

**Topological Material Search via
Symmetry Indicator and Filling Anomaly**

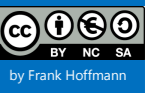
+

Revisiting criteria for topological phases

Haruki Watanabe
University of Tokyo

Variety of materials

230 The Space Group List Project



BY NC SA
by Frank Hoffmann

PERIODIC TABLE OF ELEMENTS

1 H Hydrogen Nonmetal																	2 He Helium Noble Gas	
3 Li Lithium Alkali Metal	4 Be Beryllium Alkaline Earth Metal																	10 Ne Neon Noble Gas
11 Na Sodium Alkali Metal	12 Mg Magnesium Alkaline Earth Metal																	18 Ar Argon Noble Gas
19 K Potassium Alkali Metal	20 Ca Calcium Alkaline Earth Metal	21 Sc Scandium Transition Metal	22 Ti Titanium Transition Metal	23 V Vanadium Transition Metal	24 Cr Chromium Transition Metal	25 Mn Manganese Transition Metal	26 Fe Iron Transition Metal	27 Co Cobalt Transition Metal	28 Ni Nickel Transition Metal	29 Cu Copper Transition Metal	30 Zn Zinc Transition Metal	31 Ga Gallium Post-Transition Metal	32 Ge Germanium Metalloid	33 As Arsenic Metalloid	34 Se Selenium Nonmetal	35 Br Bromine Halogen	36 Kr Krypton Noble Gas	
37 Rb Rubidium Alkali Metal	38 Sr Strontium Alkaline Earth Metal	39 Y Yttrium Transition Metal	40 Zr Zirconium Transition Metal	41 Nb Niobium Transition Metal	42 Mo Molybdenum Transition Metal	43 Tc Technetium Transition Metal	44 Ru Ruthenium Transition Metal	45 Rh Rhodium Transition Metal	46 Pd Palladium Transition Metal	47 Ag Silver Transition Metal	48 Cd Cadmium Transition Metal	49 In Indium Post-Transition Metal	50 Sn Tin Post-Transition Metal	51 Sb Antimony Metalloid	52 Te Tellurium Metalloid	53 I Iodine Halogen	54 Xe Xenon Noble Gas	
55 Cs Cesium Alkali Metal	56 Ba Barium Alkaline Earth Metal		72 Hf Hafnium Transition Metal	73 Ta Tantalum Transition Metal	74 W Tungsten Transition Metal	75 Re Rhenium Transition Metal	76 Os Osmium Transition Metal	77 Ir Iridium Transition Metal	78 Pt Platinum Transition Metal	79 Au Gold Transition Metal	80 Hg Mercury Transition Metal	81 Tl Thallium Post-Transition Metal	82 Pb Lead Post-Transition Metal	83 Bi Bismuth Post-Transition Metal	84 Po Polonium Metalloid	85 At Astatine Halogen	86 Rn Radon Noble Gas	
87 Fr Francium Alkali Metal	88 Ra Radium Alkaline Earth Metal		104 Rf Rutherfordium Transition Metal	105 Db Dubnium Transition Metal	106 Sg Seaborgium Transition Metal	107 Bh Bohrium Transition Metal	108 Hs Hassium Transition Metal	109 Mt Meitnerium Transition Metal	110 Ds Darmstadtium Transition Metal	111 Rg Roentgenium Transition Metal	112 Cn Copernicium Transition Metal	113 Nh Nihonium Post-Transition Metal	114 Fl Flerovium Post-Transition Metal	115 Mc Moscovium Post-Transition Metal	116 Lv Livermorium Post-Transition Metal	117 Ts Tennessine Halogen	118 Og Oganesson Noble Gas	
			57 La Lanthanum Lanthanide	58 Ce Cerium Lanthanide	59 Pr Praseodymium Lanthanide	60 Nd Neodymium Lanthanide	61 Pm Promethium Lanthanide	62 Sm Samarium Lanthanide	63 Eu Europium Lanthanide	64 Gd Gadolinium Lanthanide	65 Tb Terbium Lanthanide	66 Dy Dysprosium Lanthanide	67 Ho Holmium Lanthanide	68 Er Erbium Lanthanide	69 Tm Thulium Lanthanide	70 Yb Ytterbium Lanthanide	71 Lu Lutetium Lanthanide	
			89 Ac Actinium Actinide	90 Th Thorium Actinide	91 Pa Protactinium Actinide	92 U Uranium Actinide	93 Np Neptunium Actinide	94 Pu Plutonium Actinide	95 Am Americium Actinide	96 Cm Curium Actinide	97 Bk Berkelium Actinide	98 Cf Californium Actinide	99 Es Einsteinium Actinide	100 Fm Fermium Actinide	101 Md Mendelevium Actinide	102 No Nobelium Actinide	103 Lr Lawrencium Actinide	



1
H
Hydrogen
Nonmetal

Atomic Number
Symbol
Name
Chemical Group Block

Diagram illustrating the 230 space groups, showing various crystal structures and their corresponding space group symbols and numbers.

From <https://pubchem.ncbi.nlm.nih.gov/>

Unified classification?

More information at crystalsymmetry.wordpress.com

Classification based on low-E spectrum

S=1
Heisenberg
model

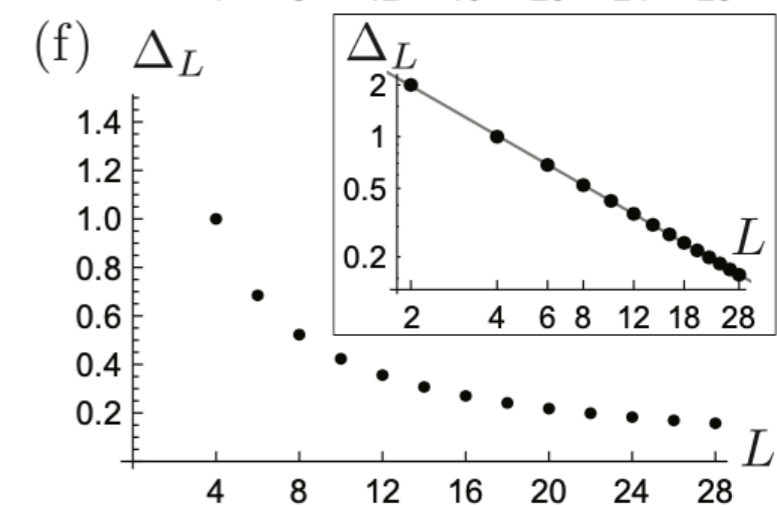
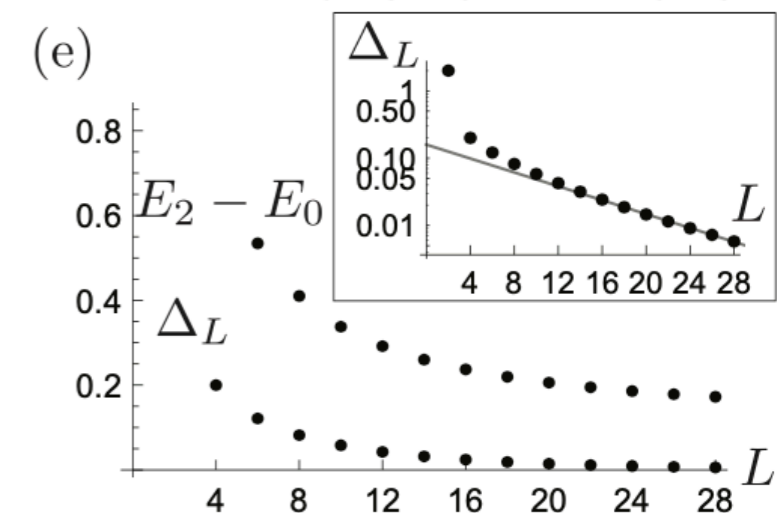
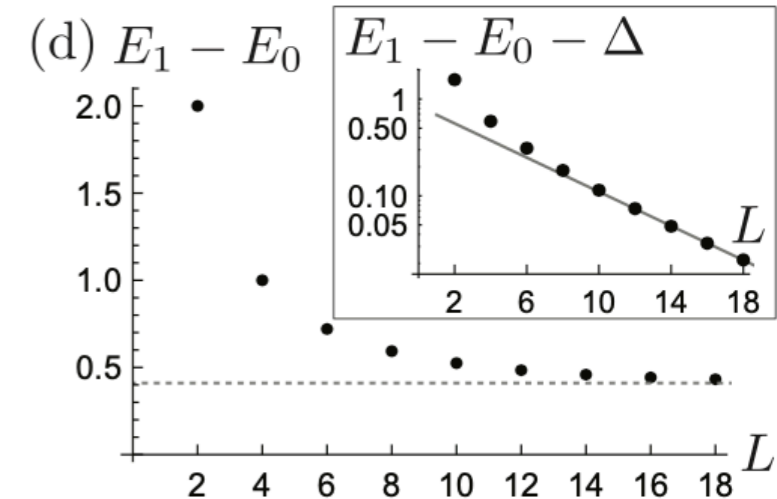
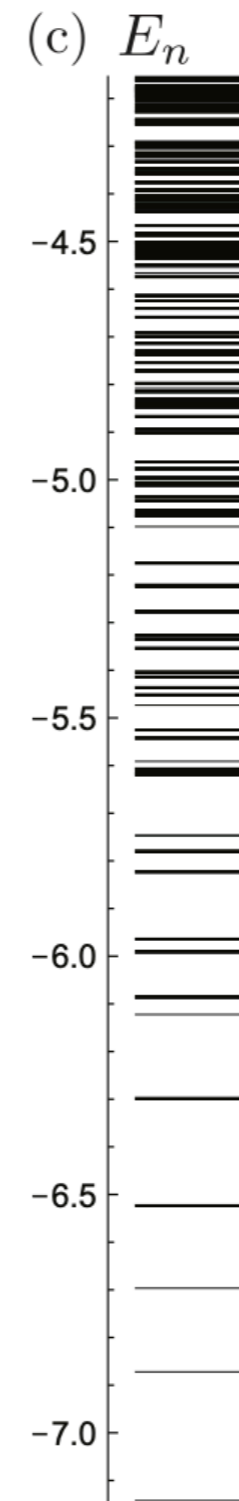
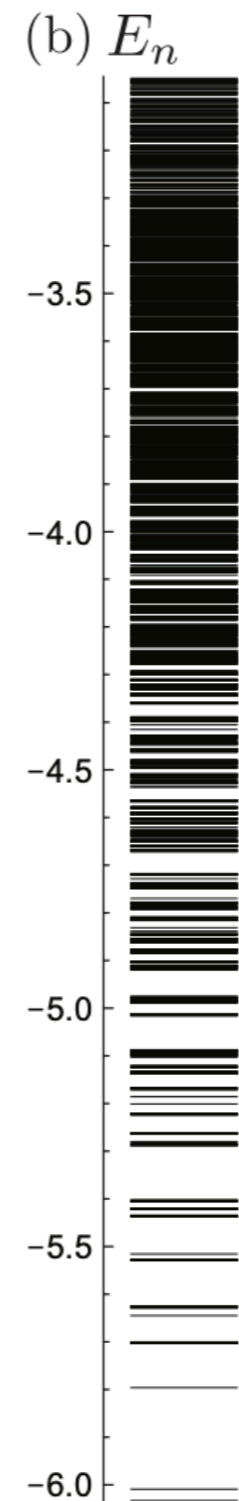
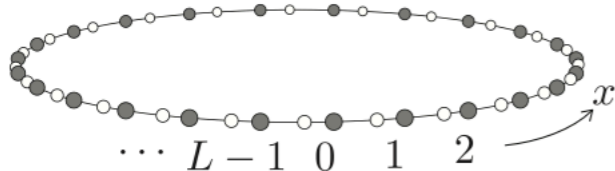
S=1/2
MG
model

S=1/2
Heisenberg
model

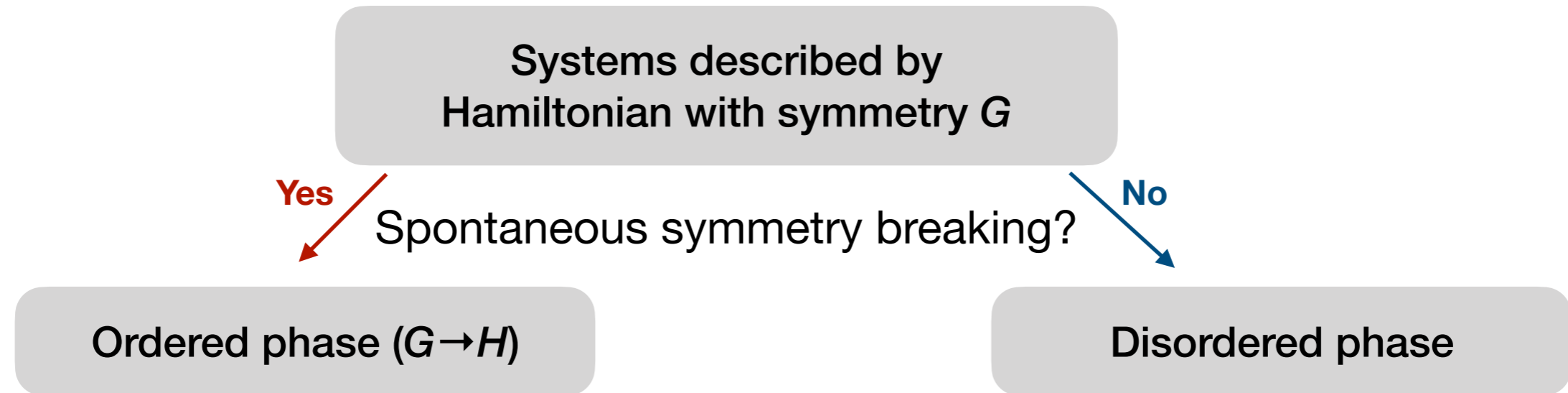
$$\hat{H}_{\text{Heisenberg}} := J \sum_{m=0}^{L-1} \hat{\mathbf{s}}_{m+1} \cdot \hat{\mathbf{s}}_m$$

$$\hat{H}_{\text{MG}} = \hat{H}_{\text{Heisenberg}} + \frac{J}{2} \sum_{m=0}^{L-1} \hat{\mathbf{s}}_{m+2} \cdot \hat{\mathbf{s}}_m$$

Periodic boundary condition



Classification of $T=0$ phases



Classification of $T=0$ phases

Systems described by
Hamiltonian with symmetry G

Yes
Spontaneous symmetry breaking?

No

Ordered phase ($G \rightarrow H$)

Disordered phase

Yes
Excitation gap?

No

Yes
Excitation gap?

No

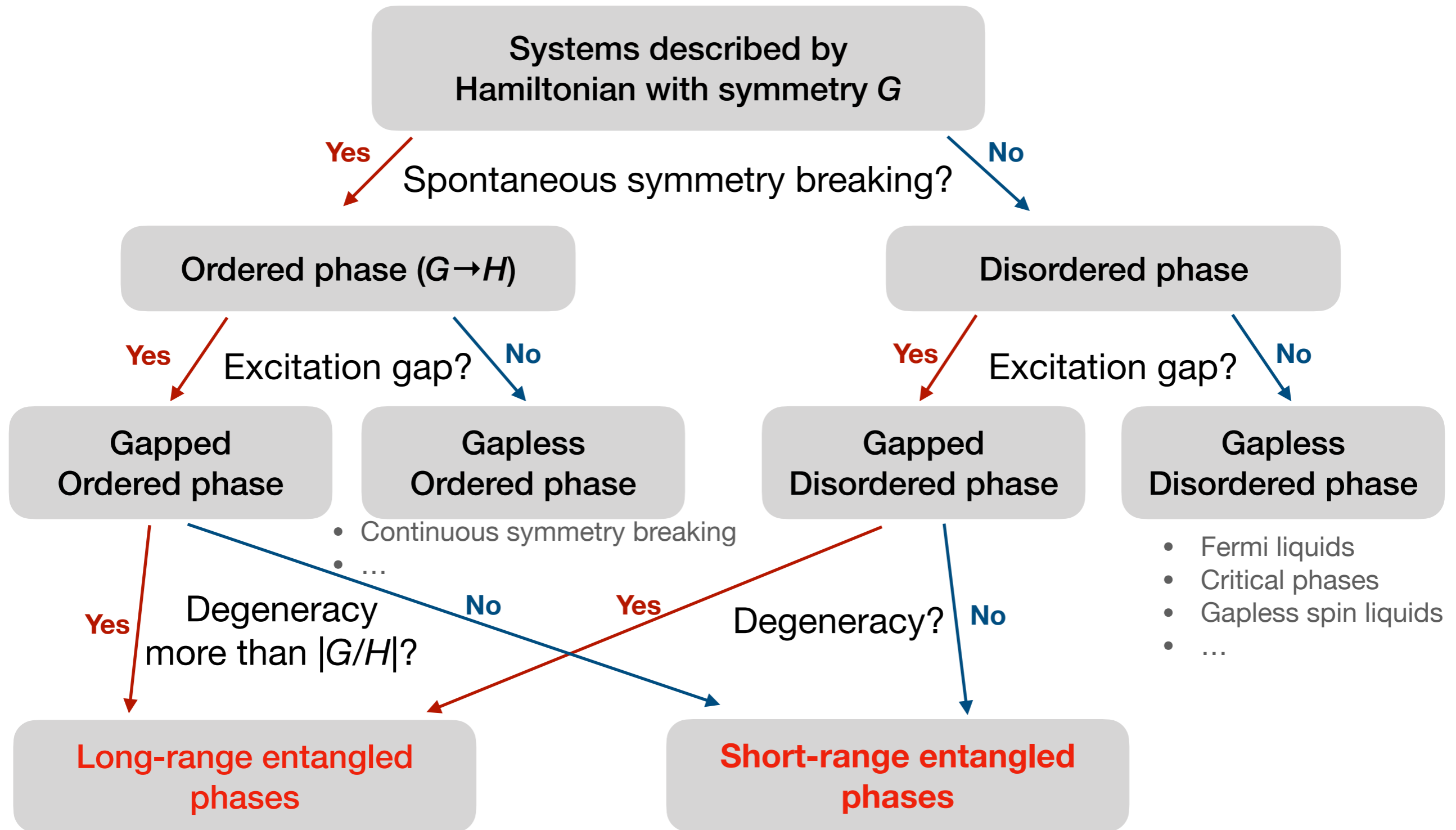
Gapped
Ordered phase

Gapless
Ordered phase

Gapped
Disordered phase

Gapless
Disordered phase

Classification of $T=0$ phases

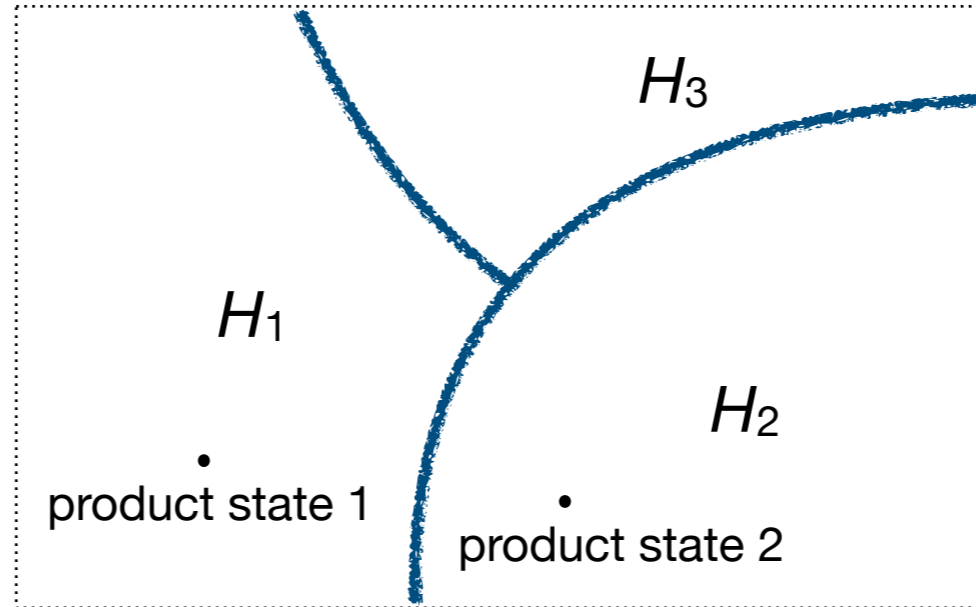


Topologically ordered phases (FQHE, QSL, ...)
Fracton topological orders

- Trivial phases
- Topological insulators
- Symmetry-protected topological phases

Features of short-range entangled phases

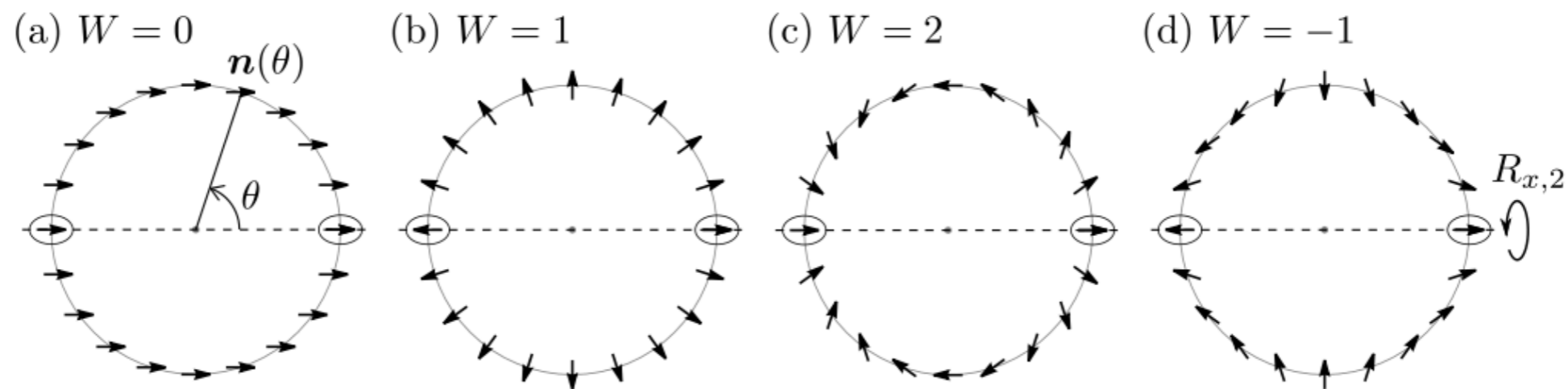
- Unique ground state with excitation gap Δ .
- With symmetry G , $H_1 \sim H_2$ if H_1 and H_2 are connected without breaking symmetry G or closing gap Δ (with or without ancillas)



- *Trivial phases* are connected to a real-space **product state**.
- *Topological phases* contain irremovable **quantum entanglement**.

Symmetry indicators

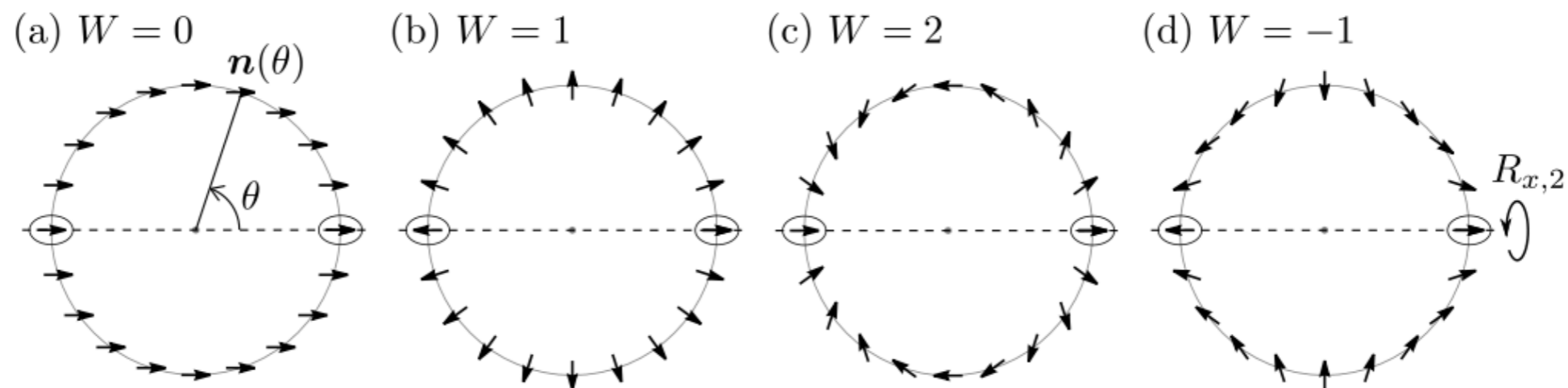
- Quick & partial diagnosis of topology
- Example: Winding number of in-plane spins on a ring



$$W[\mathbf{n}] := \int_0^{2\pi} \frac{d\theta}{2\pi} [\mathbf{n}(\theta) \times \partial_\theta \mathbf{n}(\theta)]_z$$

Symmetry indicators

- Quick & partial diagnosis of topology
- Example: Winding number of in-plane spins on a ring



$$W[\mathbf{n}] := \int_0^{2\pi} \frac{d\theta}{2\pi} [\mathbf{n}(\theta) \times \partial_\theta \mathbf{n}(\theta)]_z$$

- Winding number can be partially deduced by representation at symmetric points

$$(-1)^{W[\mathbf{n}]} = \mathbf{n}(\pi) \cdot \mathbf{n}(0)$$

Lieb-Schultz-Mattis theorem

Necessary condition for **unique ground state** with **excitation gap**.

Violation implies degeneracy or gapless excitations.

- In U(1) symmetric systems with translation symmetry, filling ν (= charge per unit cell) must be integral.

Examples:

- Band insulators with fractional filling are gapless.
- Fractional quantum Hall states has topological degeneracy.

- In systems with discrete symmetry group G , all projective representations must be removable.

Examples:

- $S=1/2$ Heisenberg model with $Z_2 \times Z_2$ and translation is gapless / degeneracy
- Toric code (with inversion) has topological degeneracy.



Violation of LSM conditions in symmetric gapped phases

→ Topological degeneracy on torus

Today's talk

- (brief) **Symmetry indicators for superconductors**
- **Revisiting criteria for topological phases**
 - **Symmetry indicators** → topological (crystalline) insulators
The converse is certainly not true.
 - Chern number $C=2n$ with C_2 rotation
 - fragile topology
 - ...
 - **Product states** → not interesting.
A counter example.
 - **Topological degeneracy on torus** → topological orders
Is the converse true?

Symmetry Indicators for topological superconductors



Seishiro Ono
U Tokyo

Getting PhD soon!

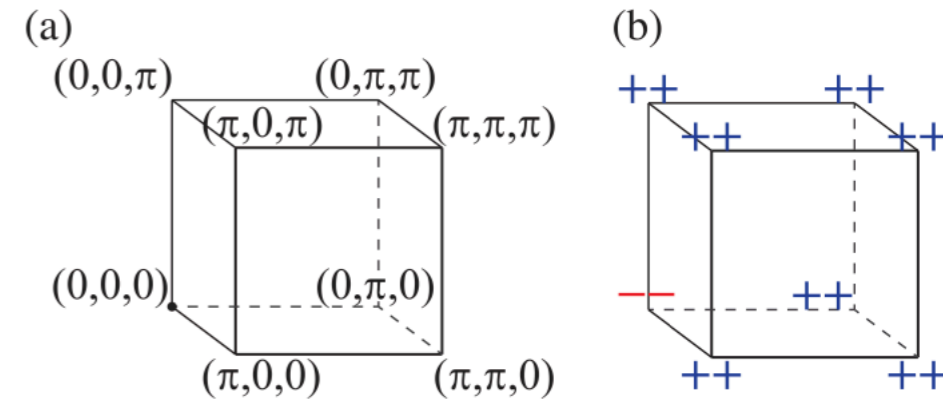
F. Tang*, S. Ono*, X. Wan, [HW](#), *High-Throughput Investigations of Topological and Nodal Superconductors*, PRL (2022). [Editors' Suggestion](#)

Symmetry indicators for topological insulators

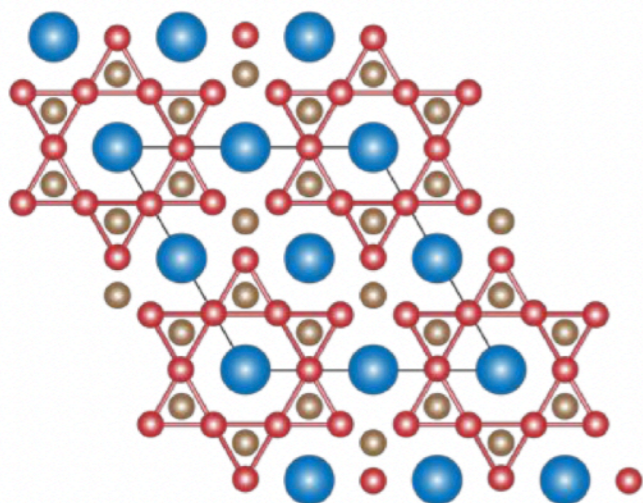
- Topological properties via representations of crystalline symmetries e.g. Fu-Kane formula for Z2 index via inversion parities

- All (magnetic) space groups & Various topology

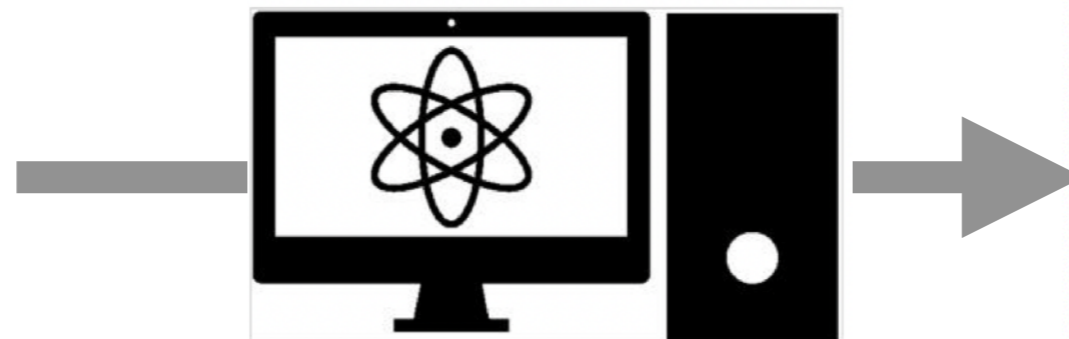
- H. C. Po, A. Vishwanath, [HW](#), Nat. Commun. (2017)
- B. Bradlyn, L. Elcoro, J. Cano, M. G. Vergniory, Z. Wang, C. Felser, M. I. Aroyo & B. A. Bernevig, Nature (2017)
- J. Kruthoff, J. de Boer, J. van Wezel, C. L. Kane, and R.-J. Slager, PRX (2017)
- Z. Song, T. Zhang, Z. Fang, C. Fang, Nat Comm (2018)
- ...



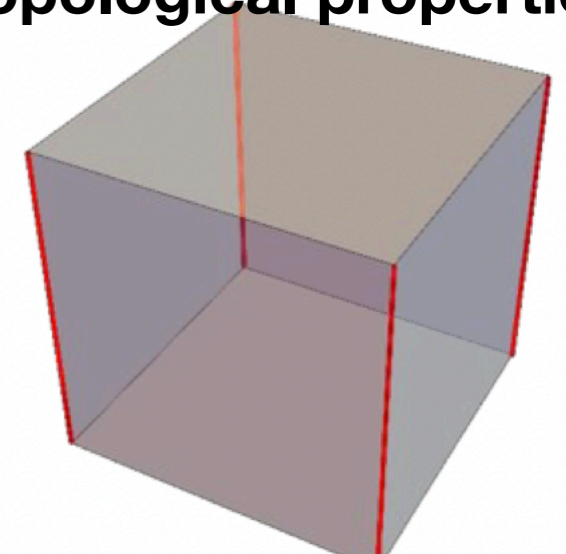
Input: Material data



DFT calculations



**Output:
Topological properties**



Comprehensive search for topological materials using symmetry indicators

Feng Tang^{1,2}, Hoi Chun Po^{3,4}, Ashvin Vishwanath³ & Xiangang Wan^{1,2*}

Catalogue of topological electronic materials

Tiantian Zhang^{1,2,9}, Yi Jiang^{1,2,9}, Zhida Song^{1,2,9}, He Huang³, Yuqing He^{2,3}, Zhong Fang^{1,4}, Hongming Weng^{1,5,6,7,8*} & Chen Fang^{1,4,6,7,8*}

Over the past decade, topological materials have attracted much attention for their unconventional surface states, proposed topological properties, as well as their potential for quantum interference from trivial states. However, the discovery of suitable nonmagnetic topological materials, either with or without noticeable full bandgaps, has been limited. We list 692 topological semiconductors and open up the possibility

Topological electronic materials such as Dirac and Weyl semimetals have a linear response in the bulk, as well as many other interesting properties of applied interest, with the potential for quantum computing. However, their discovery has so far been hindered by the difficulty of identifying new materials. This requires both experience with materials and an efficient and fully automated algorithm for searching through large databases of materials. Our algorithm is based on topological quantum chemistry, which is applied to occupied bands and topological invariants to identify new topological materials and find that as many as 8,056 of them exist in the Inorganic Crystal Structure Database with an interactive user interface.

A complete catalogue of high-quality topological materials

M. G. Vergniory^{1,2,3,11}, L. Elcoro^{4,11}, Claudia Felser⁵, Nicolas Regnault⁶, B. Andrei Bernevig^{7,8,9*} & Zhijun Wang^{7,10*}

Using a recently developed formalism called topological quantum chemistry, we perform a high-throughput search of 'high-quality' materials (for which the atomic positions and structure have been measured very accurately) in the Inorganic Crystal Structure Database in order to identify new topological phases. We develop codes to compute all

78 topological materials, including some new materials. Our source code that

Topological Materials Database

- Total Materials: 38184
- Topological Insulators: 6109
- Semi-Metals: 13985

NAVIGATION

- Search
- Predict
- About

SETTINGS

UI Mode:

Compound Contains: Only these elements Exclude - or - ICSD Number

[Show Advanced Search](#)

1 H																	2 He
3 Li	4 Be										5 B	6 C	7 N	8 O	9 F	10 Ne	
11 Na	12 Mg										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Ts	112 Og	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

Extension to topological superconductors?

- Symmetry indicator method itself needs to be modified (\mathbb{Z}_2 index in 0D)

AZ	0	1	2	3	4	5	6	7
A	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0
AIII	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}
AI	\mathbb{Z}	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2
BDI	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2
D	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}	0
DIII	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}
AII	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0
CII	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0
C	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0
CI	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}

- **Pairing symmetry** (s-wave, p-wave, ...) becomes an additional data.

M. Geier, P. W. Brouwer, and L. Trifunovic, Symmetry-based indicators for topological Bogoliubov–de Gennes Hamiltonians, PRB (2020)

S. Ono, H. Chun Po, K. Shiozaki, \mathbb{Z}_2 -enriched symmetry indicators for topological superconductors in the 1651 magnetic space groups, PRR (2021)

Pairing symmetries

- Pairing symmetry

$$\hat{H} \simeq (\hat{c}_{\mathbf{k}}^\dagger \ \hat{c}_{-\mathbf{k}}) H_{\mathbf{k}}^{\text{BdG}} \begin{pmatrix} \hat{c}_{\mathbf{k}} \\ \hat{c}_{-\mathbf{k}}^\dagger \end{pmatrix}$$

$$U_{\mathbf{k}}(g) h_{\mathbf{k}} U_{\mathbf{k}}^\dagger(g) = h_{p_g \mathbf{k}},$$

$$U_{\mathbf{k}}(g) \Delta_{\mathbf{k}} U_{-\mathbf{k}}^T(g) = \chi_g \Delta_{p_g \mathbf{k}} \quad (\chi_g \in \text{U}(1)).$$

$$H_{\mathbf{k}}^{\text{BdG}} = \begin{pmatrix} h_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^\dagger & -h_{-\mathbf{k}}^* \end{pmatrix},$$

$$U_{\mathbf{k}}^{\text{BdG}}(g) = \begin{pmatrix} U_{\mathbf{k}}(g) & 0 \\ 0 & \chi_g U_{-\mathbf{k}}^*(g) \end{pmatrix},$$

$\chi_g = 1$: conventional

$\chi_g \neq 1$: unconventional

- Unconventional pairing symmetry is recipe for TSC.
- Symmetry indicators are all trivial for conventional pairing symmetries in time-reversal symmetric case.
- We investigate symmetry indicators for materials **for each** unconventional pairing symmetry.

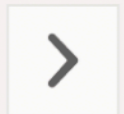
Editors' Suggestion Open Access

High-Throughput Investigations of Topological and Nodal Superconductors

Feng Tang, Seishiro Ono, Xiangang Wan, and Haruki Watanabe
Phys. Rev. Lett. **129**, 027001 – Published 6 July 2022



Article  PDF HTML Export Citation



ABSTRACT

The theory of symmetry indicators has enabled database searches for topological materials in normal conducting phases, which has led to several encyclopedic topological material databases. To date, such a database for topological superconductors is yet to be achieved because of the lack of information about pairing symmetries of realistic materials. In this Letter, sidestepping this issue, we tackle an alternative problem: the predictions of topological and nodal superconductivity in materials for each single-valued representation of point groups. Based on recently developed symmetry indicators for superconductors, we provide comprehensive mappings from pairing symmetries to the

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Periodic Table Compound Doping

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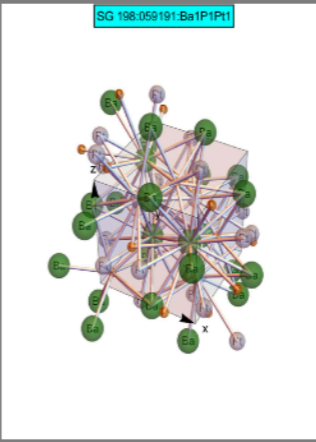
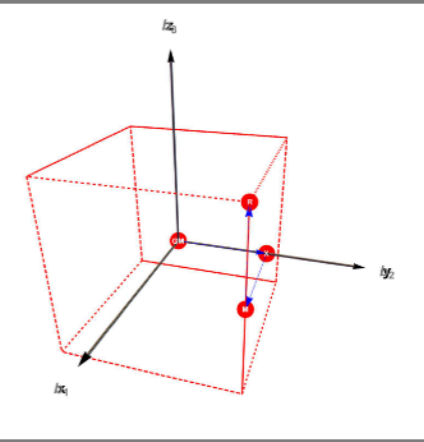
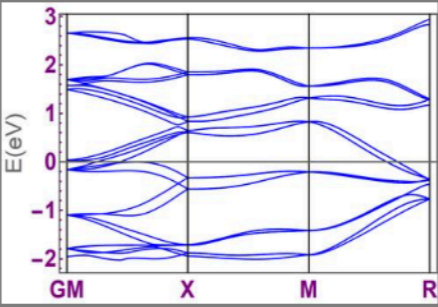
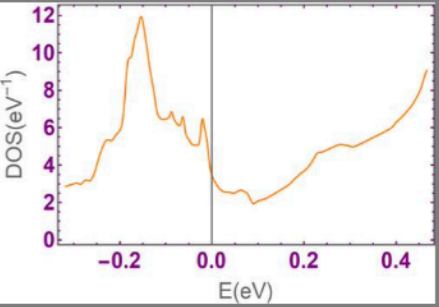
Database of topological and nodal superconductors

P Ba Pt Space Group number ICSD number

Space Group number	ICSD number	Chemical formula
1. 198	059191	Ba1P1Pt1
2. 14	062520	Ba1P3Pt2

Ba1P1Pt1

SG 198.059191.Ba1P1Pt1

Periodic Table Compound Doping

ν	Γ_5	Γ_6	Γ_7	X_2	X_3	X_4	X_5	M_5	R_4	R_5	R_6	R_7
180	31	30	30	45	45	45	45	90	14	16	16	46

2E
1E
A

Γ_5	Γ_6	Γ_7	X_2	X_3	X_4	X_5	M_5	R_4	R_5	R_6	R_7
1	0	-1	0	0	0	0	0	-2	0	2	0
C	A	A	A	A	A	A	D	A	A	D	D
Γ_6	Γ_7	Γ_5	X_2	X_3	X_4	X_5	M_5	R_5	R_6	R_4	R_7

Case I

? Γ -R[(0, 0, 0)-(1/2, 1/2, 1/2)](S)
? Γ -R[(0, 0, 0)-(1/2, 1/2, 1/2)](S)

Topological Supercon

User guide

For a given input file containing symmetry operations and characters of irreducible representations for each band, the program perform several procedures to diagnose nodes and topology.

The input files for normal conducting phases (i.e., without Fermi energy) are generated by external programs: [vasp2trace](#), [irvsp](#), and [qeirreps](#).

To generate input files for the superconducting phases, users should manually add the Fermi energy to the first line of the input. Please see [README.pdf](#) and [Sample.txt](#).

If you use this program in your work, please cite the following references:

S. Ono, H.C. Po*, H. Watanabe*, Sci. Adv. 6, eaaz8367 (2020),
S. Ono, H.C. Po, K. Shiozaki, Phys. Rev. Research 3, 023086 (2021),
S. Ono, K. Shiozaki, arXiv:2102.07676,
F. Tang*, S. Ono*, X. Wan, H. Watanabe, arXiv:2106.11985.
(* equally contributed)

If you have any trouble, please contact [toposupercon\[at\]gmail.com](mailto:toposupercon[at]gmail.com).

We have confirmed the operation with Google Chrome [version 90.0.4430.93 (64bit)] browser and Microsoft Edge [version 90.0.818.51 (64bit)] browser under Windows10.

Upload your input .txt file

no file selected

Choose the conditions you consider

SC phase or normal phase?	<input type="radio"/> normal	<input checked="" type="radio"/> SC ($C^2 = +1$)	<input type="radio"/> SC ($C^2 = -1$)
TRS	<input checked="" type="radio"/> Yes	<input type="radio"/> No	
SOC	<input checked="" type="radio"/> Yes	<input type="radio"/> No	

Results

Choose the pairing symmetry you consider

B_u, B_g, A_u, A_g

[.irreps of PG](#)
[.irreps of SG](#)



Topological Supercon

Results

This material is Case II, whose entry of symmetry indicators is $\{1, 1, 2, 0\}$ in $\{2, 4, 4, 8\}$.
The vector n_{SC} is
 $n_{SC} = \{-3, 3, -3, 3\}, \{0, 0, 0, 0\}, \{-1, 1, -1, 1\}, \{0\}, \{0\}, \{0\}, \{2, -2, 2, -2\}, \{0\}$,
and the basis vectors are
 $\{1, -1, 1, -1\}, \{1, -1, 1, -1\}, \{1, -1, 1, -1\}, \{0\}, \{0\}, \{0\}, \{1, -1, 1, -1\}, \{0\}$
 $\{0, 0, 0, 0\}, \{-1, 1, -1, 1\}, \{0, 0, 0, 0\}, \{0\}, \{0\}, \{0\}, \{-1, 1, -1, 1\}, \{0\}$
 $\{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \{-1, 1, -1, 1\}, \{0\}, \{0\}, \{0\}, \{-1, 1, -1, 1\}, \{0\}$
 $\{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \{0\}, \{0\}, \{0\}, \{1, -1, 1, -1\}, \{0\}$



Topological superconductors with conventional pairing symmetries

- **Symmetry indicators** → topological (crystalline) insulators.
The converse is not true.
- Time-reversal & inversion symmetric superconductors
can be topological even with conventional pairing symmetry

S. Qin, C. Fang, F.-C. Zhang, J. Hu, Topological Superconductivity in an Extended s-Wave Superconductor and Its Implication to Iron-Based Superconductor, PRX (2022)

This study examined only a few examples

- The majority of SCs have conventional pairing symmetries
→ There might be TSCs in known materials
overlooked because they have conventional pairing symmetries.

Classification of topological superconductors with conventional pairing symmetries

K. Shiozaki, et al arXiv:1810.00801
Z. Song, et al, Sci. (2019)

K-theory type classification via
Real-space Atiyah-Hirzebruch spectral sequence (AHSS)
Also known as “topological crystals”

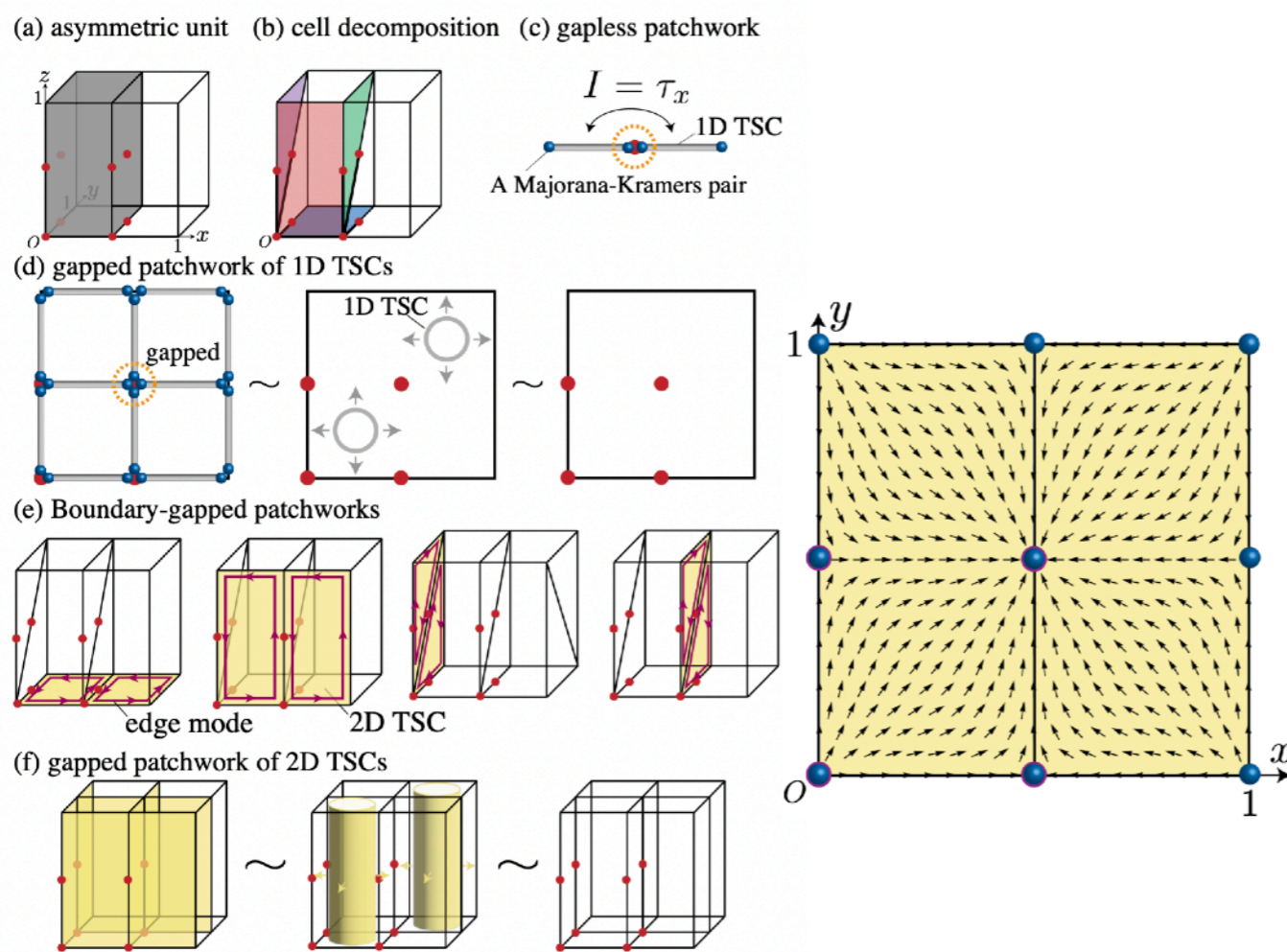


FIG. 1. Illustration of 3D patchworks in space group $P\bar{1}$. (a) A

TABLE XVIII: Classification table of topological phases in space groups.

Space group	pairing symmetry	$E_{3,-3}^\infty$	$E_{2,-2}^\infty$	$E_{1,-1}^\infty$	$\phi K_G^{(z,c)-n}(T^3)$
1	A	\mathbb{Z}	\mathbb{Z}_2^3	\mathbb{Z}_2^3	$\mathbb{Z}_2^6 \times \mathbb{Z}$
2	A_g	0	0	0	0
3	A	\mathbb{Z}	\mathbb{Z}_2^4	$\mathbb{Z}_2^3 \times \mathbb{Z}^4$??
4	A	\mathbb{Z}	\mathbb{Z}_2^3	\mathbb{Z}_2^3	??
5	A	\mathbb{Z}	\mathbb{Z}_2^3	$\mathbb{Z}_2^2 \times \mathbb{Z}^2$??
6	A'	0	\mathbb{Z}_2^2	$\mathbb{Z}_2 \times \mathbb{Z}^4$	$\mathbb{Z}_2 \times \mathbb{Z}^4$
7	A'	0	\mathbb{Z}_2^3	\mathbb{Z}_2^3	$\mathbb{Z}_2^4 \times \mathbb{Z}_4$
8	A'	0	\mathbb{Z}_2^2	$\mathbb{Z}_2 \times \mathbb{Z}^2$	$\mathbb{Z}_2^2 \times \mathbb{Z}^2$
9	A'	0	\mathbb{Z}_2^2	\mathbb{Z}_2^2	\mathbb{Z}_2^4
10	A_g	0	0	0	0
11	A_g	0	0	\mathbb{Z}^2	\mathbb{Z}^2
12	A_g	0	0	0	0
13	A_g	0	\mathbb{Z}_2	$\mathbb{Z}_2 \times \mathbb{Z}^2$	$\mathbb{Z}_2 \times \mathbb{Z}^2$
14	A_g	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}_2^2
15	A_g	0	\mathbb{Z}_2	\mathbb{Z}	\mathbb{Z}
16	A_1	\mathbb{Z}	\mathbb{Z}_2^5	\mathbb{Z}^{12}	??
17	A_1	\mathbb{Z}	\mathbb{Z}_2^4	$\mathbb{Z}_2^3 \times \mathbb{Z}^4$??
18	A_1	\mathbb{Z}	\mathbb{Z}_2^3	$\mathbb{Z}_2^2 \times \mathbb{Z}^2$??
19	A_1	\mathbb{Z}	\mathbb{Z}_2^2	\mathbb{Z}_2^2	??
20	A_1	\mathbb{Z}	\mathbb{Z}_2^3	$\mathbb{Z}_2^2 \times \mathbb{Z}^2$??
21	A_1	\mathbb{Z}	\mathbb{Z}_2^4	$\mathbb{Z}_2 \times \mathbb{Z}^7$??
22	A_1	\mathbb{Z}	\mathbb{Z}_2^4	$\mathbb{Z}_2 \times \mathbb{Z}^6$??
23	A_1	\mathbb{Z}	\mathbb{Z}_2^3	\mathbb{Z}^6	??
24	A_1	\mathbb{Z}	\mathbb{Z}_2^3	$\mathbb{Z}_2^2 \times \mathbb{Z}^3$??
25	A_1	0	\mathbb{Z}_2	\mathbb{Z}^4	\mathbb{Z}^4
26	A_1	0	\mathbb{Z}_2	$\mathbb{Z}_2 \times \mathbb{Z}^2$	$\mathbb{Z}_2 \times \mathbb{Z}^2$

S. Ono, K. Shiozaki, HW, arXiv:2206.02489

Please invite Ono-kun for the detailed talk!

2. Fractional corner charges in trivial insulators



Hoi Chun Po

The Hong Kong University
of Science and Technology



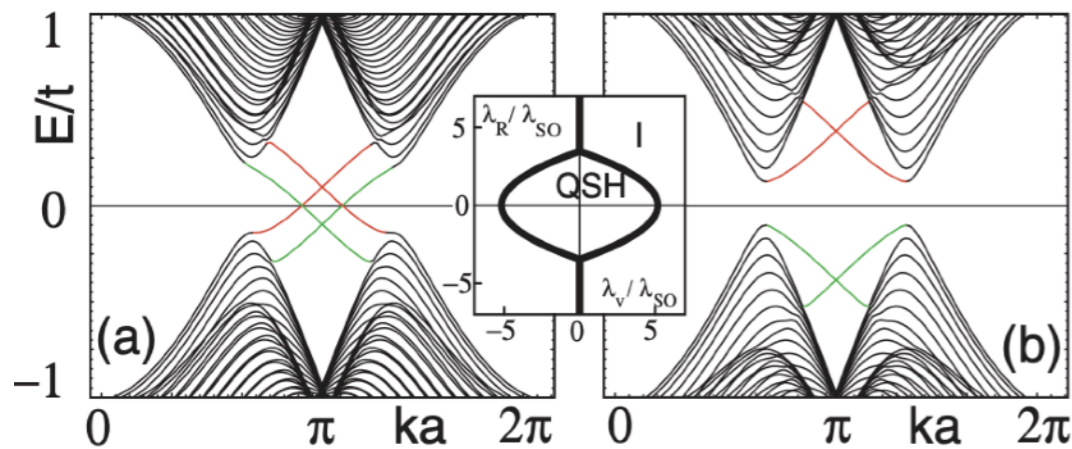
Seishiro Ono

U Tokyo

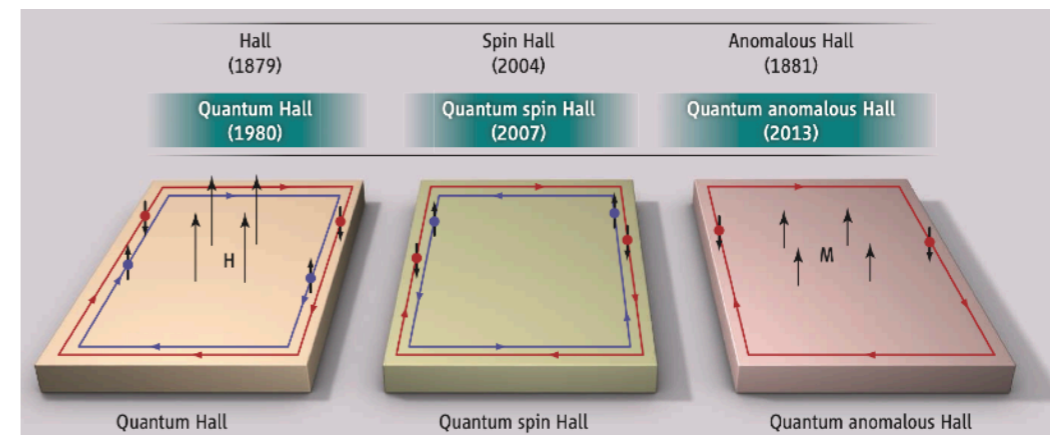
- [HW](#), S. Ono, Corner charge and bulk multipole moment in periodic systems, PRB (2020).
- [HW](#), H. C. Po, *Fractional Corner Charge of Sodium Chloride*, PRX (2021).

Bulk-boundary correspondence of topological phases

- 2D topological insulator

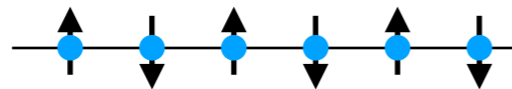


C. L. Kane and E. J. Mele, PRL (2005)



S. Oh, Science (2013)

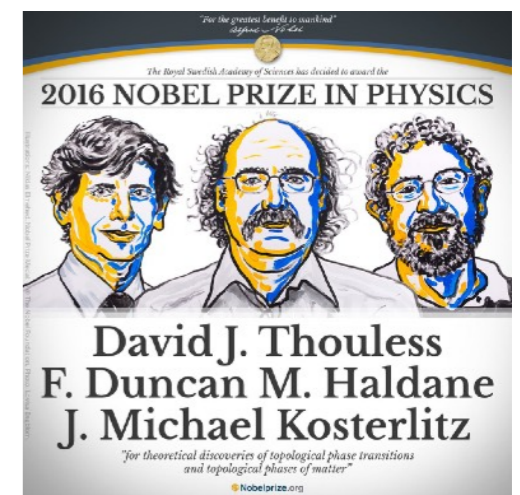
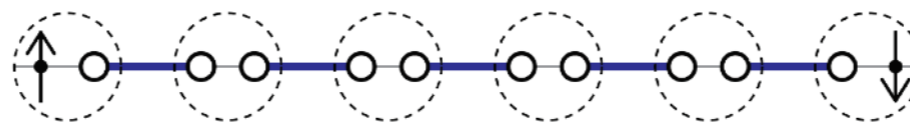
- Haldane phase



$S = 1$ Heisenberg model

$$\hat{H} = J \sum_n \hat{\mathbf{s}}_n \cdot \hat{\mathbf{s}}_{n+1}$$

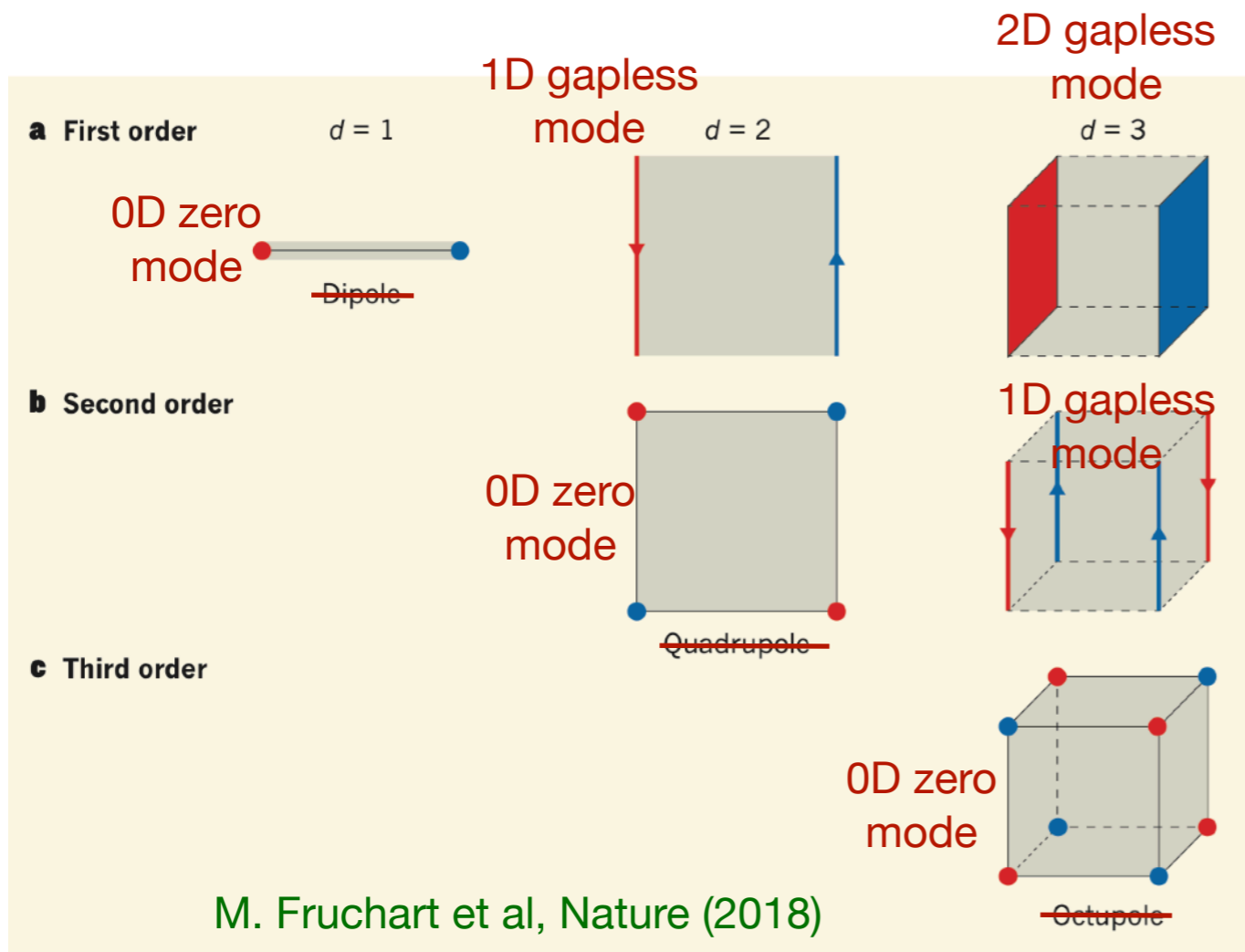
$S = 1/2$ edge spin



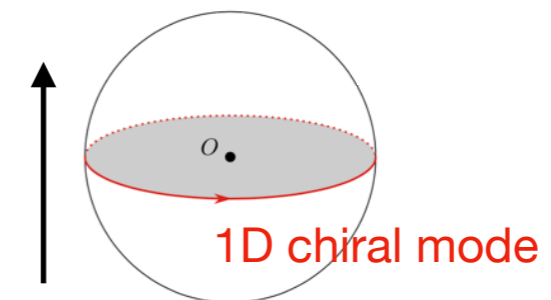
Bulk topology implies nontrivial boundary.

Boundary states(=degrees of freedom) / surface topological order

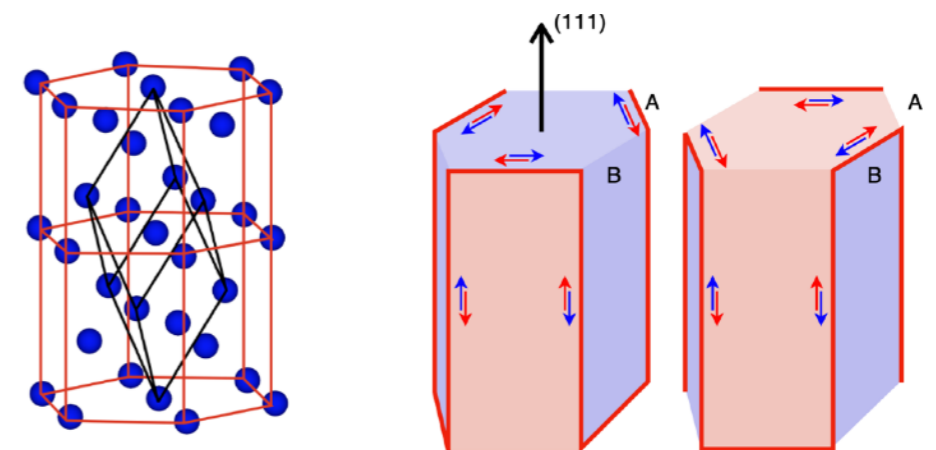
Bulk-boundary correspondence for higher-order topology



Inversion symmetric 3D topological insulator under magnetic field



Higher order topology in Bismuth

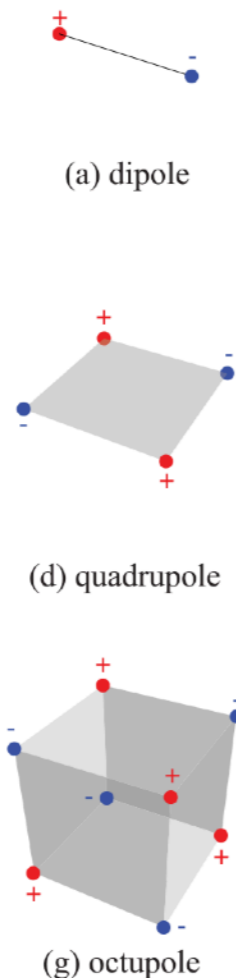


F. Schindler et al, Nature Physics (2018)
F. Schindler et al, Science Advances (2018)

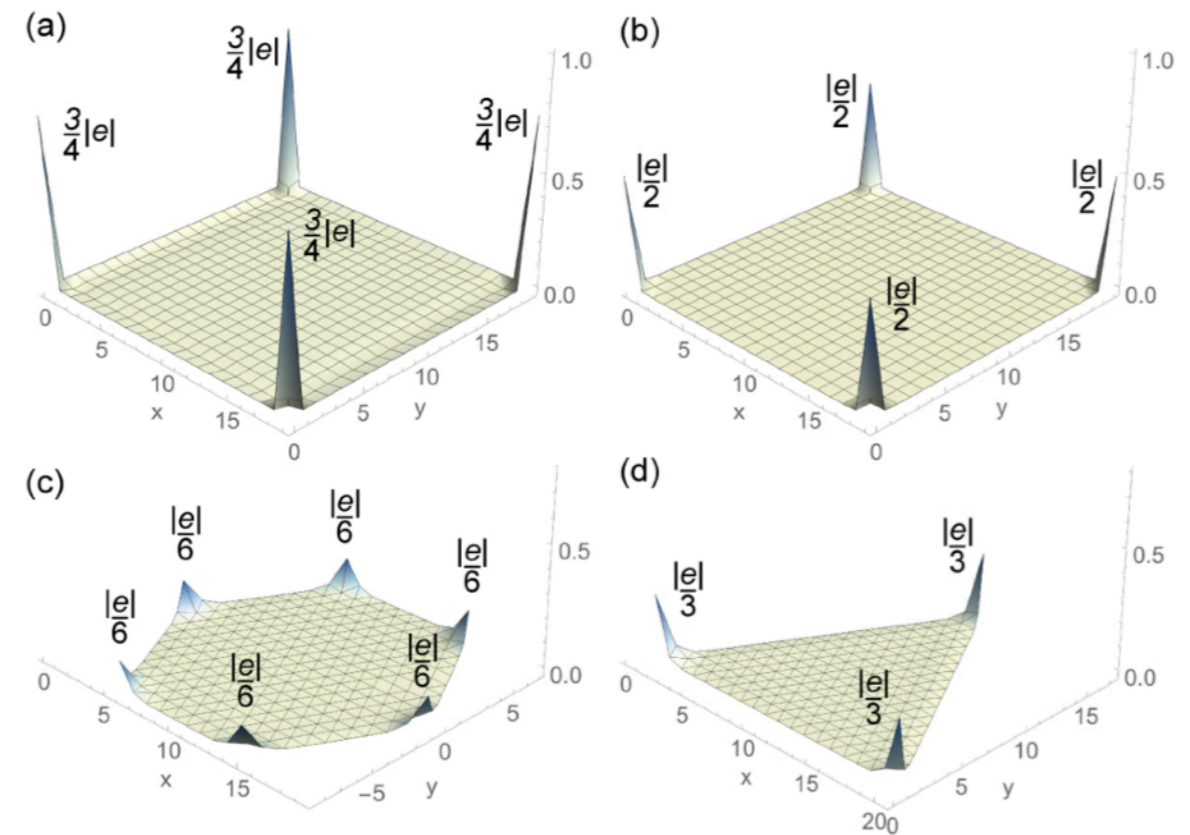
Boundary states can be localized to **corners** and **hinges** depending on the bulk topology.

Bulk-boundary correspondence of *trivial* insulators

- Even trivial insulators may have interesting signature on their boundary.
- No known material realization of fractional corner charge.



W. A. Benalcazar, B. A. Bernevig, T. L. Hughes,
Science (2017) / PRB (2017)



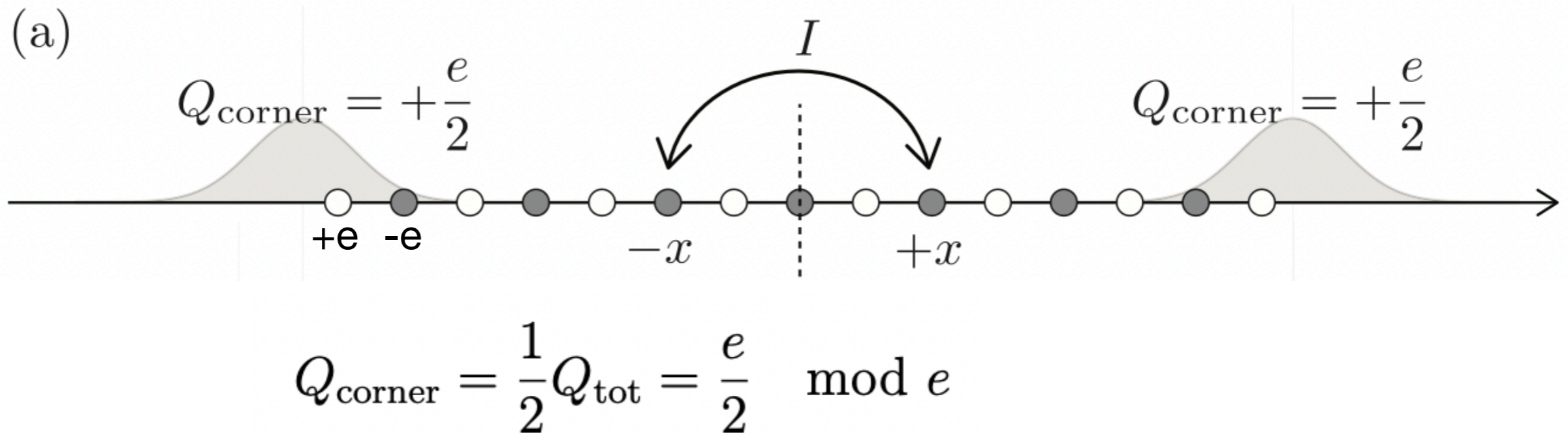
W. A. Benalcazar, T. Li, T. L. Hughes,
PRB (2019)

Charges are “frozen” i.e., *not* degrees of freedom

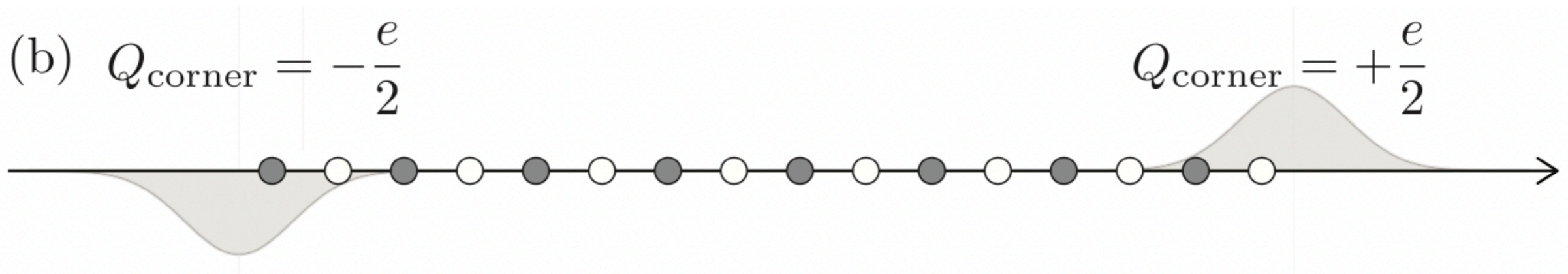
Filling anomaly

W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)

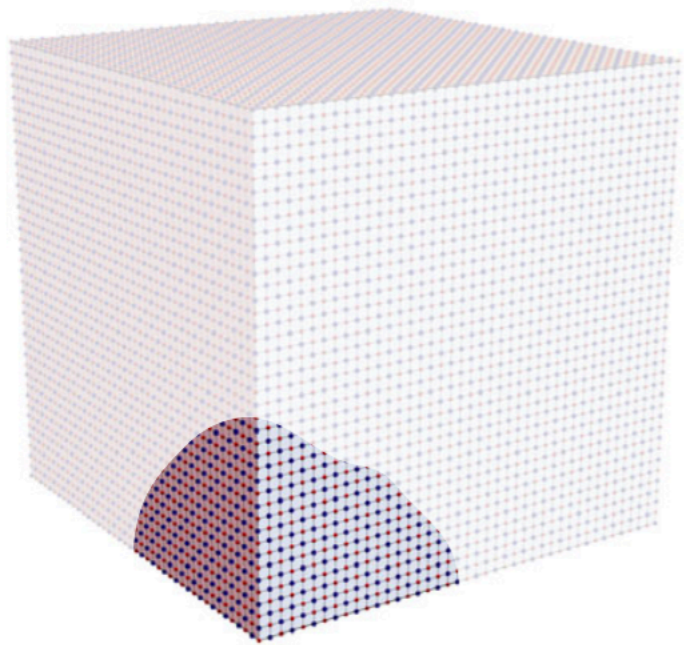
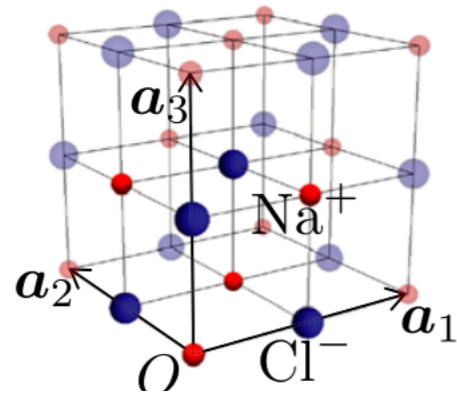
- Sometimes, **point group symmetry** and **charge neutrality** cannot be simultaneously respected.



- Surface charge is a local property.

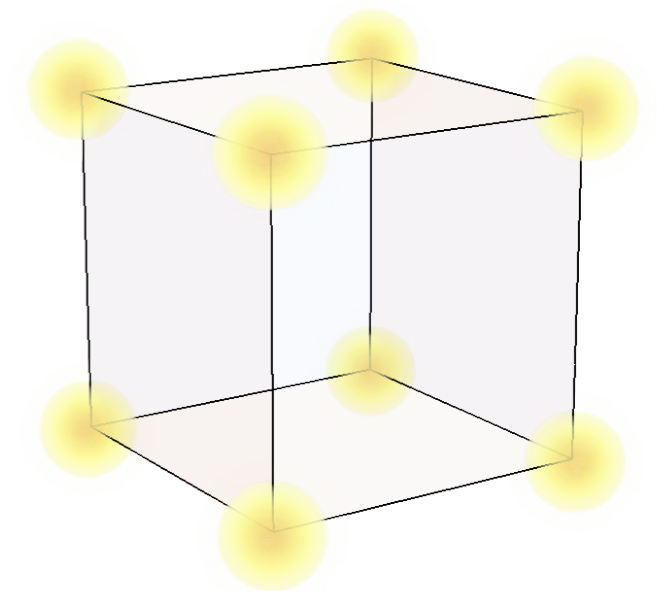
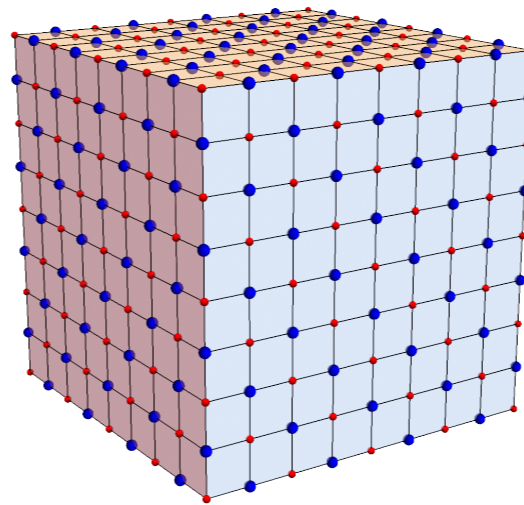


Fractional corner charge in sodium chloride (NaCl)



Filling anomaly

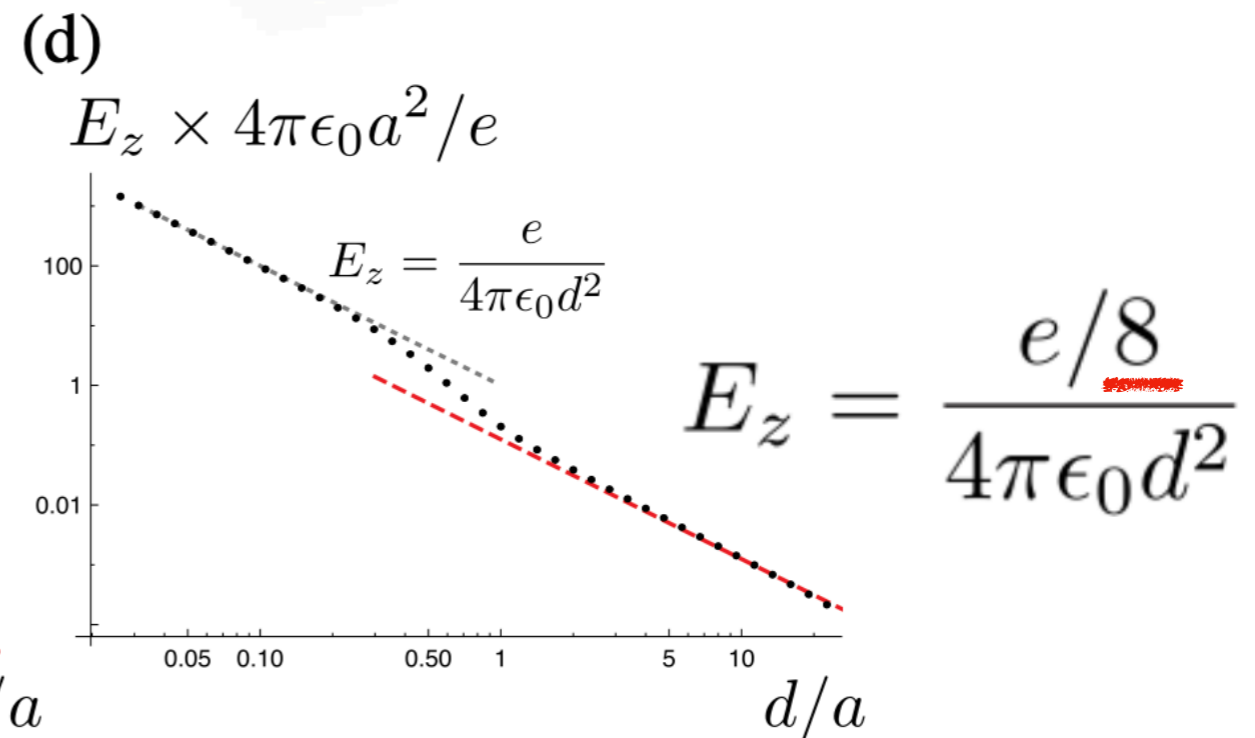
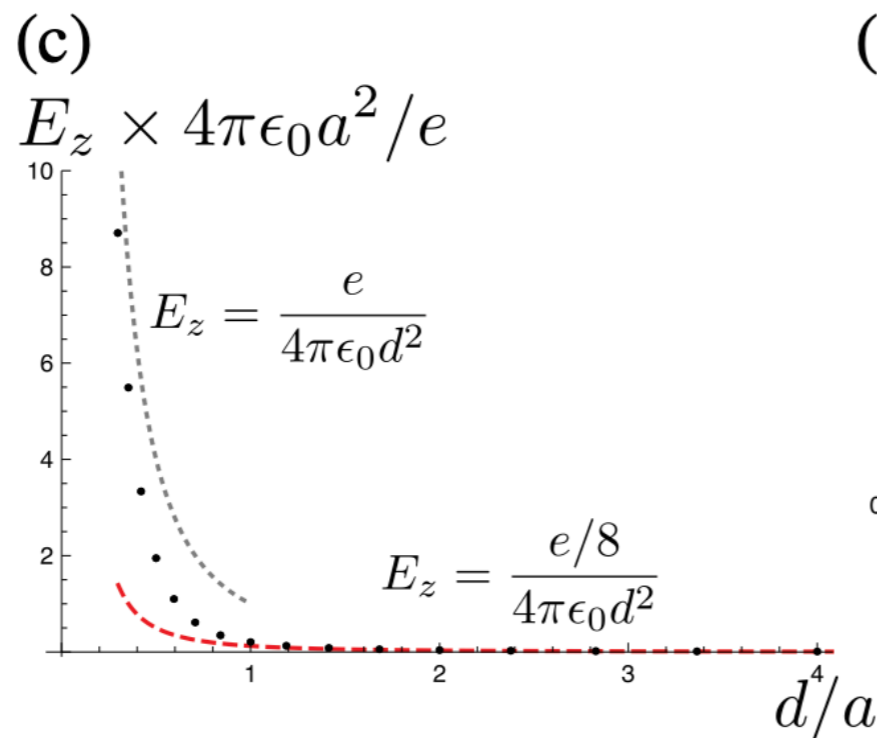
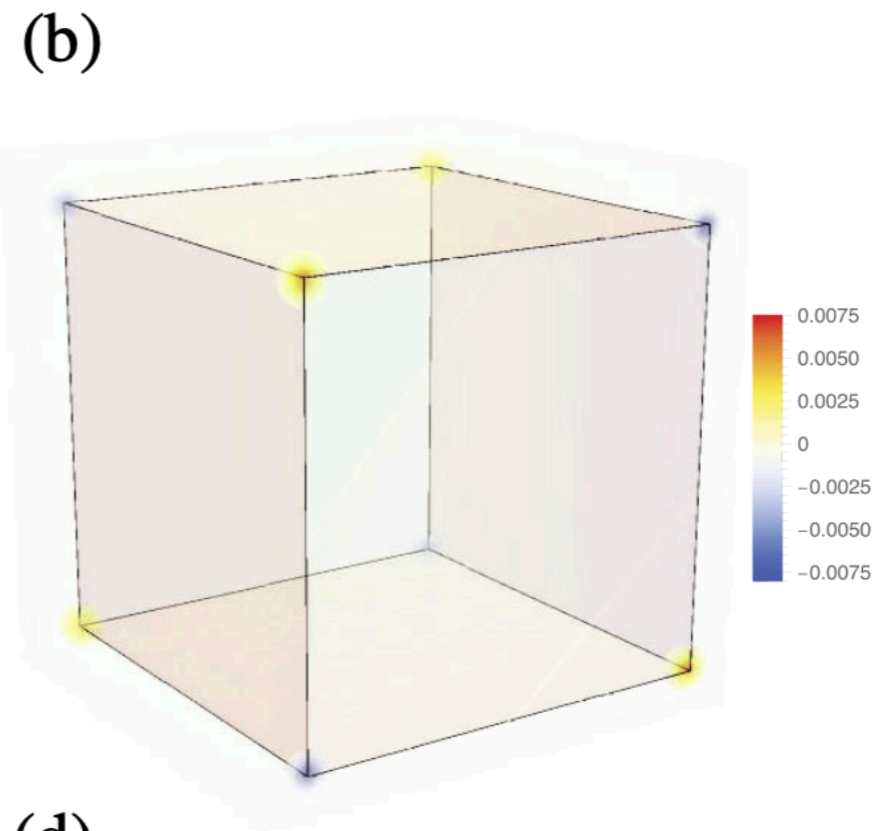
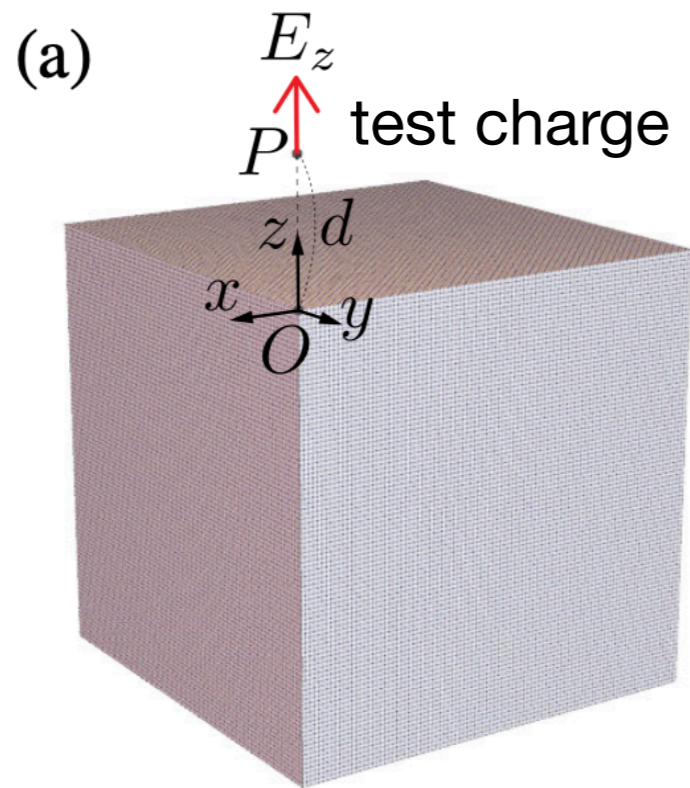
$$Q_{\text{corner}} = Q_{\text{tot}} / N_{\text{corner}}$$



$$Q_{\text{tot}} = +e, \quad Q_{\text{corner}} = \frac{1}{8}e \pmod{\frac{1}{4}e}$$

- [HW](#), S. Ono, Corner charge and bulk multipole moment in periodic systems, PRB (2020).
- [HW](#), H. C. Po, *Fractional Corner Charge of Sodium Chloride*, PRX (2021).
- K. Naito, R. Takahashi, [HW](#), S. Murakami, *Fractional hinge and corner charges in various crystal shapes with cubic symmetry*, PRB (2022).

Possible direct measurement via Coulomb force



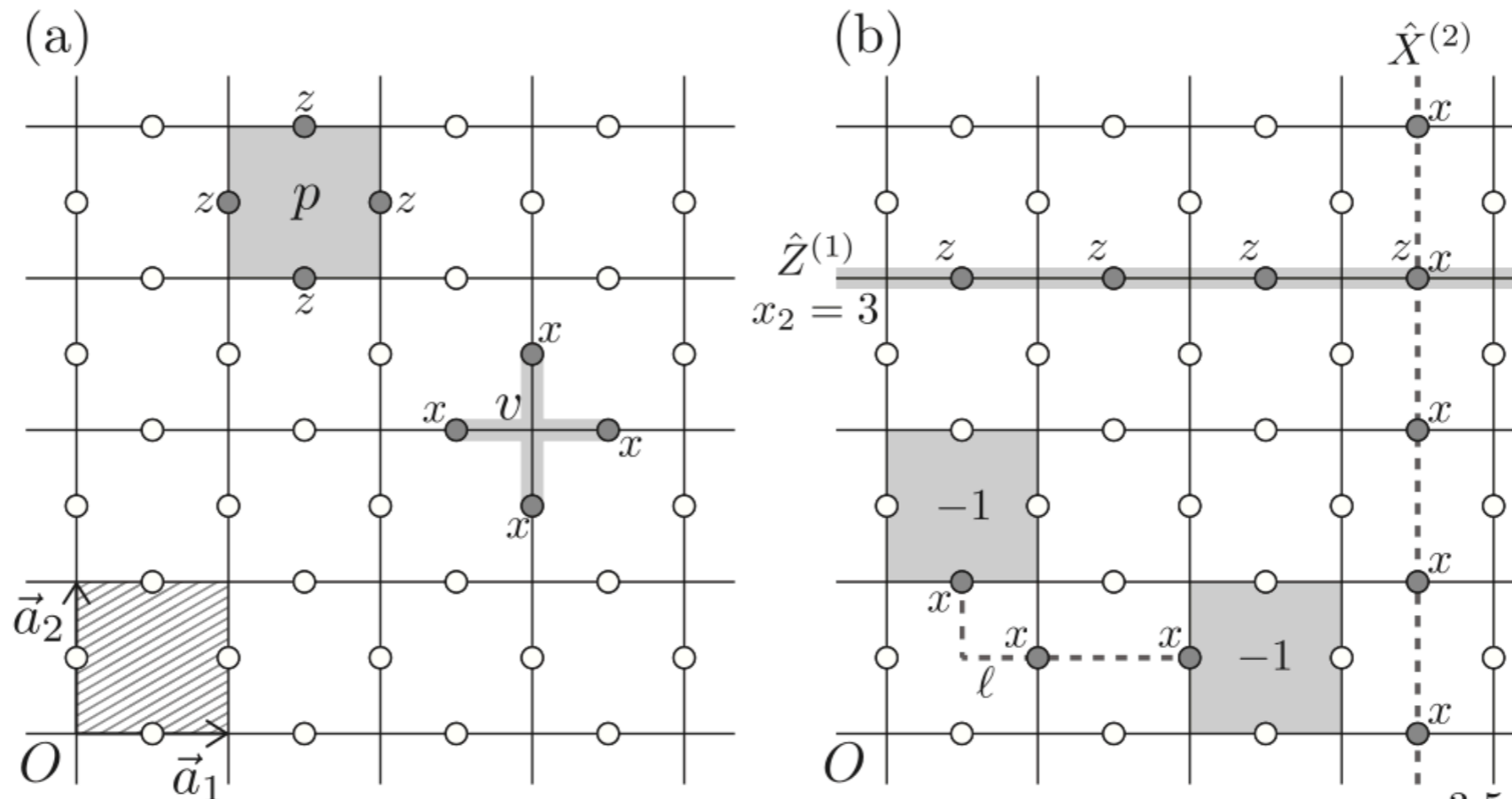
3. Topological orders “without” ground state degeneracy

Meng Cheng, Yohei Fuji, HW, in prep

Features of topologically ordered phases

- Topological ground state degeneracy
- Fractional excitations (anyons) and their statistics
- Topological entanglement entropy

- ...



Z_N toric code (1)

N-level spins

$$X \equiv \begin{pmatrix} 1 & & & & 1 \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix},$$

$$Z^N = X^N = 1,$$

$$Z \equiv \begin{pmatrix} 1 & & & & \\ & \omega & & & \\ & & \omega^2 & & \\ & & & \ddots & \\ & & & & \omega^{N-1} \end{pmatrix},$$

$$ZX = \omega XZ = \begin{pmatrix} \omega & & & & \\ & \omega^2 & & & \\ & & \ddots & & \\ & & & \omega^{N-1} & \\ & & & & 1 \end{pmatrix}$$

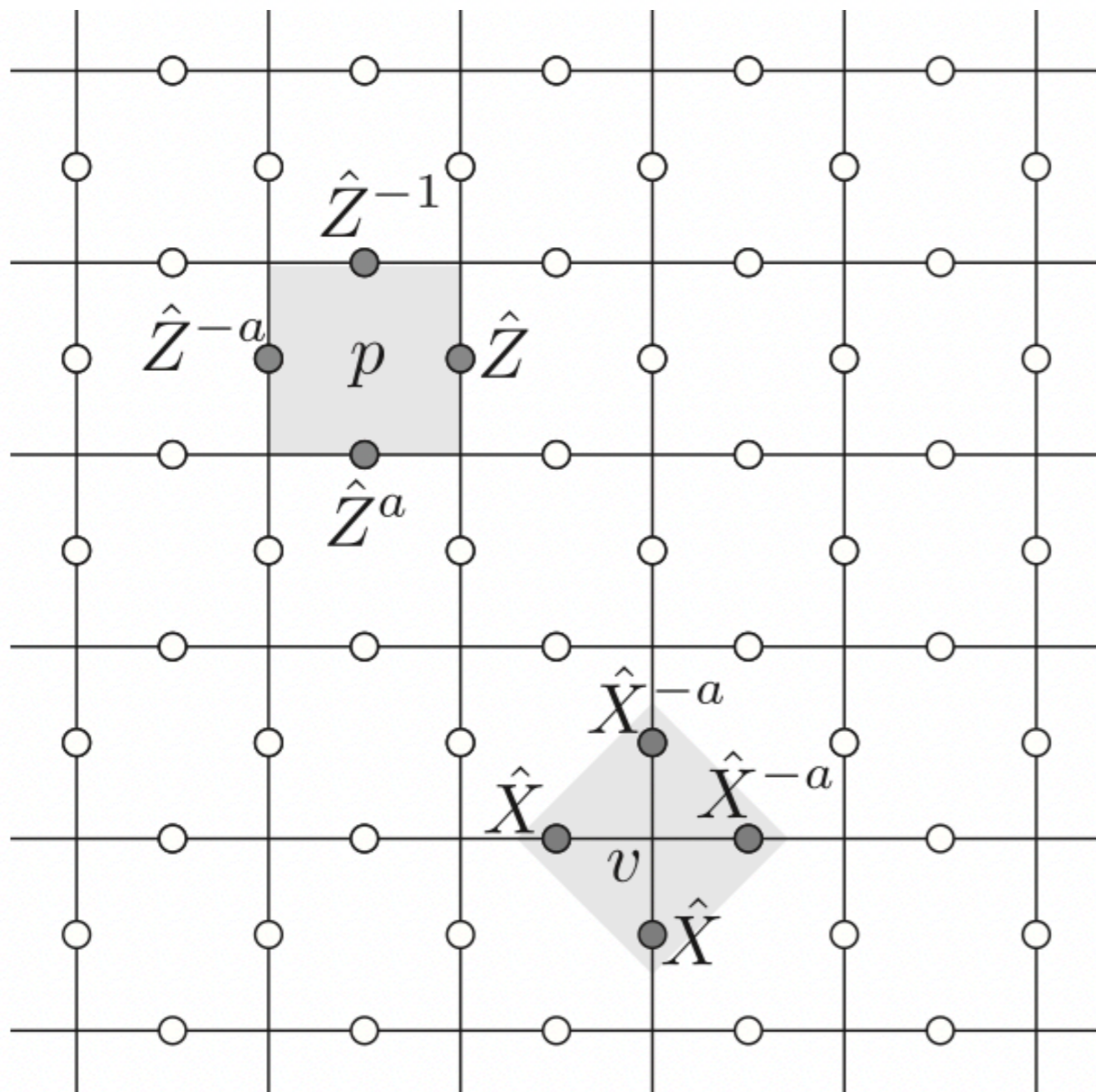
$$\omega \equiv e^{\frac{2\pi i}{N}},$$

Z_N toric code (2)

Hamiltonian

Kitaev (2003)

$$\hat{H}^{(L_1, L_2)} = - \sum_{v \in \mathcal{V}} \frac{1}{2} (\hat{A}_v + \text{h.c.}) - \sum_{p \in \mathcal{P}} \frac{1}{2} (\hat{B}_p + \text{h.c.}).$$



- $a=1$ is the standard model
- $a=-1$ is the simplest nontrivial example

M. Barkeshli, et al CMP (2020)
(preprint in 2016)

J. C. Bridgeman et al, PRB (2017)

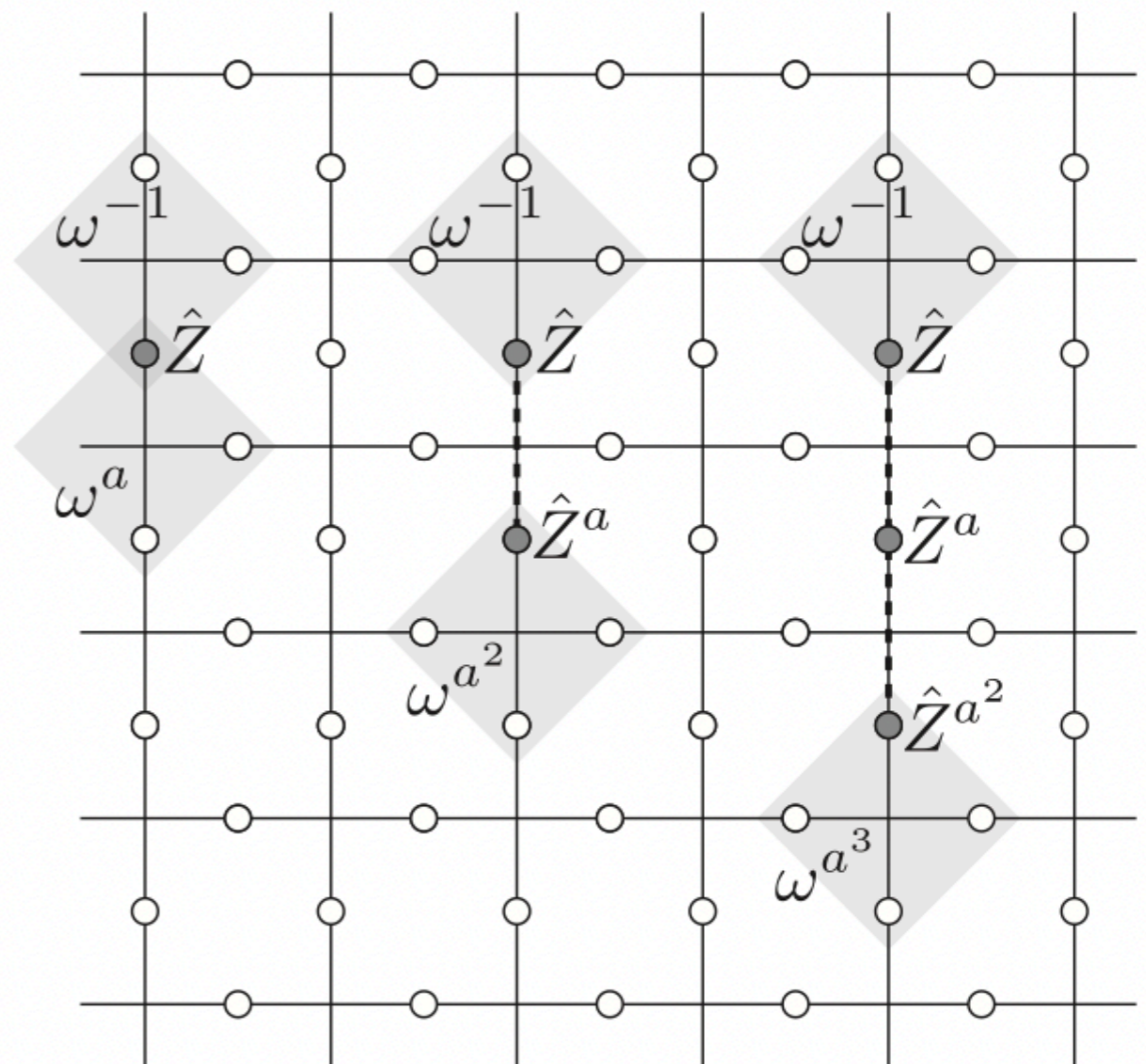
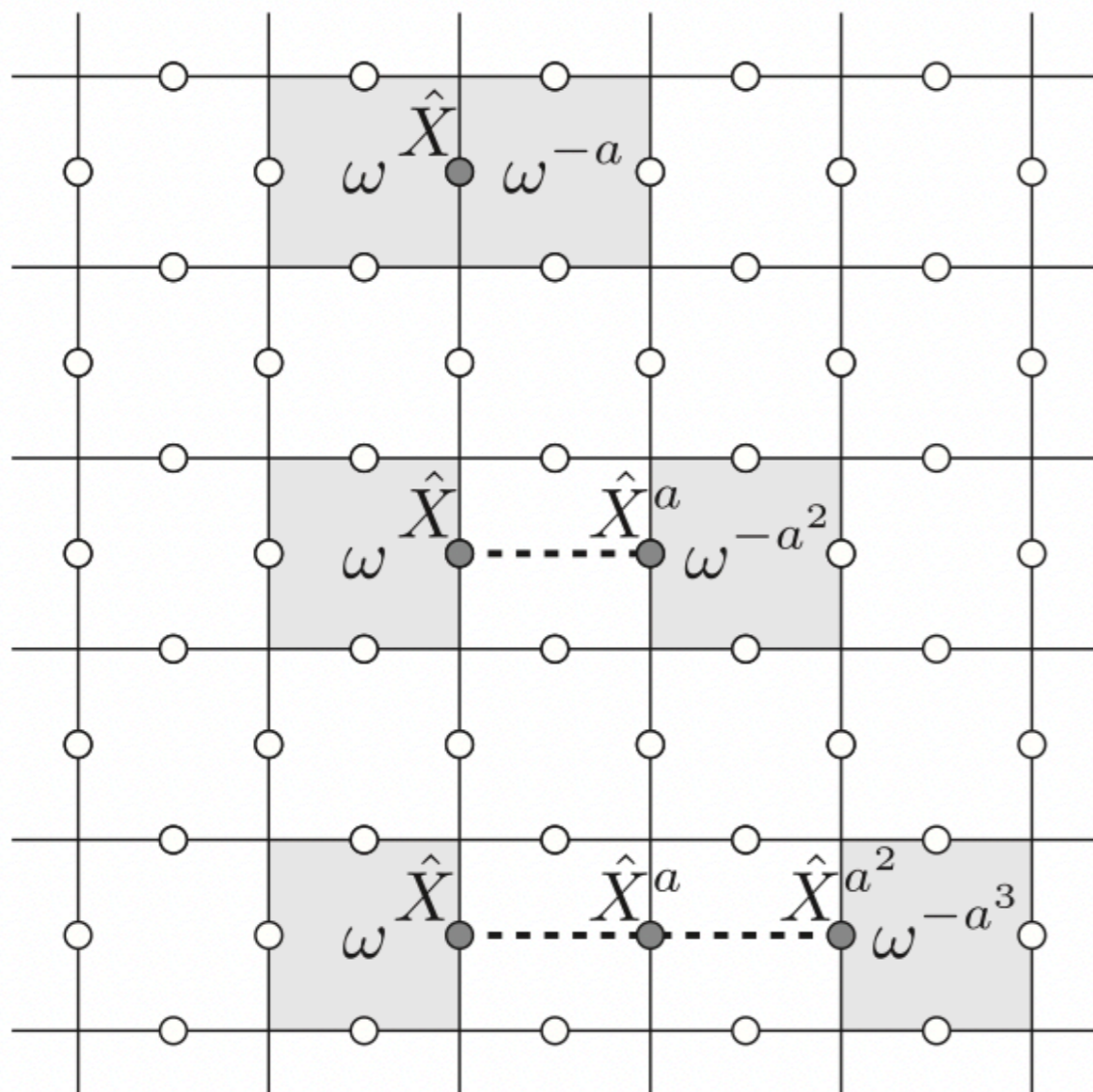
Y. Fuji, PRB (2019)

...

- Other values of a are also interesting.

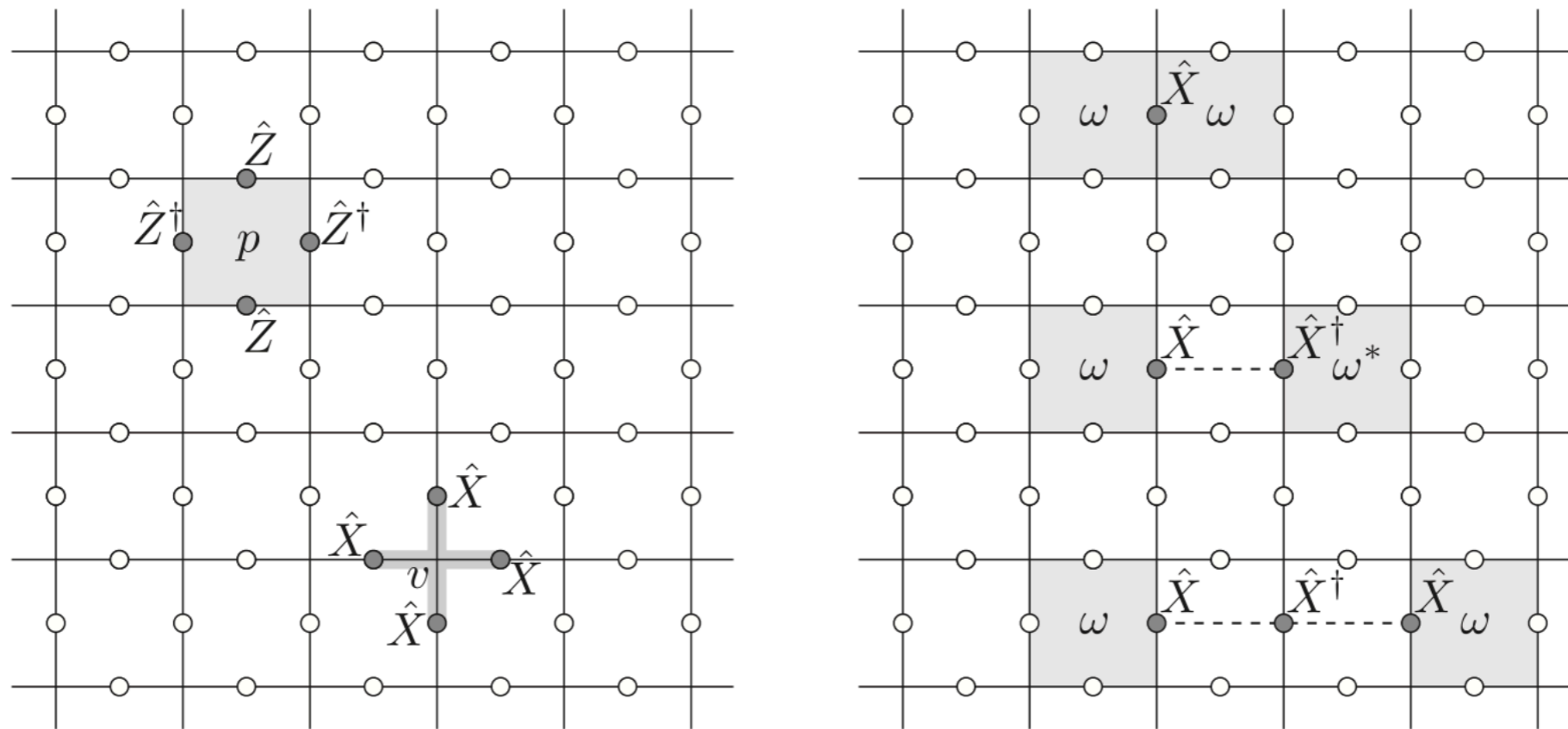
Z_N toric code (3)

String operators



- Strings can be closed only when L_1, L_2 are multiple of the period.
- Translation permutes anyons.

Ground state degeneracy on torus for $a=-1$



$$N_{\text{deg}}^{(L_1, L_2)} = \begin{cases} N^2 & (L_1 \text{ and } L_2 \text{ are even}) \\ 4 & (L_1 \text{ or } L_2 \text{ is odd \& } N \text{ is even}) \\ 1 & (L_1 \text{ or } L_2 \text{ is odd \& } N \text{ is odd}) \end{cases}$$

- Ground state can be unique and gapped!!

Topological entanglement entropy

- Entanglement entropy

$$S_R \equiv -\text{tr}[\hat{\rho}_R \log \hat{\rho}_R]$$

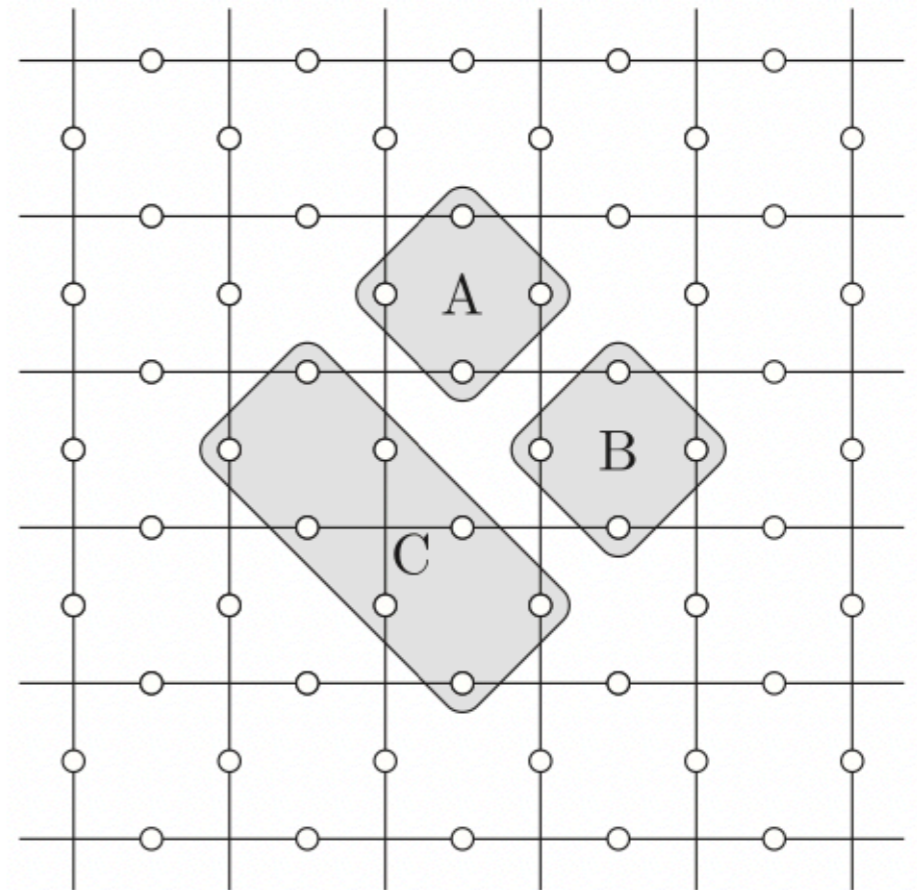
$$\hat{\rho}_R \equiv \text{tr}_{\bar{R}} |\Phi_0\rangle\langle\Phi_0|$$

- Topological entanglement entropy

$$S_R = \alpha \partial R + S_{\text{topo}}^{(L_1, L_2)}$$

$$S_{\text{topo}}^{(L_1, L_2)} = S_A + S_B + S_C - (S_{AB} + S_{BC} + S_{CA}) + S_{ABC}$$

$$S_{\text{topo}}^{(L_1, L_2)} = -\log N \quad \text{regardless of } a, L_1, L_2$$



Conclusions

- **Symmetry indicators for superconductors**

New database & subroutine

F. Tang*, S. Ono*, X. Wan, HW, PRL (2022)

- **Revisiting criteria for topological phases**

- **Symmetry indicators** → topological (crystalline) insulators

The converse is not true.

For example, many TSCs with conventional pairing symmetries.

S. Ono, K. Shiozaki, HW, arXiv:2206.02489

- **Product states** → not interesting.

NaCl as a counter example. HW, H. C. Po, PRX (2021).

- **Topological degeneracy on torus** → topological orders

There can be topological order without degeneracy on torus for a sequence of L_1, L_2 .