bar{1}$	A_g	{BDI}	0	0	$\{\}$
$\bar{1}$	$\bar{1}$	A_u	{DIII}	$\mathbb{Z}$	0	$\{4\}$
$\bar{1}1'$	$\bar{1}$	A_g	{D_T}	0	0	$\{\}$
$\bar{1}1'$	$\bar{1}$	A_u	{DIII^2}	$\mathbb{Z}^{\times 2}$	1	$\{4\}$
$\vdots$						
$m\bar{3}m'$	$m\bar{3}$	A_g	{D_T^2,DIII}	$\mathbb{Z}$	0	$\{\}$
$m\bar{3}m'$	$m\bar{3}$	E_g	{D_T^2,DIII}	$\mathbb{Z}$	0	$\{\}$
$m\bar{3}m'$	$m\bar{3}$	A_u	{DIII^5}	$\mathbb{Z}^{\times 5}$	3	$\{\}$
$m\bar{3}m'$	$m\bar{3}$	E_u	{DIII^5}	$\mathbb{Z}^{\times 5}$	3	$\{\}$
$m'\bar{3}'m'$	432	A_1	{D^{10}}	0	0	$\{\}$
$m'\bar{3}'m'$	432	A_2	{D^2,A_C}	0	0	$\{\}$

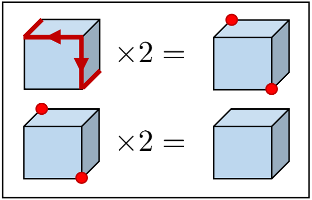
Ex: SCs with TRS and inversion symmetry ($\bar{1}1'$)

- Even parity SCs (A_g rep) $\Rightarrow K/K''' = 0$.
  - No surface state.
- Odd parity SCs (A_u rep) $\Rightarrow K/K''' = \mathbb{Z} \times \mathbb{Z}_4$.
  - $\mathbb{Z}$: $2d$ Majorana-Weyl surface states.
  - $\mathbb{Z}_4$: generated by the helical henge Majorana state. Doubling it yields to $0d$ Majorana bound state.

$\mathbb{Z}$



$\mathbb{Z}_4$



Summary

- Using the Cornfeld-Chapman's trick, we completed the classification of topological insulators/superconductors with point group symmetry.
- By identifying the atomic insulators at the point group center and dD Dirac Hamiltonians with hedgehog-mass potential with a unit winding number, one can compute the group $K^{(d)}$ of dth-order TIs/TSCs from the irreducible character.
- We presented the complete list of the effective AZ classes for insulators/superconductors with 122 magnetic point group and their surface states.

Wigner criterion

- Let α be an irrep of G_0 with the factor system $\tilde{z}_{g,h}$.
- The TRS-type operator $\hat{a}$ acts on the representation vector space V of the irrep α in three ways.
- Let $|i\rangle$ be the basis of the representation vector space V, that is

$$\hat{g}\,|i\rangle = |j\rangle\,[\tilde{D}_\alpha(g)]_{ji},$$

with $D_\alpha(g)$ the representation matrix.
- We want to consider how the TRS-type operator $\hat{a}$ acts on V, which can be checked by looking the formal basis $\hat{a}\,|i\rangle$.
- The irrep $a(\alpha)$ mapped by $\hat{a}$ has the following representation matrices

$$\hat{g}(\hat{a}\,|i\rangle) = (\hat{a}\,|j\rangle)[\tilde{D}_{a(\alpha)}(g)]_{ji}, \qquad \tilde{D}_{a(\alpha)}(g) = \frac{\tilde{z}_{g,a}}{\tilde{z}_{a,a^{-1}ga}}\tilde{D}_\alpha(a^{-1}ga)^*.$$

- $a(\alpha)$ is unitary equivalent to α or not, which can be checked by the orthogonality relation of the irreducible character $\tilde{\chi}_\alpha(g) = \mathrm{Tr}\tilde{D}_\alpha(g)$.

$$O^T_{\alpha\beta} := (a(\alpha), \beta) = \frac{1}{|G_0|}\sum_{g\in G_0}\left[\frac{\tilde{z}_{g,a}}{\tilde{z}_{a,a^{-1}ga}}\tilde{\chi}_\alpha(a^{-1}ga)^*\right]^*\tilde{\chi}_\beta(g) \in \{0,1\}.$$

- If $O^T_{\alpha\alpha} = 0$, $\hat{a}$ does not preserve the irrep α, and transforms α to another irrep $\beta = a(\alpha)$ satisfying $O^T_{\alpha\beta} = 1$.
- When $O^T_{\alpha\alpha} = 1$, the TRS-type operator $\hat{a}$ preserves the irrep α, but there still remain two situations: $\hat{a}$ produces the Kramers degeneracy or not, which can be checked by the Wigner criterion

$$W^T_\alpha := \frac{1}{|G_0|} \sum_{g \in G_0} \tilde{z}_{ag,ag} \tilde{\chi}_\alpha((ag)^2) \in \{0, \pm 1\}.$$

- We can see

$$\begin{array}{lcl} W^T_\alpha = 1 & \Rightarrow & a(\alpha) = \alpha \text{ and } \hat{a} \text{ is non-Kramers (class AI)}, \\ W^T_\alpha = -1 & \Rightarrow & a(\alpha) = \alpha \text{ and } \hat{a} \text{ is Kramers (class AII)}, \\ W^T_\alpha = 0 & \Rightarrow & a(\alpha) \neq \alpha. \end{array}$$

- Therefore, the Wigner criterion W^T_α alone gives us how $\hat{a}$ acts on the irrep α.

(The detail)

- If $a(\alpha) = \alpha$, there exists a unitary matrix U such that

$$\tilde{D}_{a(\alpha)}(g) = \frac{\tilde{z}_{g,a}}{\tilde{z}_{a,a^{-1}ga}} [\tilde{D}_\alpha(a^{-1}ga)]^*_{ji} = U^\dagger \tilde{D}_\alpha(g) U, \qquad g \in G_0.$$

- The matrix U behaves as a matrix representation of a.
- Form the Schor's lemma, one can show that $UU^* = \xi \tilde{D}_\alpha(a^2)$ with ξ a $U(1)$ phase and $\xi / z_{a,a} \in \{\pm 1\}$.
- Introduce a new basis $\widetilde{|i\rangle} = (\hat{a}\,|j\rangle) U^\dagger_{ji}$ that obeys the same matrix rep $\hat{g}\widetilde{|i\rangle} = \widetilde{|j\rangle}[\tilde{D}_\alpha(g)]_{ji}$.
- Taking the same transformation twice yields

$$\widetilde{\widetilde{|i\rangle}} = \xi / z_{a,a}\,|i\rangle\,.$$

- Therefore,

$$\begin{array}{lcl} \xi / z_{a,a} = 1 & \Rightarrow & \hat{a} \text{ is non-Kramers (class AI)} \\ \xi / z_{a,a} = -1 & \Rightarrow & \hat{a} \text{ is Kramers (class AII)} \end{array}$$

- One can show

$$W^T_\alpha = \begin{cases} \xi / z_{a,a} & (\hat{a}\,|i\rangle \text{ is unitary equivalent to } |i\rangle), \\ 0 & (\hat{a}\,|i\rangle \text{ is unitary inequivalent to } |i\rangle). \end{cases}$$

- In the same way, we introduce the Wigner criterion for the PHS-type operator $\hat{b}$ by

$$W_\alpha^C = \frac{1}{|G_0|} \sum_{g \in G_0} \tilde{z}_{bg,bg} \tilde{\chi}_\alpha((bg)^2) \in \{0, \pm 1\},$$

and we have

$$\begin{aligned} W_\alpha^C = 1 \quad &\Rightarrow \quad b(\alpha) = \alpha, \text{ and } \hat{b} \text{ behaves as class D PHS,} \\ W_\alpha^C = -1 \quad &\Rightarrow \quad a(\alpha) = \alpha, \text{ and } \hat{b} \text{ behaves as class C PHS,} \\ W_\alpha^C = 0 \quad &\Rightarrow \quad b(\alpha) \neq \alpha. \end{aligned}$$

- For the chiral-type operator $\widehat{ab}$, we ask if the mapped irrep $ab(\alpha)$ is unitary equivalent to α or not, which can be checked by the orthogonal test

$$O_{\alpha\alpha}^\Gamma = \frac{1}{|G_0|} \sum_{g \in G_0} \left[\frac{\tilde{z}_{g,ab}}{\tilde{z}_{ab,(ab)^{-1}gab}} \tilde{\chi}_\alpha((ab)^{-1}gab) \right]^* \tilde{\chi}_\alpha(g) \in \{0, 1\}.$$

We have

$$\begin{aligned} O_{\alpha\alpha}^\Gamma = 1 \quad &\Rightarrow \quad ab(\alpha) = \alpha, \text{ and } \widehat{ab} \text{ behaves as chiral symmetry,} \\ O_{\alpha\alpha}^\Gamma = 0 \quad &\Rightarrow \quad ab(\alpha) \neq \alpha. \end{aligned}$$

Application I. $3d$ insulators with magnetic point group symmetry

- There are 122 crystallographic magnetic point groups in $3d$.
- Let G be a magnetic point group equipped with the data $(O_g, \phi_g, z_{g,h})$. $(c_g \equiv 1.)$
- The factor system is given as

$$z_{g,h} = \begin{cases} 1 & \text{(spinless)} \\ (-1)^{\frac{1-\phi_g}{2}\frac{1-\phi_h}{2}} & \text{(spinful)} \end{cases}$$

- We get the complete list of the effective AZ classes for 122 magnetic point groups. [KS]
- Spinful systems:

MPG	EAZ	$K_0^G(\mathbb{R}^3)$	$K_{-1}^G(\mathbb{R}^3)$	$K_{-2}^G(\mathbb{R}^3)$	$\cdots$
1	{A}	0	$\mathbb{Z}$	0	
$11'$	{AII}	$\mathbb{Z}_2$	$\mathbb{Z}$	0	
$\bar{1}$	{AIII}	$\mathbb{Z}$	0	$\mathbb{Z}$	
$\bar{1}1'$	{DIII}	$\mathbb{Z}$	0	0	
$\bar{1}'$	{D}	0	0	0	
$\vdots$					
$m\bar{3}m'$	{DIII^4}	$\mathbb{Z}^{\times 4}$	0	0	
$m'\bar{3}m'$	{D^5}	0	0	0	