

# Complete Theory of Symmetry-Based Indicators of the Band Topology

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University of Tokyo



Ashvin Vishwanath  
moved to Harvard

This talk is based on:

Sci. Adv. (2016) (feQBI)

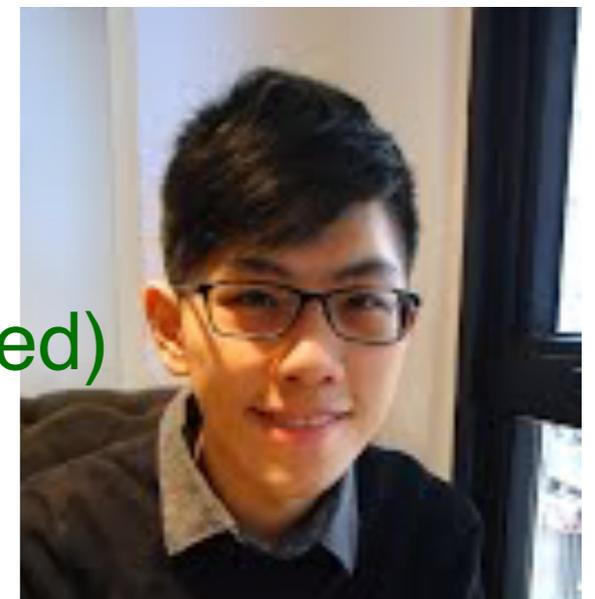
Phys. Rev. Lett. (2016) (filling-enforced)

**Nat. Commun. (2017) (Indicator)**

arXiv: 1707.01903 (MSG)

arXiv: 1709.06551 (fragile topo.)

**(new) arXiv: 1710.07012 (Chern #)**  
with my students and Ken Shiozaki



Hoi Chun Po (Adrian)  
Ashvin's student

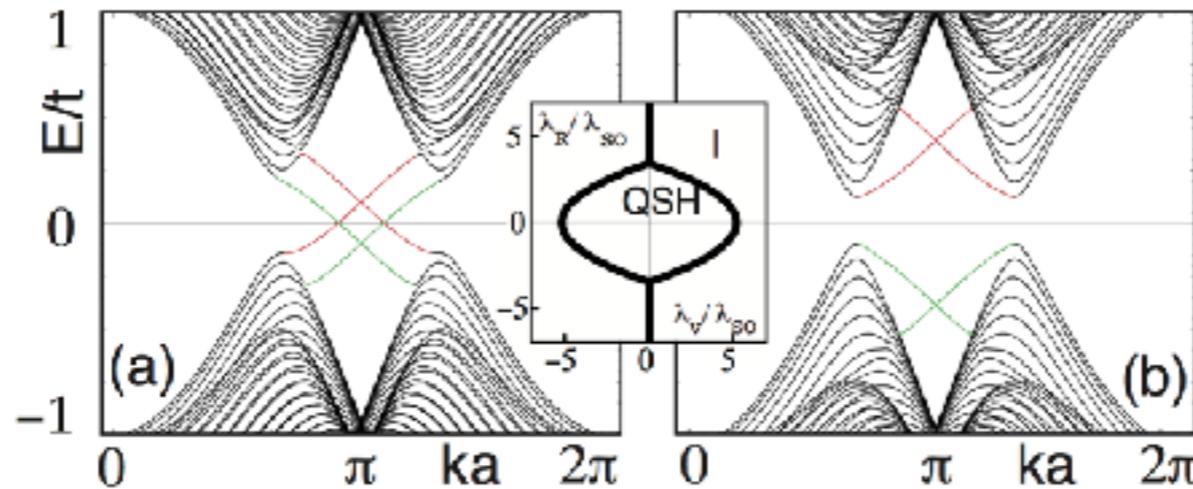
# Plan

- Brief intro
- Symmetry-based indicator of band topology (noninteracting)
- Interaction effect (LSM theorem + recent development)

# Three definitions of Topological insulators

Topological insulators

Trivial insulators



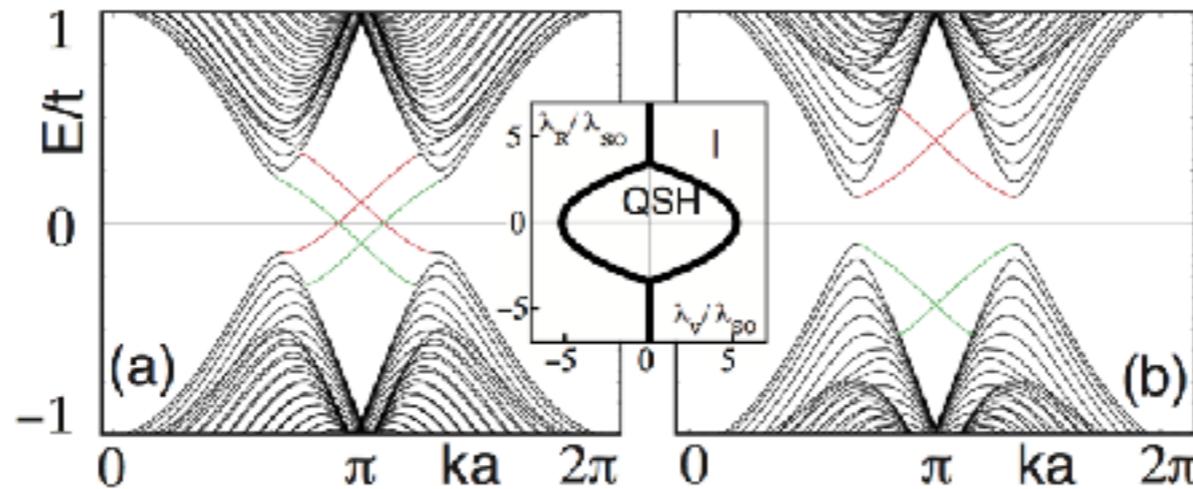
Kane-Mele PRL (2005)

- Have edge states?
- Topological Index? (e.g. Chern number, Z2 QSH index)
- Adiabatically connected to atomic limit (i.e. no hopping)?  
= Valence bands can form good\* Wannier orbitals?

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**No**

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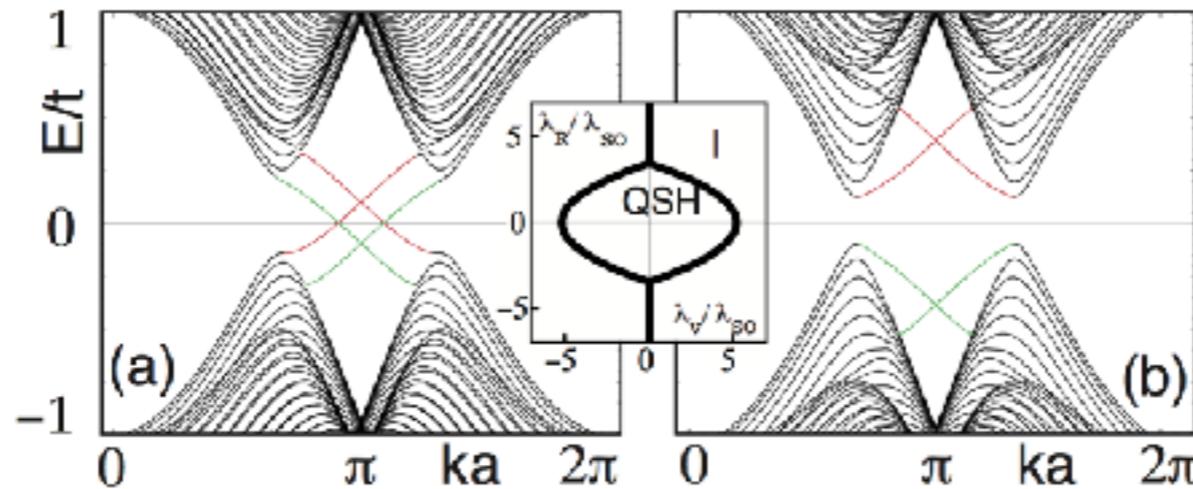
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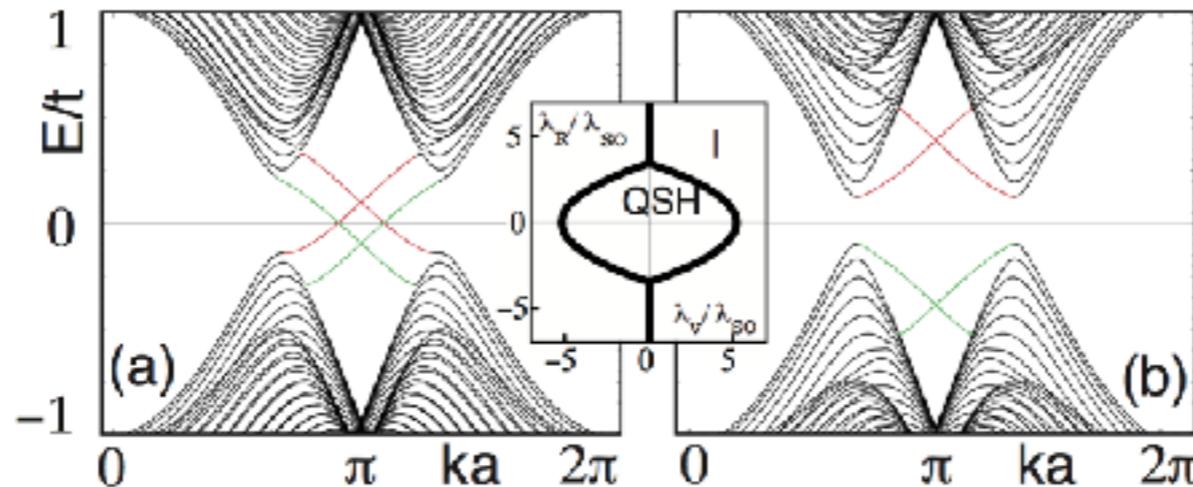
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# Three definitions of Topological insulators

**Topological insulators**

**Trivial insulators**



Kane-Mele PRL (2005)

- Have edge states?

**Yes**

**No**

\*exponentially localized & symmetric

- Topological Index? (e.g. Chern number, Z2 QSH index)

**Yes**

**No**

**Weakest definition**

- Adiabatically connected to atomic limit (i.e. no hopping)?  
= Valence bands can form good\* Wannier orbitals?

**No**

**Yes**

# Generalization of Fu-Kane Formula

- $Z_2$  index for Quantum Hall Spin insulators

Requires a careful gauge fixing and integration of Pfaffian in  $k$  space

# Generalization of Fu-Kane Formula

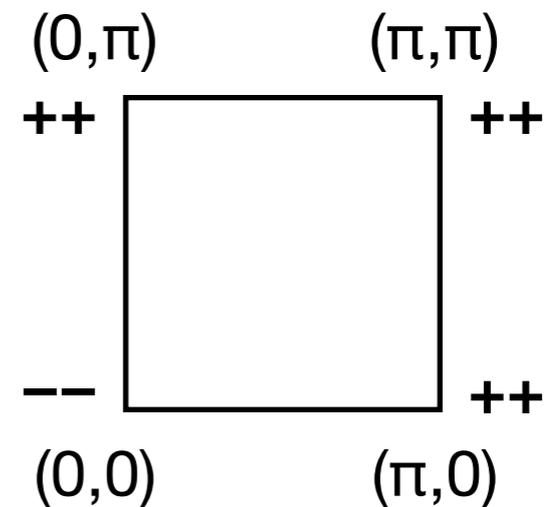
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- For inversion-symmetric TI

Fu-Kane formula:  $\nu = \prod_{k=\text{TRIMs}} \xi_k = \pm 1$

Easy & Helpful for material search!



# Generalization of Fu-Kane Formula

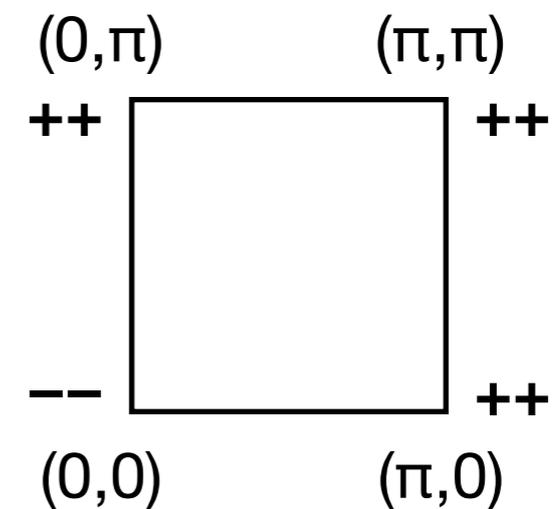
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**Combination of inversion eigenvalues *indicates* the band insulator is  $Z_2$  QSH.**

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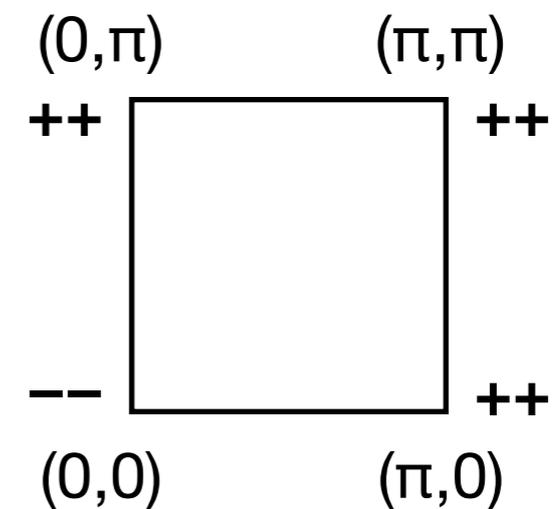
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**Irreducible representations at high-sym momenta**  
**Combination of inversion eigenvalues *indicates***  
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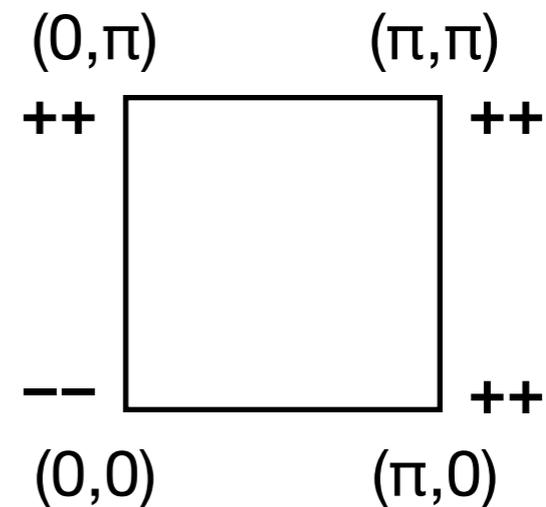
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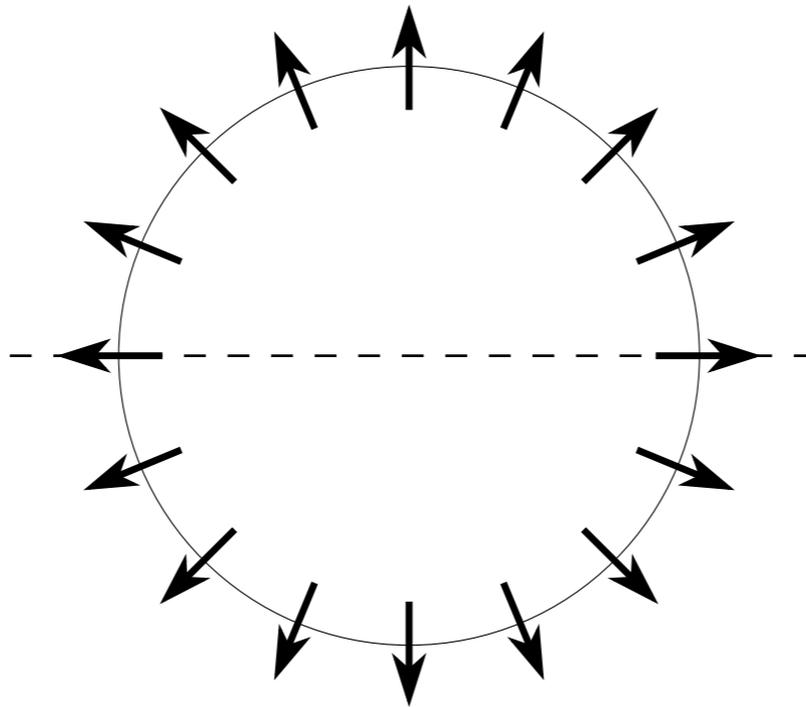
**Irreducible representations at high-sym momenta**  
**Combination of ~~inversion eigenvalues~~ *indicates***  
**the band insulator is  ~~$Z_2$  QSH.~~**

**Nontrivial (not adiabatically connected to the atomic limit)**

# Symmetry and Topology

Example: Winding number of the map  $S^1$  to  $S^1 \rightarrow \pi_1(S^1) = \mathbb{Z}$

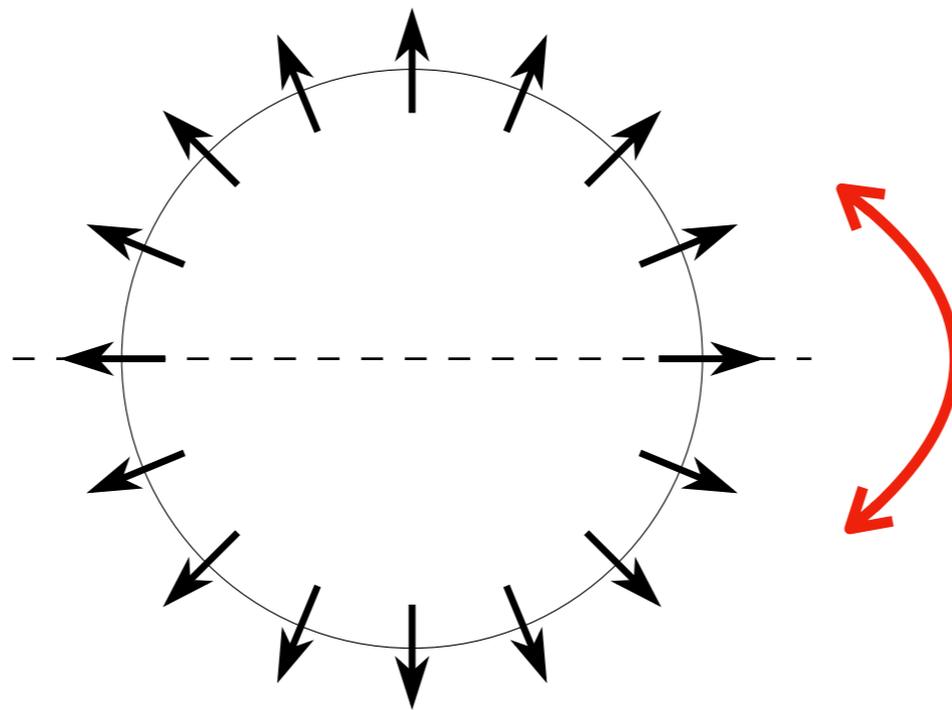
$$W[\mathbf{n}(\theta)] = \frac{1}{2\pi} \int_0^{2\pi} d\theta \hat{z} \cdot \mathbf{n} \times \partial_\theta \mathbf{n}$$



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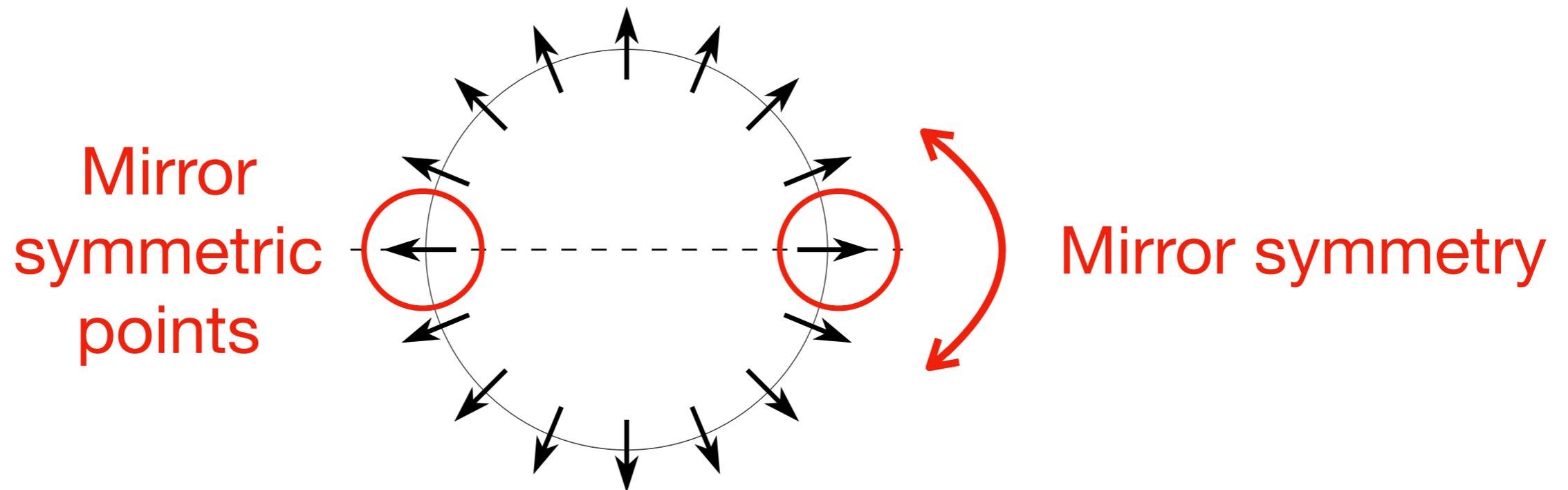


Mirror symmetry

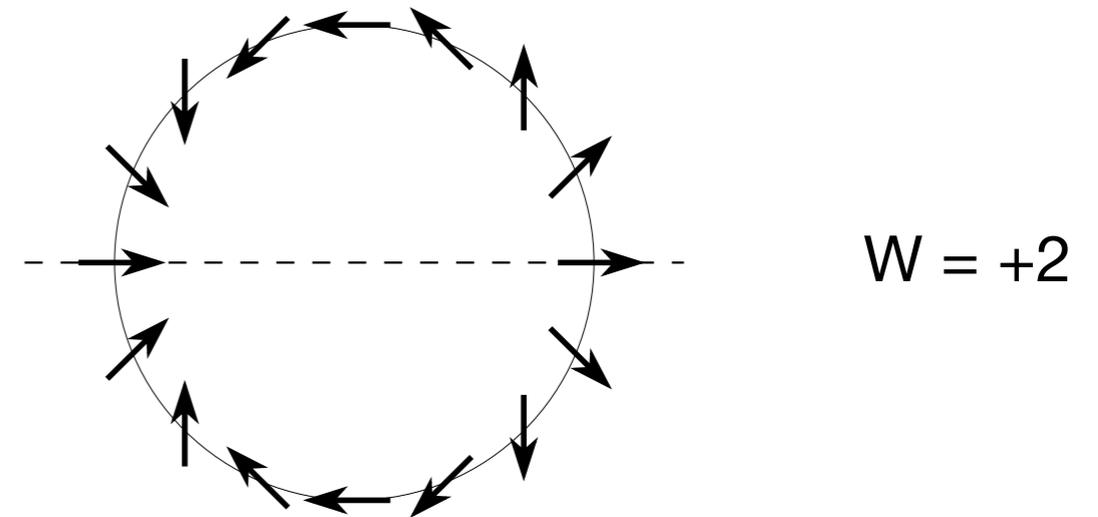
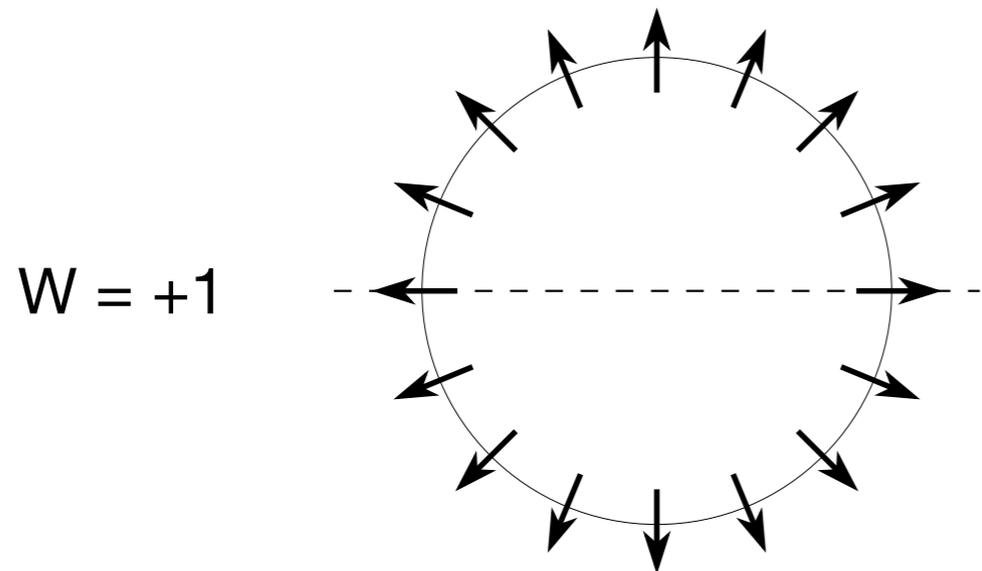
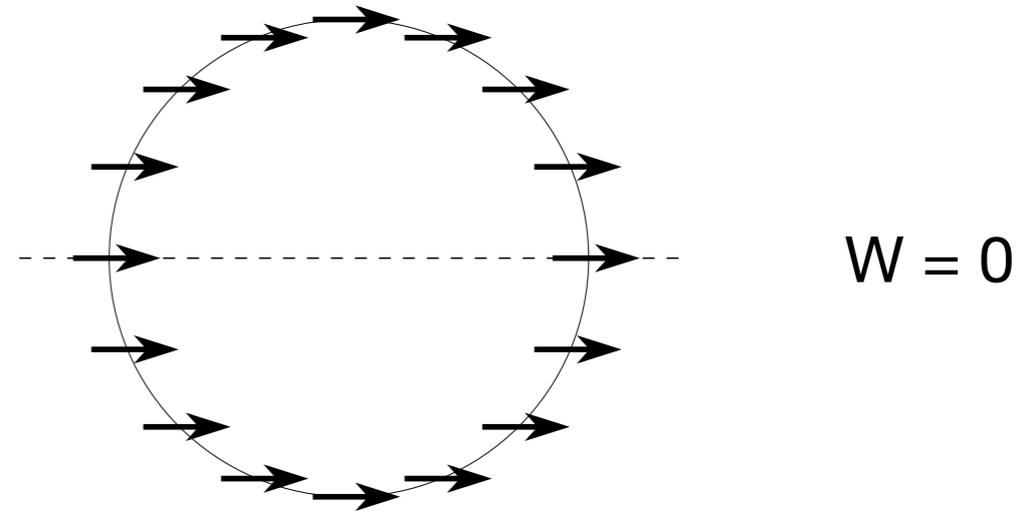
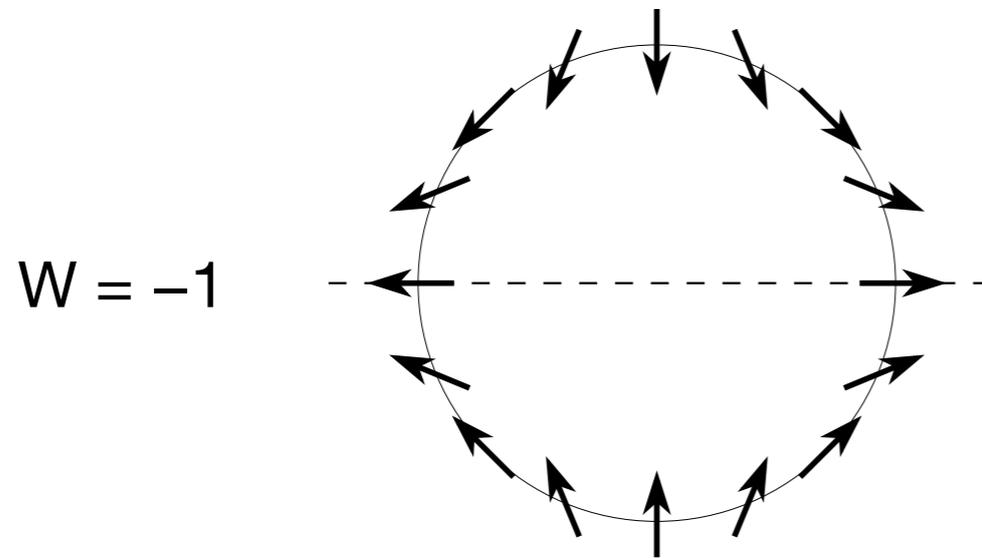
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# Symmetry and Topology

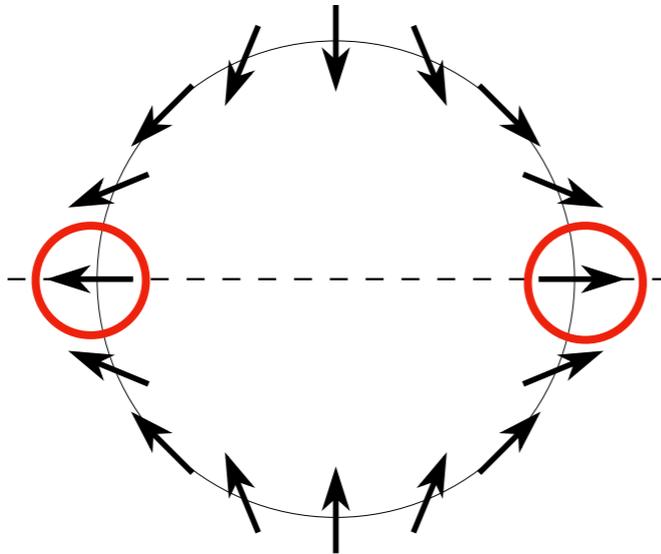


Opposite direction  
→  $W = \text{odd}$

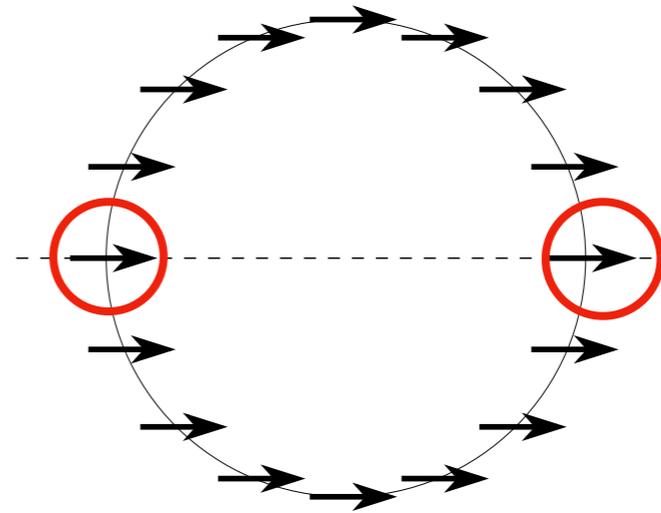
Same direction  
→  $W = \text{even}$

# Symmetry and Topology

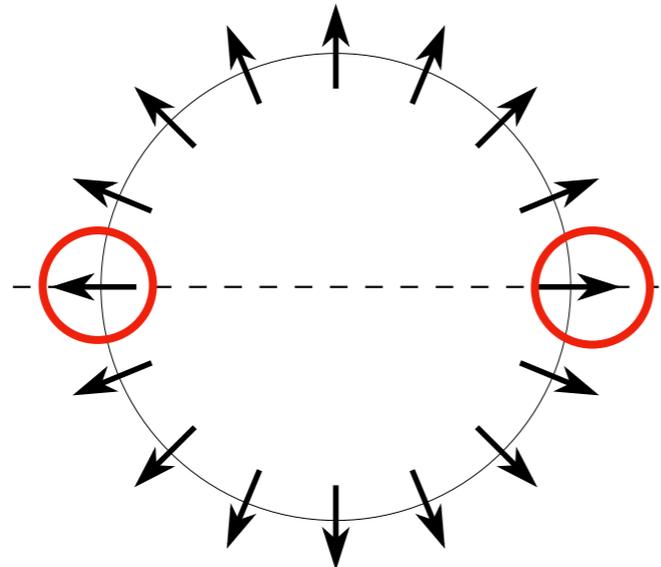
$$W = -1$$



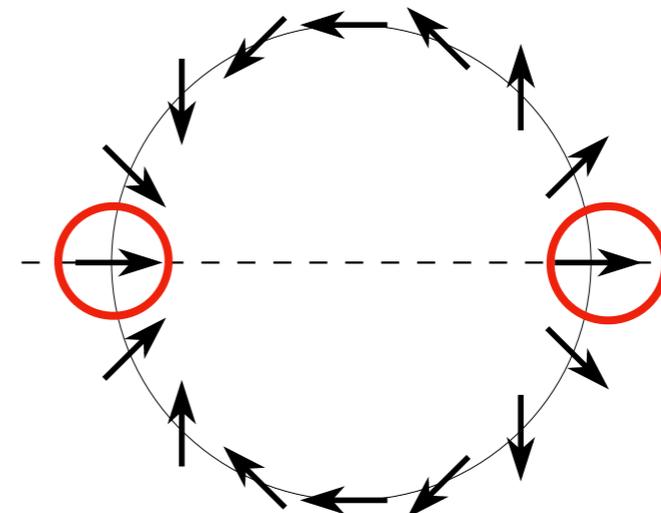
$$W = 0$$



$$W = +1$$



$$W = +2$$

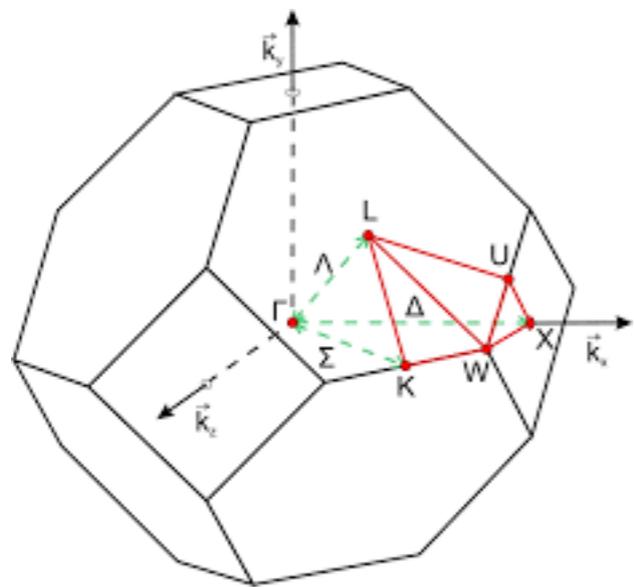


Opposite direction  
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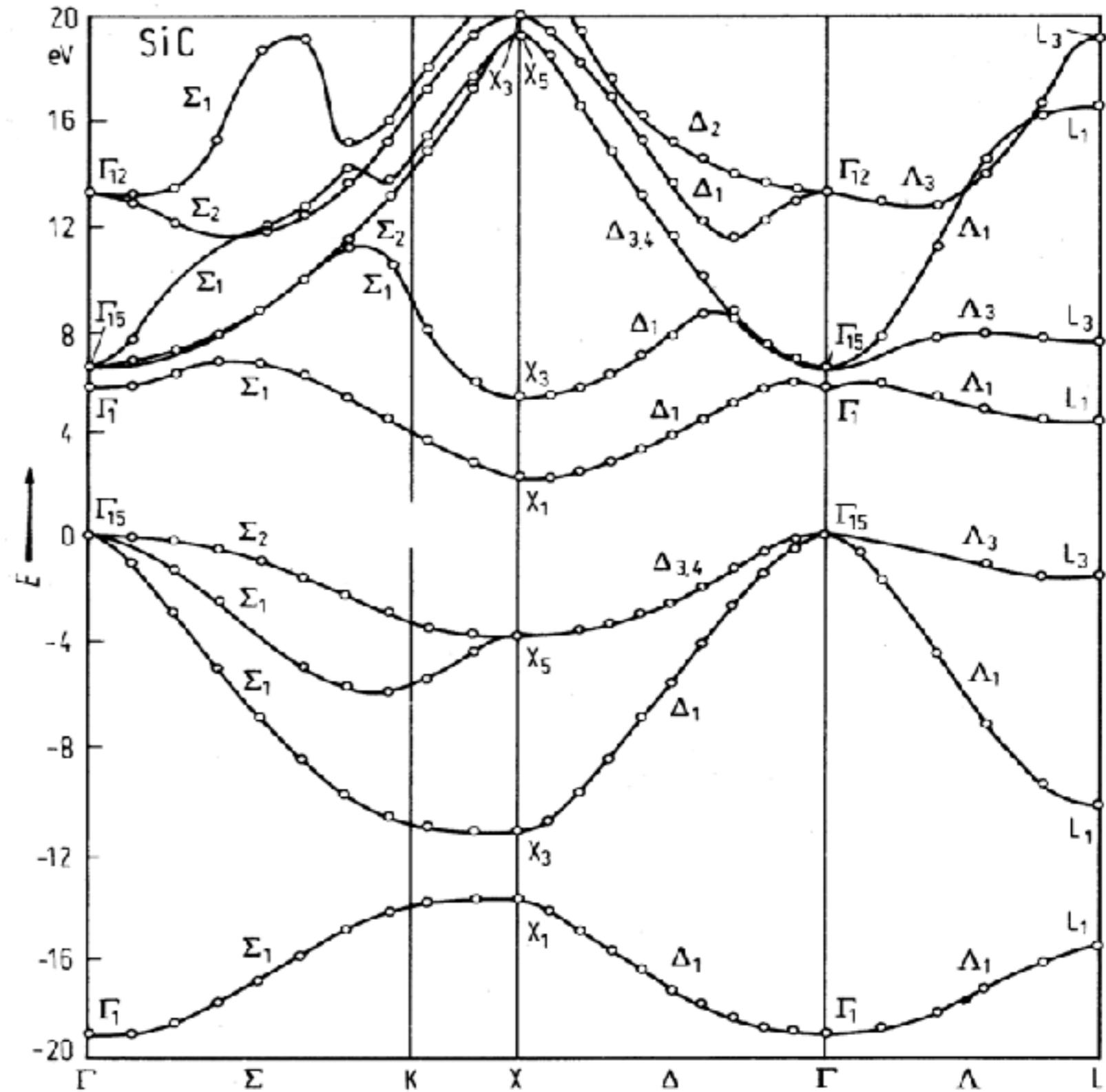
Same direction  
→  $W = \text{even}$

# Symmetry Representation of Band Structures (momentum space)

# Irreducible Representation in Band Structure

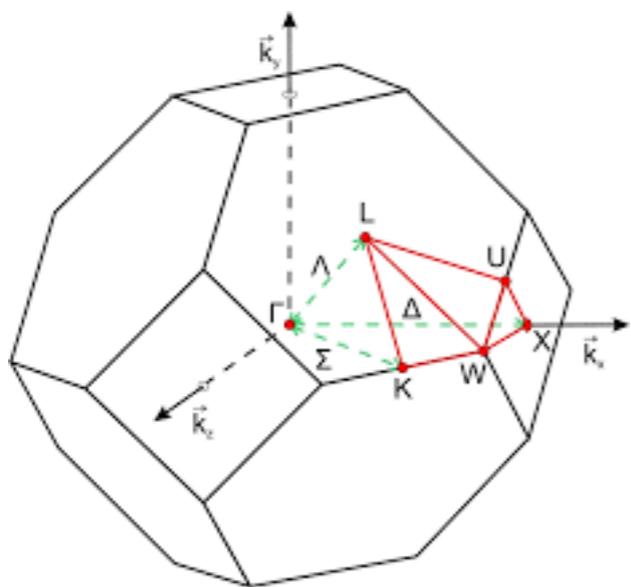


Hemstreet & Fong (1974)

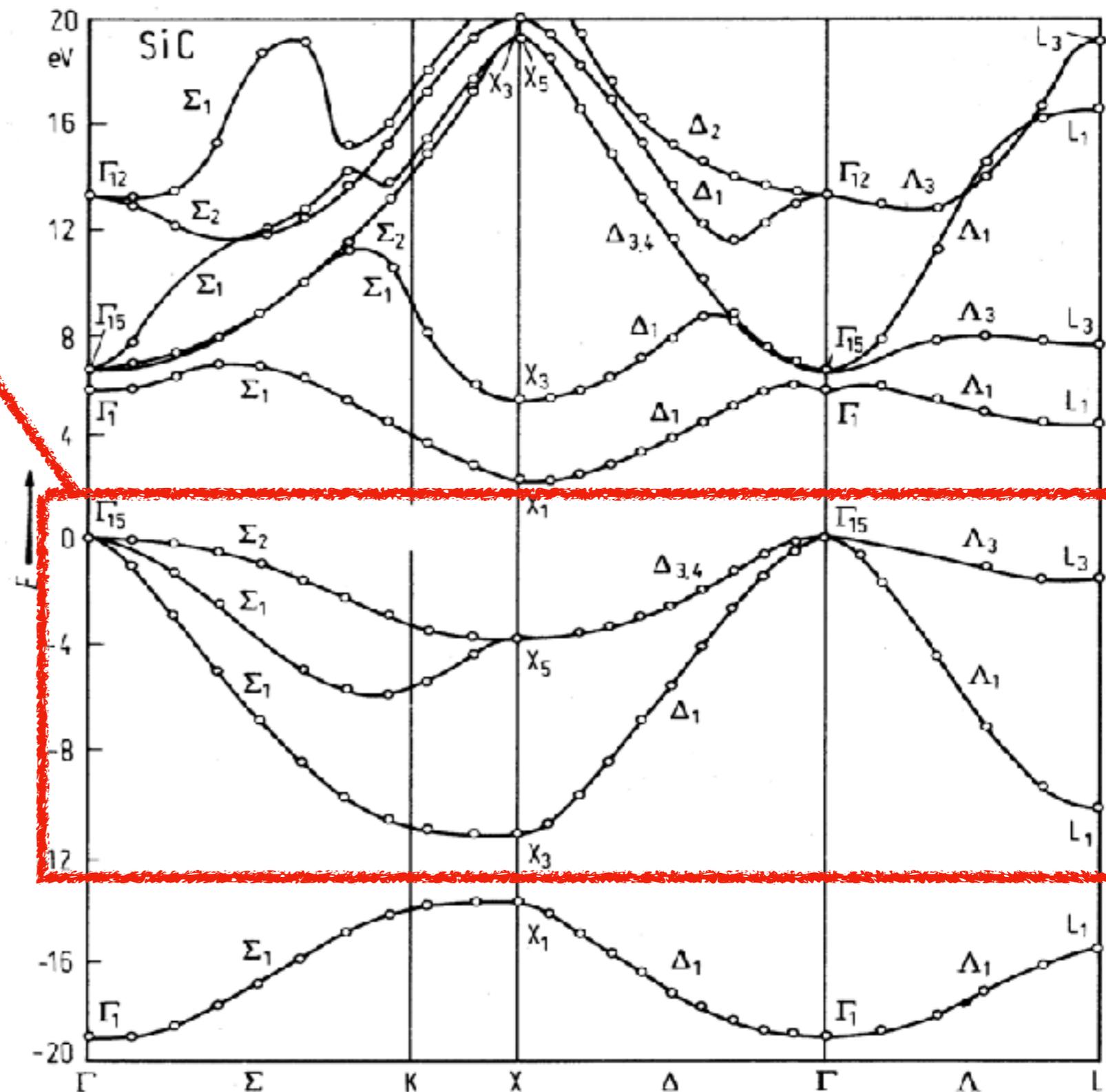


# Irreducible Representation in Band Structure

Focus on a set of bands with band gap above and below at all high-symmetry momenta

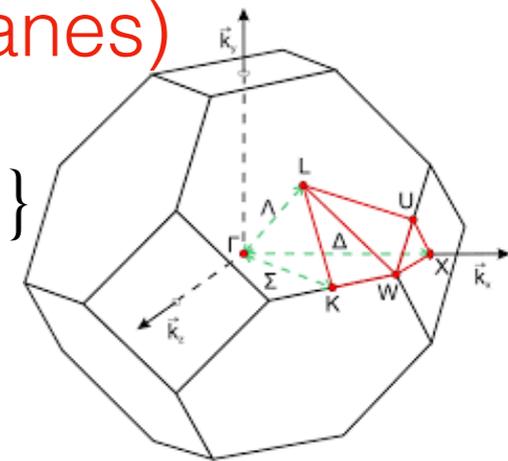


Hemstreet & Fong (1974)



# Characterizing Band Structure by its representation contents

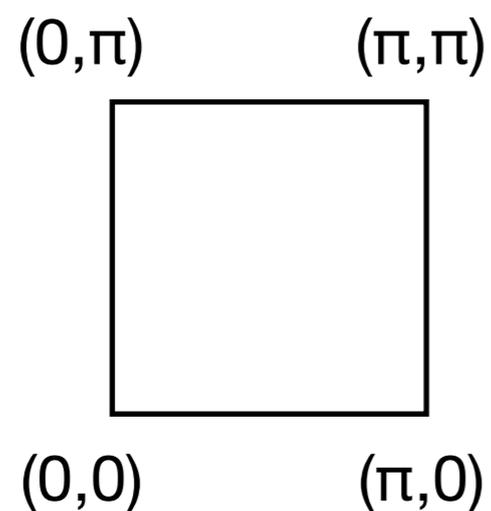
1. Collect all different types of high-sym  $\mathbf{k}$  (points, lines, planes)
  2. For each  $\mathbf{k}$ , define little group  $G_{\mathbf{k}} = \{ g \text{ in } G \mid g\mathbf{k} = \mathbf{k} + \mathbf{G} \}$
  3. Find irreps  $u_{\mathbf{k}}^a$  ( $a = 1, 2, \dots$ ) of  $G_{\mathbf{k}}$
  4. Count the number of times  $u_{\mathbf{k}}^a$  appears in band structure  $\{n_{\mathbf{k}}^a\}$
- ※ Note *compatibility relations* among  $\{n_{\mathbf{k}}^a\}$
5. Form a vector  $\mathbf{b} = (n_{\mathbf{k}_1^1}, n_{\mathbf{k}_1^2}, \dots, n_{\mathbf{k}_2^1}, n_{\mathbf{k}_2^2}, \dots)$  for each BS
  6. Find the set of  $\mathbf{b}$ 's (Band Structure Space) :



$$\{\text{BS}\} = \{ \mathbf{b} = \{n_{\mathbf{k}}^a\} \mid \text{satisfying compat. relations} \} = \mathbb{Z}^{d_{\text{BS}}}$$

# Example: 2D lattice with inversion symmetry

1. Collect all different types of high-sym  $\mathbf{k}$  (point, line, plane)
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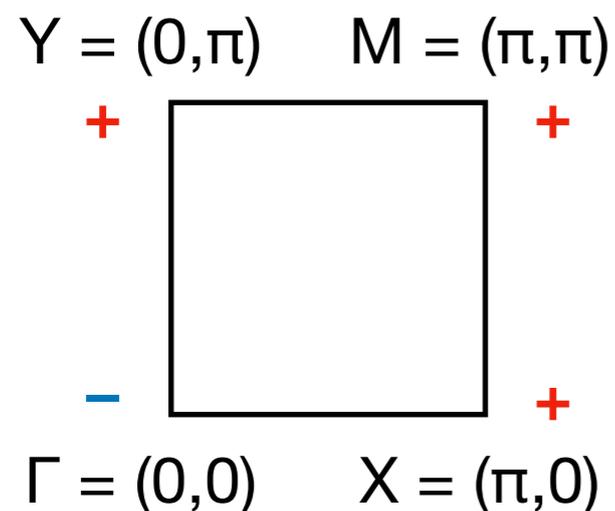


$$G_{\mathbf{k}} / \text{Translation} = \{e, I\}$$

$$u_{\mathbf{k}^+}(I) = +1, u_{\mathbf{k}^-}(I) = -1$$

# Example: 2D lattice with inversion symmetry

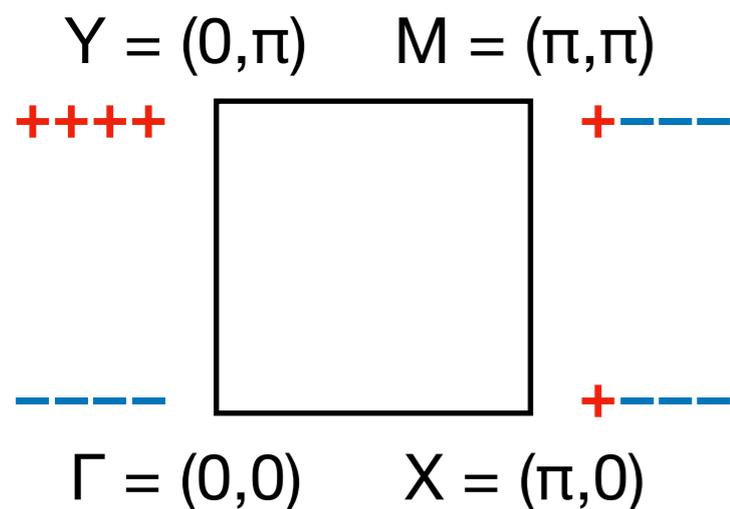
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$$\begin{aligned}\mathbf{b} &= (n_{\Gamma^+}, n_{\Gamma^-}, n_{X^+}, n_{X^-}, n_{Y^+}, n_{Y^-}, n_{M^+}, n_{M^-}) \\ &= (0, 1, 1, 0, 1, 0, 1, 0)\end{aligned}$$

# Example: 2D lattice with inversion symmetry

6. Find the set of **b**'s (Band Structure Space):  $\{\text{BS}\} = \{ \mathbf{b} = \{n_{\mathbf{k}^a}\} \} = \mathbb{Z}^{d_{\text{BS}}}$



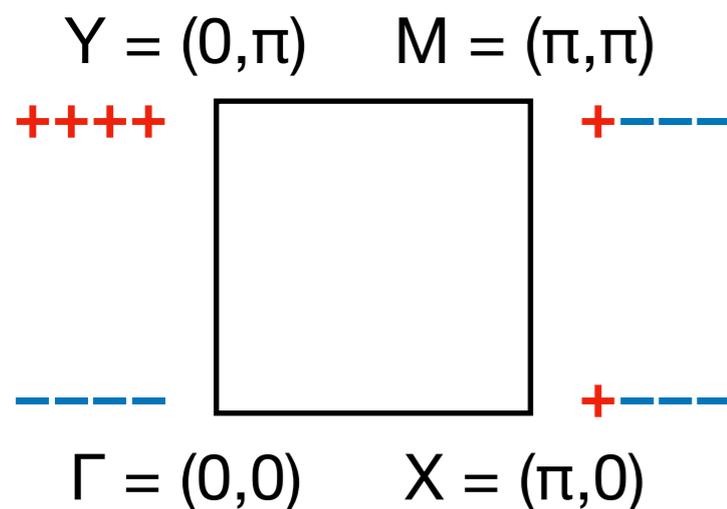
The general form of **b** in this case:

$$\mathbf{b} = (n_{\Gamma^+}, n_{\Gamma^-}, n_{X^+}, n_{X^-}, n_{Y^+}, n_{Y^-}, n_{M^+}, n_{M^-})$$

→  $8 - 3 = 5$  independent  $n$ ,  $\{\text{BS}\} = \mathbb{Z}^5$

# Example: 2D lattice with inversion symmetry

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$$\mathbf{b} = n_{\Gamma^+}(1, -1, 0, 0, 0, 0, 0, 0) + n_{X^+}(0, 0, 1, -1, 0, 0, 0, 0)$$

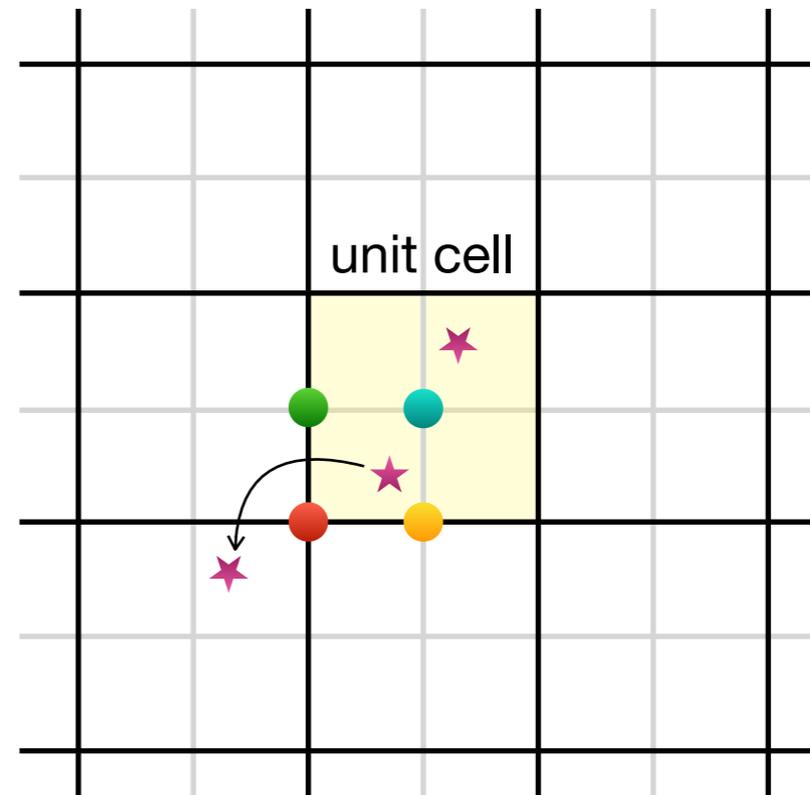
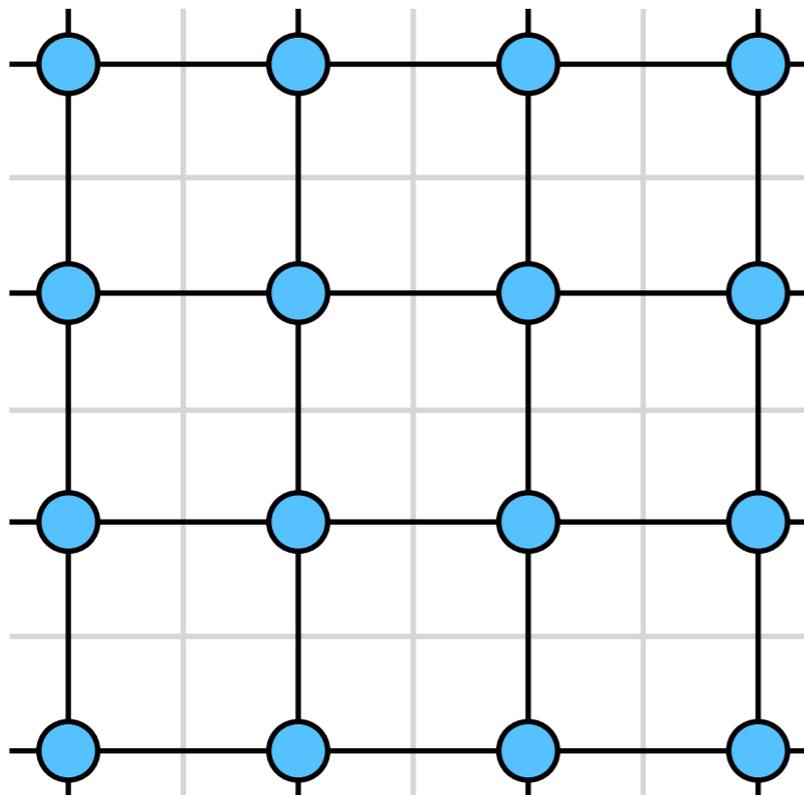
$$+ n_{Y^+}(0, 0, 0, 0, 1, -1, 0, 0) + n_{M^+}(0, 0, 0, 0, 0, 0, 1, -1) + v(0, 1, 0, 1, 0, 1, 0, 1)$$

5-dimensional lattice in an imaginary space

# Trivial Insulators (real space)

# Atomic Insulators

Product state in real space (trivial)  $\Leftrightarrow$  Wannier orbitals



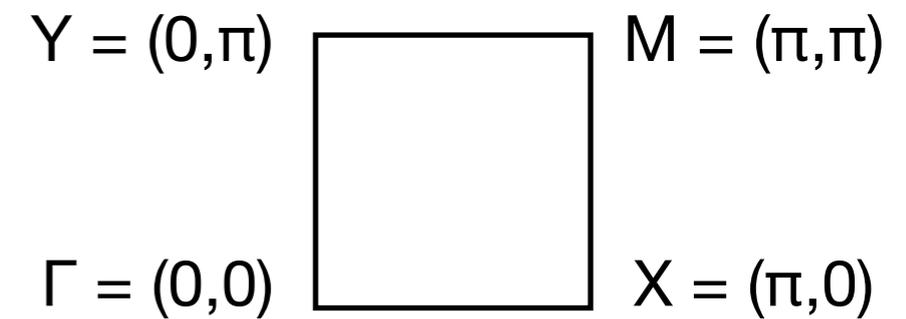
We have to specify the position  $\mathbf{x}$  and the orbital type

1. Choose  $\mathbf{x}$  in unit cell. e.g.  $\mathbf{x} = \bullet$
2. Find little group (site-symmetry gr)  $G_{\mathbf{x}}$ .  $G_{\mathbf{x}} = \{e, I\}$  at  $\mathbf{x} = \bullet$
3. Choose an orbit (an irrep of  $G_{\mathbf{x}}$ ). 
● ( $l = +1$ )
●● ( $l = -1$ )

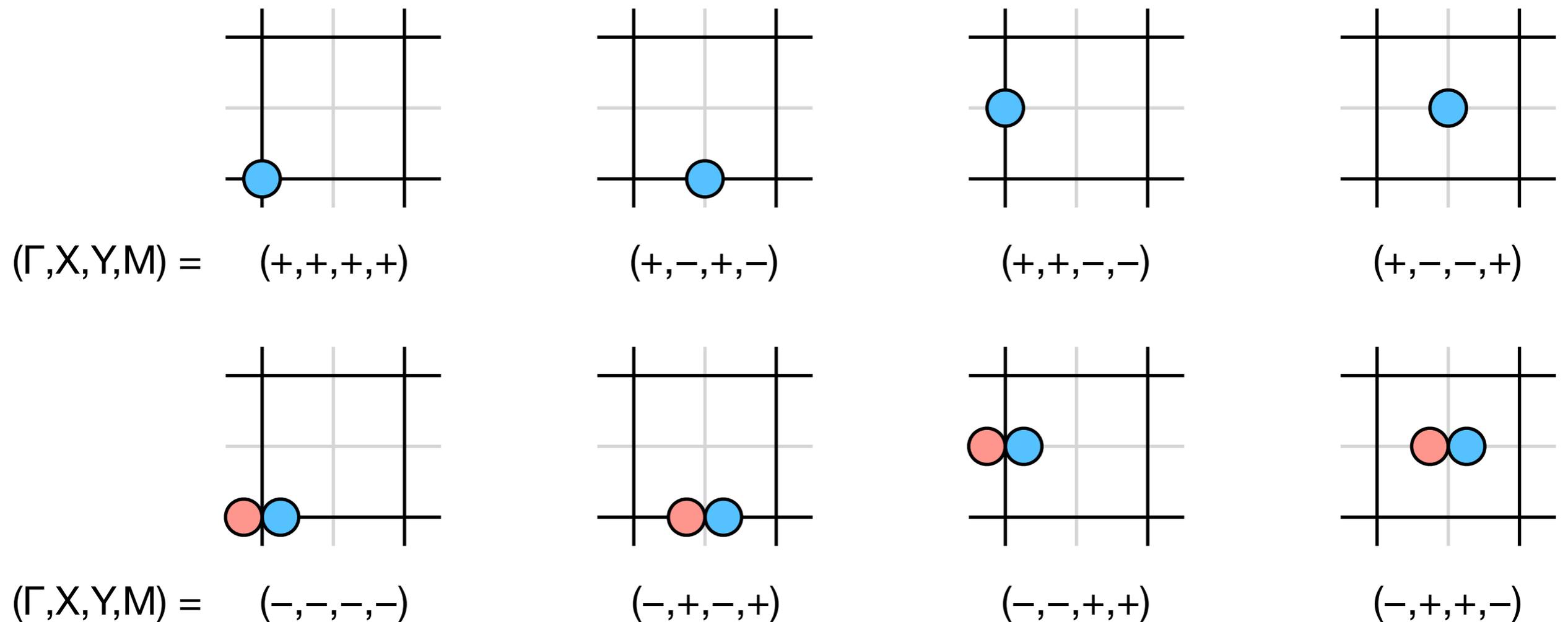
# Irrep contents of A1

Representation content changes

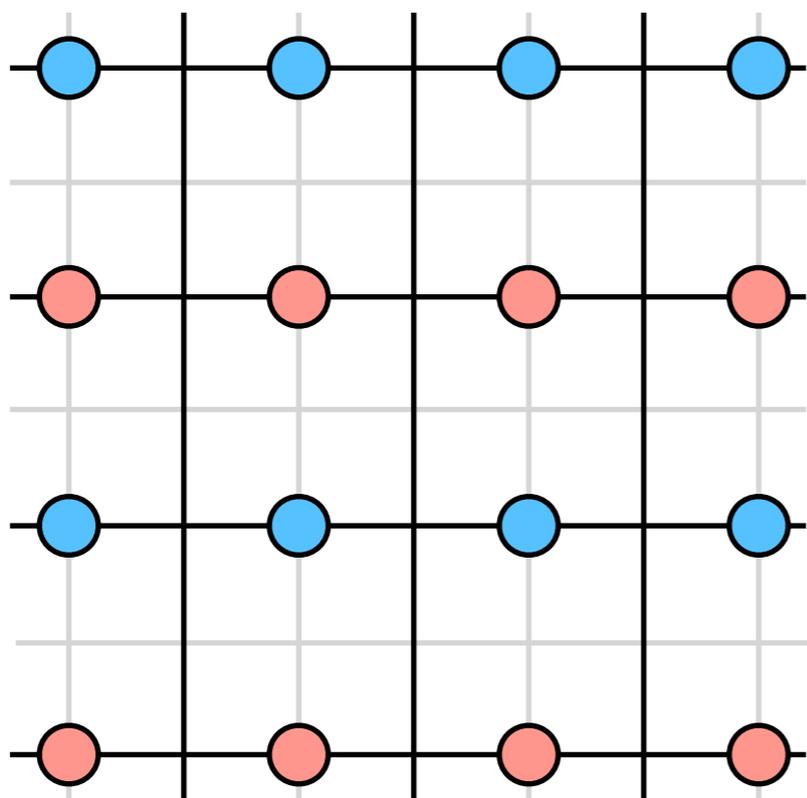
depending on the position  $\mathbf{x}$  and the orbital type



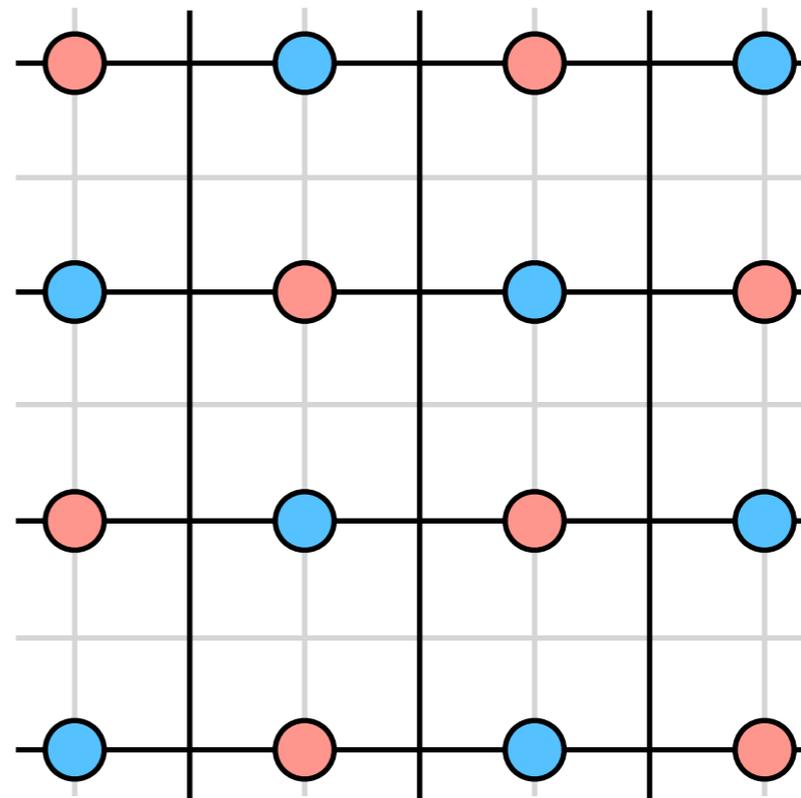
8 - 3 = 5 independent combinations



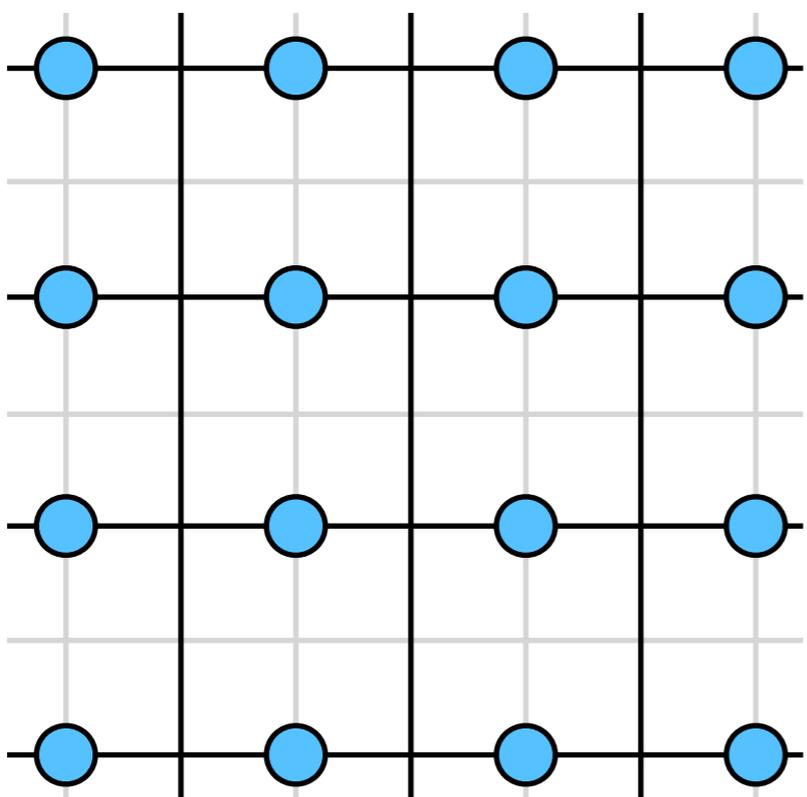
$k = (0, \pi)$   
 $l = +1$



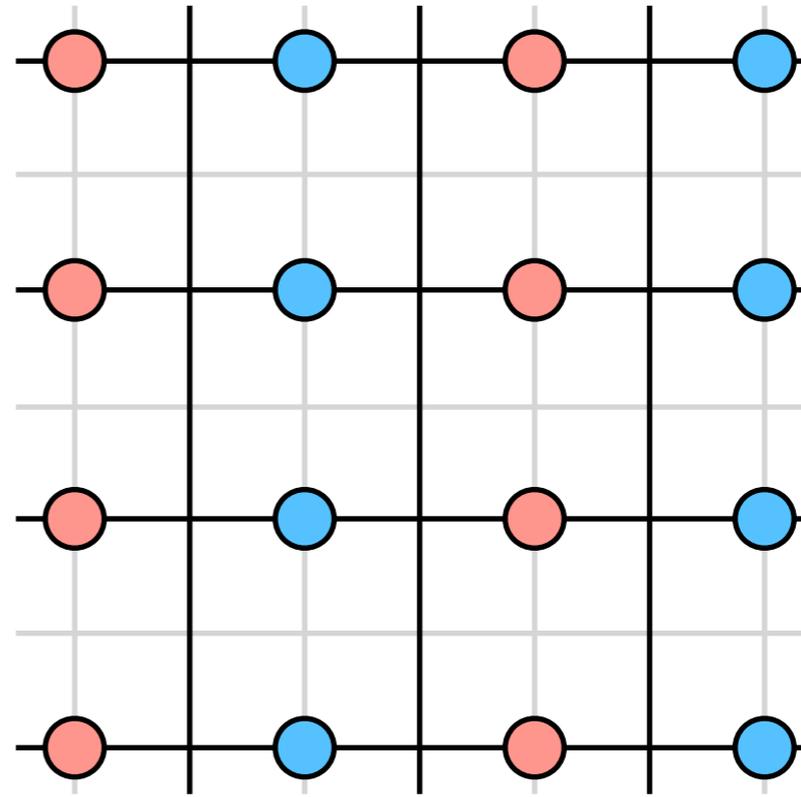
$k = (\pi, \pi)$   
 $l = -1$



$k = (0, 0)$   
 $l = +1$



$k = (\pi, 0)$   
 $l = -1$



# **Symmetry-Based Indicators of the Band Topology**

# Our main results

$$\mathbf{b} = (n_{k_1^1}, n_{k_1^2}, \dots, n_{k_2^1}, n_{k_2^2}, \dots)$$

1. Every  $\mathbf{b}$  can be expanded as  $\mathbf{b} = \sum_i q_i \mathbf{a}_i$   
(We have enough varieties of AI)

Conversly, one can get full list of  $\mathbf{b}$  by superposing  $\mathbf{a}$   
(with possibly fractional coefficients)

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(We have enough varieties of AI)

Conversly, one can get full list of  $\mathbf{b}$  by superposing  $\mathbf{a}$   
(with possibly fractional coefficients)

2. Sufficient condition to be a topological insulators

(1)  $\mathbf{b} = \sum_i n_i \mathbf{a}_i$  all  $n_i$ 's are nonnegative integers

(2)  $\mathbf{b} = \sum_i n_i \mathbf{a}_i$  all  $n_i$ 's are integers but some of them are negative

**Topological!**

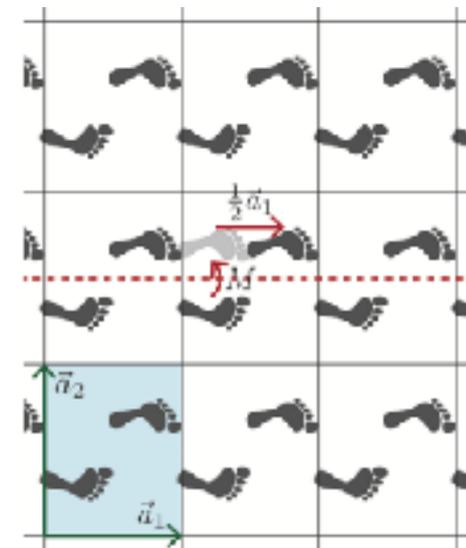
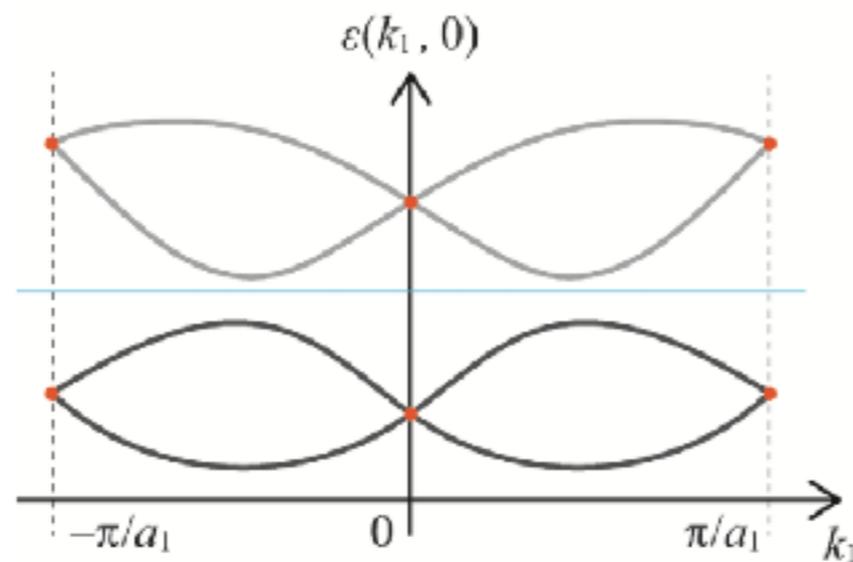
(3)  $\mathbf{b} = \sum_i q_i \mathbf{a}_i$  not all  $n_i$ 's are integers

(by product)

# Filling constraints for band insulators

Nonsymmorphic symmetries protect additional band crossing

L. Michel and J. Zak, Phys. Rep. 341, 377 (2001)

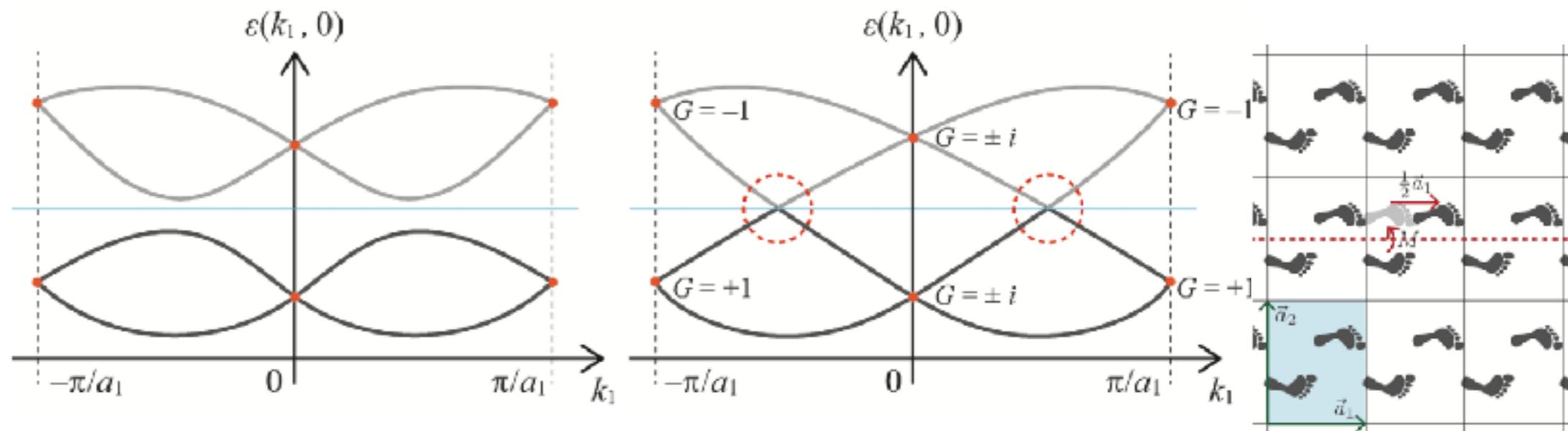


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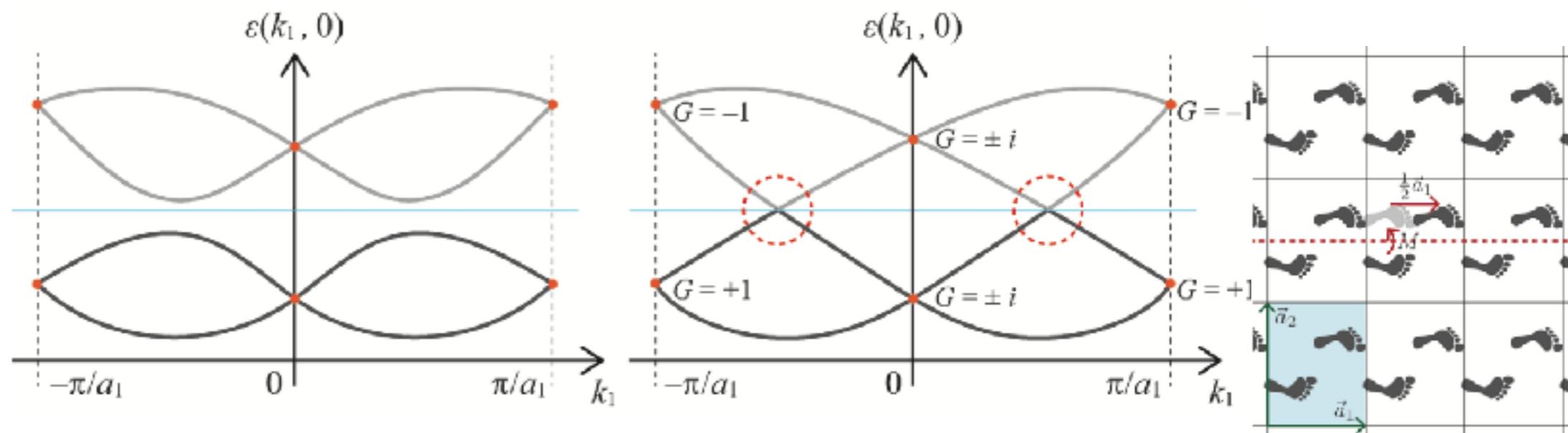


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How many number of bands do we need to realize band insulators?

Phys. Rev. Lett. (2016)

# Filling

Nonsymm

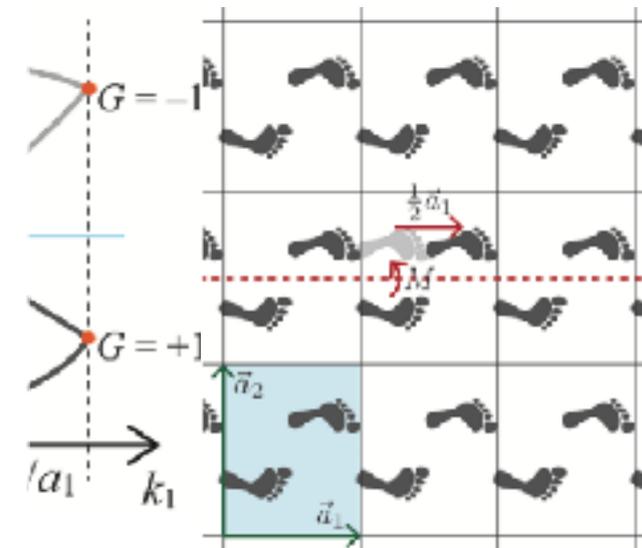


No.	$\nu$												
4	$4n$	39	$4n$	66	$4n$	100	$4n$	129	$4n$	165	$4n$	201	$4n$
7	$4n$	40	$4n$	67	$4n$	101	$4n$	130	$8n$	167	$4n$	203	$4n$
9	$4n$	41	$4n$	68	$4n$	102	$4n$	131	$4n$	169	$12n$	205	$8n$
11	$4n$	43	$4n$	70	$4n$	103	$4n$	132	$4n$	170	$12n$	206	$8n$
13	$4n$	45	$4n$	72	$4n$	104	$4n$	133	$8n$	171	$6n$	208	$4n$
14	$4n$	46	$4n$	73	$8n$	105	$4n$	134	$4n$	172	$6n$	210	$4n$
15	$4n$	48	$4n$	74	$4n$	106	$8n$	135	$8n$	173	$4n$	212	$8n$
17	$4n$	49	$4n$	76	$8n$	108	$4n$	136	$4n$	176	$4n$	213	$8n$
18	$4n$	50	$4n$	77	$4n$	109	$4n$	137	$4n$	178	$12n$	214	$4n$
19	$8n$	51	$4n$	78	$8n$	110	$8n$	138	$8n$	179	$12n$	218	$4n$
20	$4n$	52	$8n$	80	$4n$	112	$4n$	140	$4n$	180	$6n$	219	$4n$
24	$4n$	53	$4n$	84	$4n$	113	$4n$	141	$4n$	181	$6n$	220	$4n^+$
26	$4n$	54	$8n$	85	$4n$	114	$4n$	142	$8n$	182	$4n$	222	$4n$
27	$4n$	55	$4n$	86	$4n$	116	$4n$	144	$6n$	184	$4n$	223	$4n$
28	$4n$	56	$8n$	88	$4n$	117	$4n$	145	$6n$	185	$4n$	224	$4n$
29	$8n$	57	$8n$	90	$4n$	118	$4n$	151	$6n$	186	$4n$	226	$4n$
30	$4n$	58	$4n$	91	$8n$	120	$4n$	152	$6n$	188	$4n$	227	$4n$
31	$4n$	59	$4n$	92	$8n$	122	$4n$	153	$6n$	190	$4n$	228	$8n$
32	$4n$	60	$8n$	93	$4n$	124	$4n$	154	$6n$	192	$4n$	230	$8n$
33	$8n$	61	$8n$	94	$4n$	125	$4n$	158	$4n$	193	$4n$		
34	$4n$	62	$8n$	95	$8n$	126	$4n$	159	$4n$	194	$4n$		
36	$4n$	63	$4n$	96	$8n$	127	$4n$	161	$4n$	198	$8n$		
37	$4n$	64	$4n$	98	$4n$	128	$4n$	163	$4n$	199	$4n$		

How many nu

# ulators

id crossing  
 41, 377 (2001)

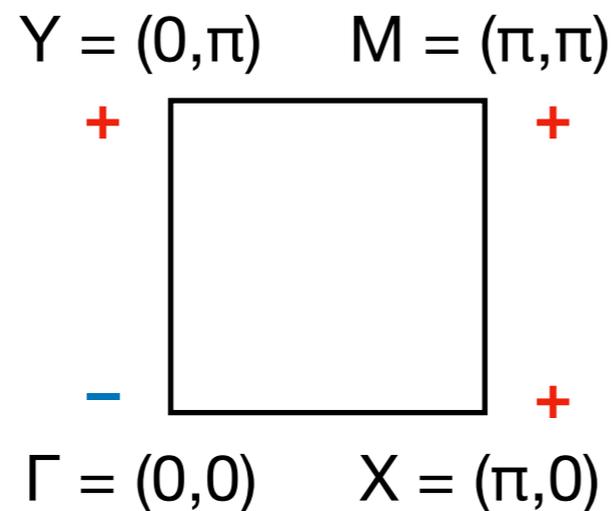


id insulators?  
 Rev. Lett. (2016)

# Example 1: Chern insulator

Chern Insulator

$$\mathbf{b} = (-, +, +, +)$$



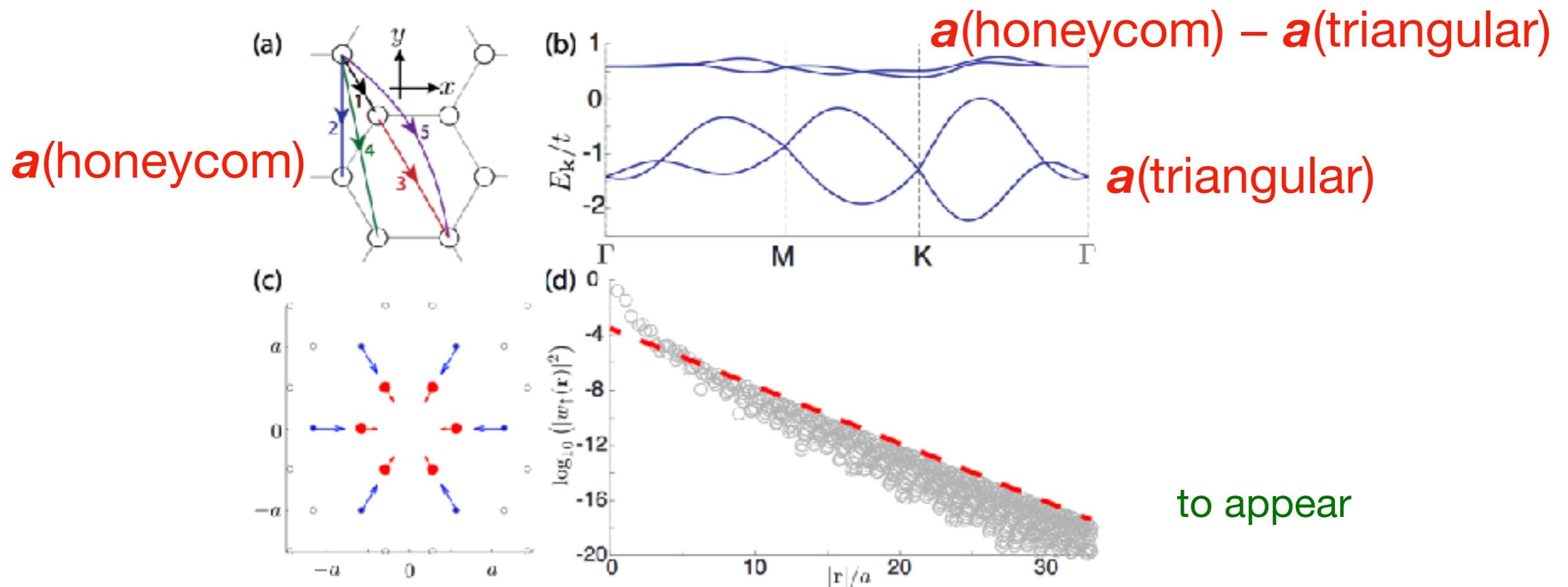
Sum of atomic Insulators

$$= \frac{1}{2} \left( \begin{array}{c} \text{Grid with blue dot at } (1,1) \\ \mathbf{a}_1 = (+, +, +, +) \end{array} - \begin{array}{c} \text{Grid with blue dot at } (2,1) \\ \mathbf{a}_2 = (+, -, +, -) \end{array} + \begin{array}{c} \text{Grid with red and blue dots at } (1,2) \\ \mathbf{a}_3 = (-, -, +, +) \end{array} + \begin{array}{c} \text{Grid with red and blue dots at } (2,2) \\ \mathbf{a}_4 = (-, +, +, -) \end{array} \right)$$

# Example 2: Fragile Topology

## “trivial = trivial + topological”

Example: TB model on honeycomb lattice with strong SOC



Not connected to atomic limit / no Wannier  $\rightarrow$  topological  
 but NO topological index or edge state  $\rightarrow$  fragile

# K-theory type classification

- Set of valid ***b***'s :  $\{\text{BS}\} = Z^{d_{\text{BS}}}$   $\{\text{BS}\} > \{\text{AI}\}$
- Set of all ***a***'s (***b***'s corresponding to AI):  $\{\text{AI}\} = Z^{d_{\text{AI}}}$

# K-theory type classification

- Set of valid  $\mathbf{b}$ 's :  $\{\text{BS}\} = \mathbb{Z}^{d_{\text{BS}}}$   $\{\text{BS}\} > \{\text{AI}\}$
- Set of all  $\mathbf{a}$ 's ( $\mathbf{b}$ 's corresponding to AI):  $\{\text{AI}\} = \mathbb{Z}^{d_{\text{AI}}}$

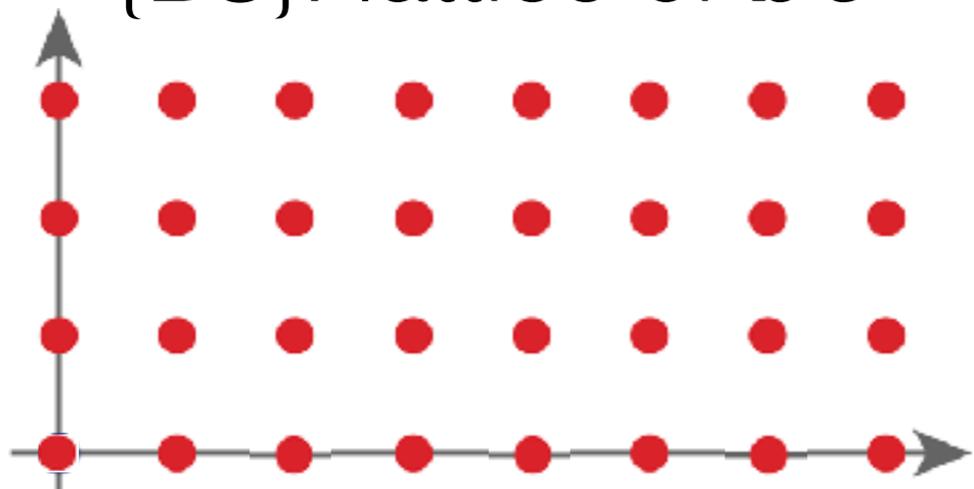
$$\begin{aligned} \text{Quotient space: } X &= \{\text{BS}\}/\{\text{AI}\} \\ &= \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \dots \times \mathbb{Z}_{n_N} \end{aligned}$$

# K-theory type classification

- Set of valid  $\mathbf{b}$ 's :  $\{\text{BS}\} = \mathbb{Z}^{d_{\text{BS}}}$   $\{\text{BS}\} > \{\text{AI}\}$
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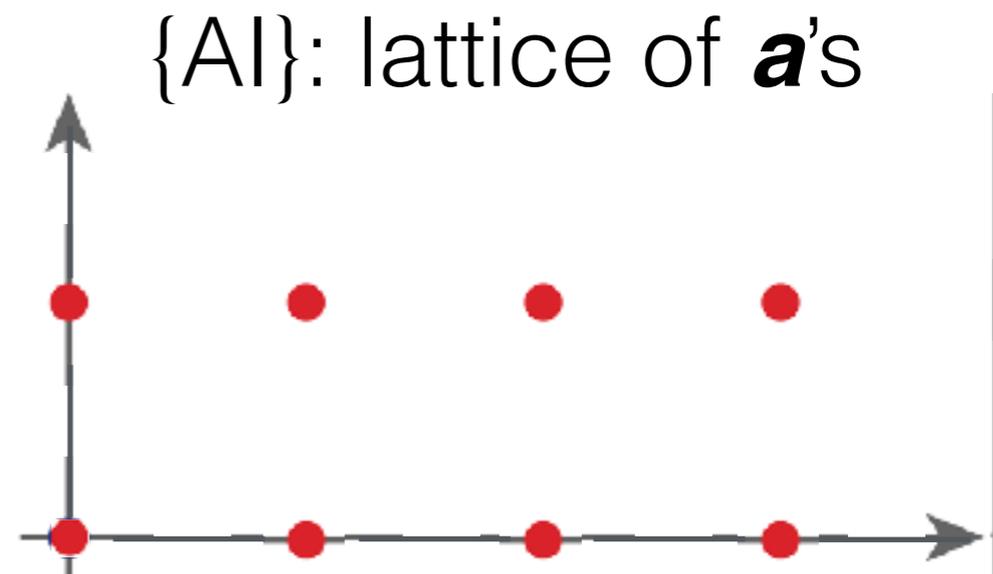
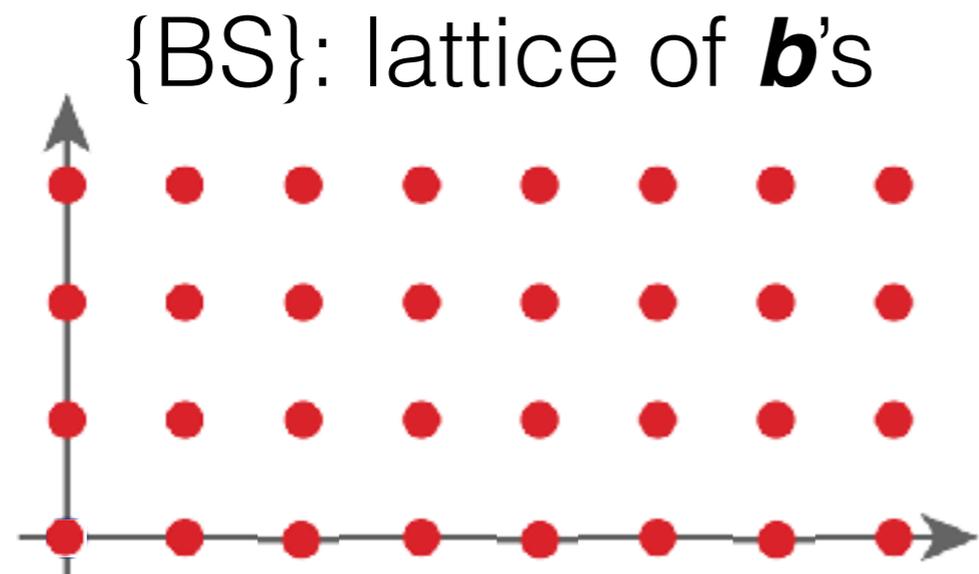
$\{\text{BS}\}$ : lattice of  $\mathbf{b}$ 's



# K-theory type classification

- Set of valid  $\mathbf{b}$ 's :  $\{\text{BS}\} = \mathbb{Z}^{d_{\text{BS}}}$   $\{\text{BS}\} > \{\text{AI}\}$
- Set of all  $\mathbf{a}$ 's ( $\mathbf{b}$ 's corresponding to AI):  $\{\text{AI}\} = \mathbb{Z}^{d_{\text{AI}}}$

$$\begin{aligned} \text{Quotient space: } X &= \{\text{BS}\} / \{\text{AI}\} \\ &= \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \dots \times \mathbb{Z}_{n_N} \end{aligned}$$

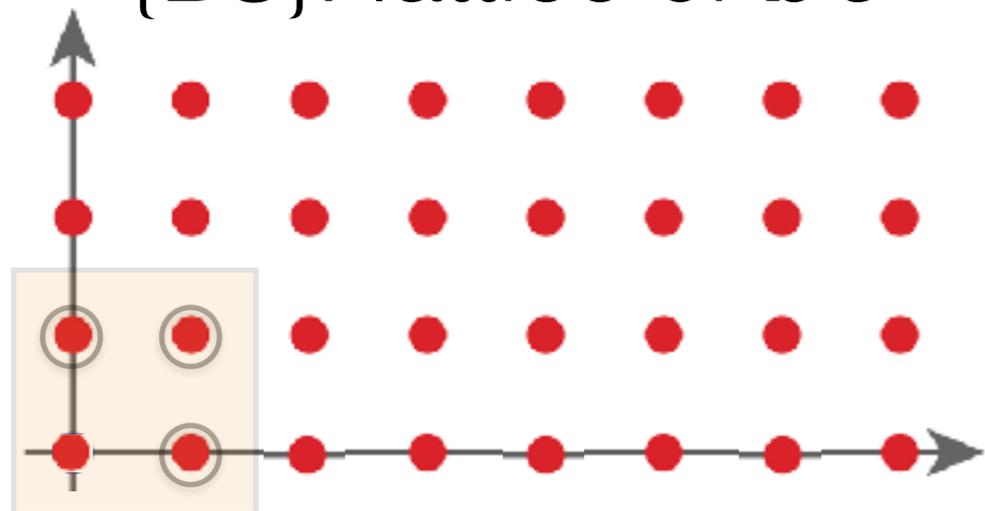


# K-theory type classification

- Set of valid  $\mathbf{b}$ 's :  $\{\text{BS}\} = \mathbb{Z}^{d_{\text{BS}}}$   $\{\text{BS}\} > \{\text{AI}\}$
- Set of all  $\mathbf{a}$ 's ( $\mathbf{b}$ 's corresponding to AI):  $\{\text{AI}\} = \mathbb{Z}^{d_{\text{AI}}}$

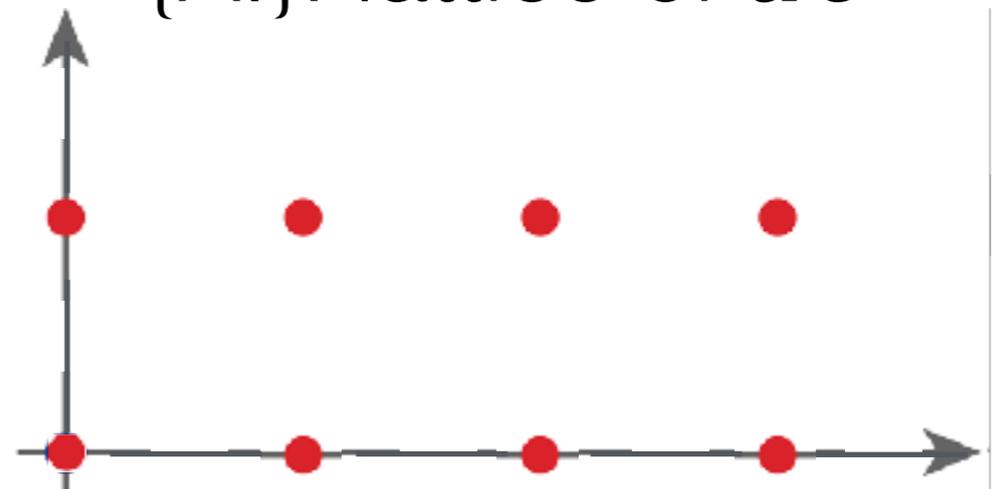
$$\begin{aligned} \text{Quotient space: } X &= \{\text{BS}\} / \{\text{AI}\} \\ &= \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \dots \times \mathbb{Z}_{n_N} \end{aligned}$$

$\{\text{BS}\}$ : lattice of  $\mathbf{b}$ 's



$$X = \mathbb{Z}_2 \times \mathbb{Z}_2$$

$\{\text{AI}\}$ : lattice of  $\mathbf{a}$ 's



# 230 SGs x TRS with SOC

$d$	SGs
1	1, 3, 4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46 76, 77, 78, 80, 91, 92, 93, 94, 95, 96, 98, 101, 102 105, 106, 109, 110, 144, 145, 151, 152, 153, 154 169, 170, 171, 172, 178, 179, 180, 181
2	79, 90, 97, 100, 104, 107, 108, 146, 155, 160, 161 195, 196, 197, 198, 199, 208, 210, 212, 213, 214
3	48, 50, 52, 54, 56, 57, 59, 60, 61, 62, 68, 70, 73 75, 89, 99, 103, 112, 113, 114, 116, 117, 118, 120 122, 133, 142, 150, 157, 159, 173, 182, 185 186, 209, 211
4	63, 64, 72, 121, 126, 130, 135, 137, 138, 143, 149 156, 158, 168, 177, 183, 184, 207, 218, 219, 220
5	11, 13, 14, 15, 49, 51, 53, 55, 58, 66, 67, 74, 81 82, 86, 88, 111, 115, 119, 134, 136, 141, 167 217, 228, 230
6	69, 71, 85, 125, 129, 132, 163, 165, 190, 201 203, 205, 206, 215, 216, 222
7	12, 65, 84, 128, 131, 140, 188, 189, 202, 204, 223
8	124, 127, 148, 166, 193, 200, 224, 226, 227
9	2, 10, 47, 87, 139, 147, 162, 164, 176, 192, 194
10	174, 187
11	225, 229
13	83, 123
14	175, 191, 221

$X_{BS}$	SGs
$\mathbb{Z}_2$	81, 82, 111, 112, 113, 114, 115, 116, 117 118, 119, 120, 121, 122, 215, 216, 217 218, 219, 220
$\mathbb{Z}_3$	188, 190
$\mathbb{Z}_4$	52, 56, 58, 60, 61, 62, 70, 88, 126 130, 133, 135, 136, 137, 138, 141, 142 163, 165, 167, 202, 203, 205, 222, 223 227, 228, 230
$\mathbb{Z}_8$	128, 225, 226
$\mathbb{Z}_{12}$	176, 192, 193, 194
$\mathbb{Z}_2 \times \mathbb{Z}_4$	14, 15, 48, 50, 53, 54, 55, 57, 59 63, 64, 66, 68, 71, 72, 73, 74, 84, 85 86, 125, 129, 131, 132, 134, 147, 148 162, 164, 166, 200, 201, 204, 206, 224
$\mathbb{Z}_2 \times \mathbb{Z}_8$	87, 124, 139, 140, 229
$\mathbb{Z}_3 \times \mathbb{Z}_3$	174, 187, 189
$\mathbb{Z}_4 \times \mathbb{Z}_8$	127, 221
$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	175, 191
$(\mathbb{Z}_2)^2 \times \mathbb{Z}_4$	11, 12, 13, 49, 51, 65, 67, 69
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	83, 123
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	2, 10, 47

# 230 SGs x TRS without SOC

$d$	SGs
1	1, 4, 7, 9, 19, 29, 33, 76, 78, 144, 145, 169, 170
2	8, 31, 36, 41, 43, 80, 92, 96, 110, 146, 161, 198
3	5, 6, 18, 20, 26, 30, 32, 34, 40, 45, 46, 61, 106 109, 151, 152, 153, 154, 159, 160, 171, 172, 173, 178, 179, 199, 212, 213
4	24, 28, 37, 39, 60, 62, 77, 79, 91, 95, 102, 104 143, 155, 157, 158, 185, 186, 196, 197, 210
5	3, 14, 17, 27, 42, 44, 52, 56, 57, 94, 98, 100, 101 108, 114, 122, 150, 156, 182, 214, 220
6	11, 15, 35, 38, 54, 70, 73, 75, 88, 90, 103, 105, 107 113, 142, 149, 167, 168, 184, 195, 205, 219
7	13, 22, 23, 59, 64, 68, 82, 86, 117, 118, 120, 130, 163 165, 180, 181, 203, 206, 208, 209, 211, 218, 228, 230
8	21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217
9	2, 25, 48, 50, 53, 55, 72, 99, 121, 126, 138, 141 147, 188, 207, 216, 222
10	12, 74, 93, 112, 119, 176, 177, 202, 204, 215
11	66, 84, 128, 136, 166, 227
12	51, 87, 89, 115, 129, 134, 162, 164, 174, 189, 193, 223, 226
13	16, 67, 111, 125, 194, 224
14	49, 140, 192, 200
15	10, 69, 71, 124, 127, 132, 187
17	225, 229
18	65, 83, 131, 139, 175
22	221
24	191
27	47, 123

$X_{BS}$	SGs
$\mathbb{Z}_2$	3, 11, 14, 27, 37, 48, 49, 50, 52, 53, 54, 56 58, 60, 66, 68, 70, 75, 77, 82, 85, 86, 88 103, 124, 128, 130, 162, 163, 164, 165, 166 167, 168, 171, 172, 176, 184, 192, 201, 203
$(\mathbb{Z}_2)^2$	12, 13, 15, 81, 84, 87
$\mathbb{Z}_2 \times \mathbb{Z}_4$	147, 148
$(\mathbb{Z}_2)^3$	10, 83, 175
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	2

# Example 3: reQBI

Inversion & TR symmetric 3D system (SG2 & TRS)

$$X = Z_2 \times Z_2 \times Z_2 \times Z_4$$

# Example 3: reQBI

Inversion & TR symmetric 3D system (SG2 & TRS)

$$X = \textcircled{Z_2} \times \textcircled{Z_2} \times \textcircled{Z_2} \times Z_4$$

weak TI

# Example 3: reQBI

Inversion & TR symmetric 3D system (SG2 & TRS)

$$X = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

weak TI      strong TI + d

# Example 3: reQBI

Inversion & TR symmetric 3D system (SG2 & TRS)

$$X = \textcircled{Z_2} \times \textcircled{Z_2} \times \textcircled{Z_2} \times \textcircled{Z_4}$$

weak TI      strong TI +  $\alpha$

Two copies of TI

No surface Dirac / no magnetoelectric response.

# Example 3: reQBI

Inversion & TR symmetric 3D system (SG2 & TRS)

$$X = \textcircled{Z_2} \times \textcircled{Z_2} \times \textcircled{Z_2} \times \textcircled{Z_4}$$

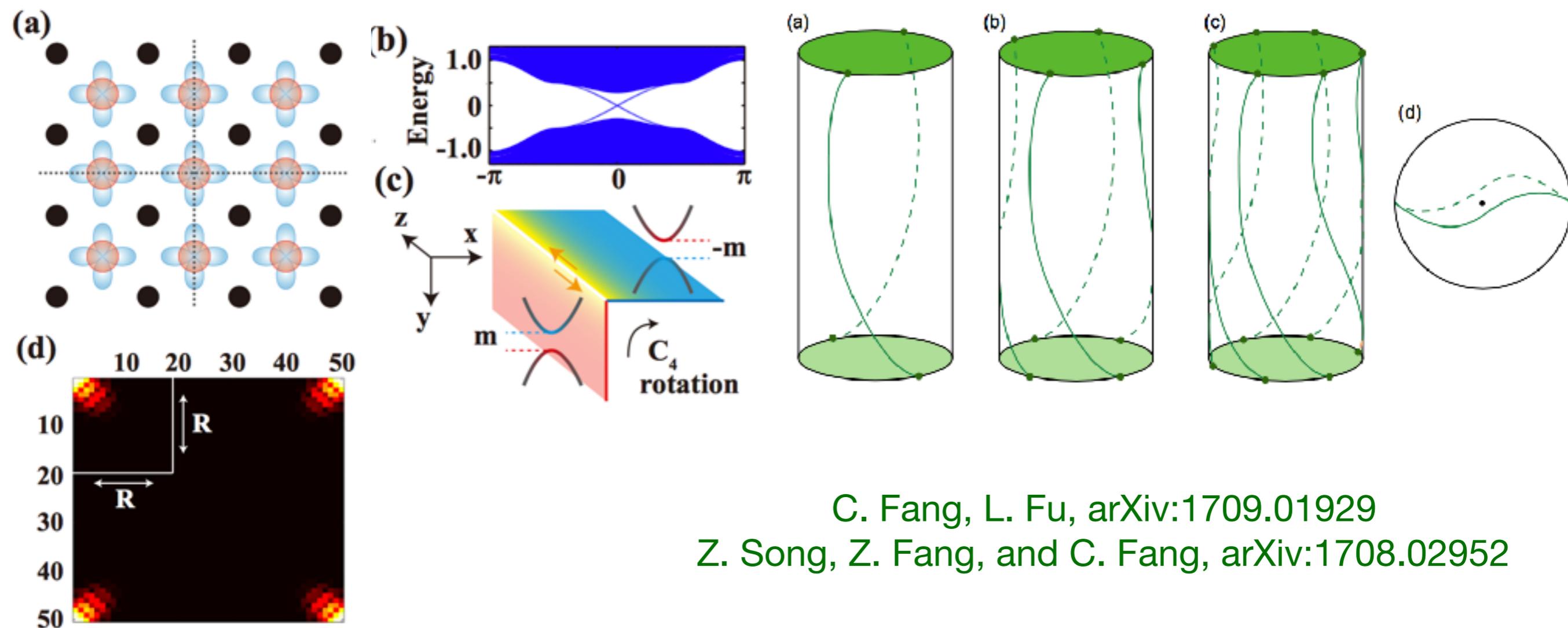
weak TI      strong TI +  $\alpha$

Two copies of TI

No surface Dirac / no magnetoelectric response.

Still topologically nontrivial.

# 1D edge state on the surface of 3D TCI



C. Fang, L. Fu, arXiv:1709.01929

Z. Song, Z. Fang, and C. Fang, arXiv:1708.02952

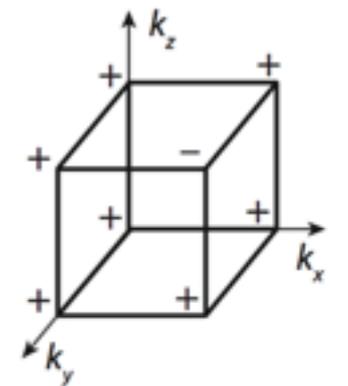
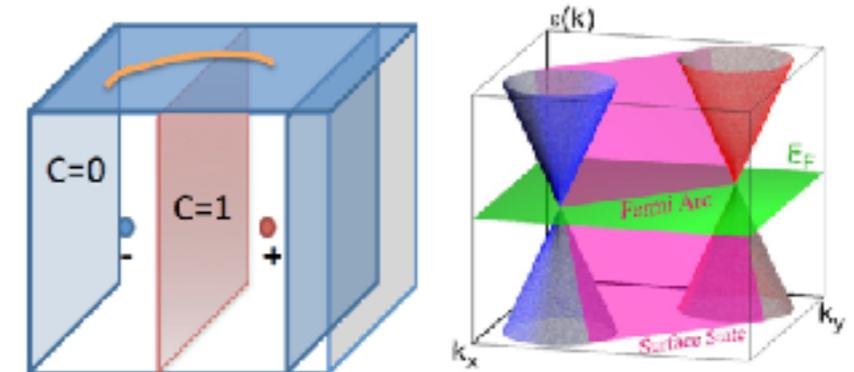
These 1D edges can be identified from the symmetry-based indicator!!

# Example 4: Representation-enforced Semimetal

Inversion symmetric but TR broken 3D system (SG2)

$$X = Z_2 \times Z_2 \times Z_2 \times \textcircled{Z_4}$$

A. Turner, ..., A. Vishwanath (2010) Weyl SM

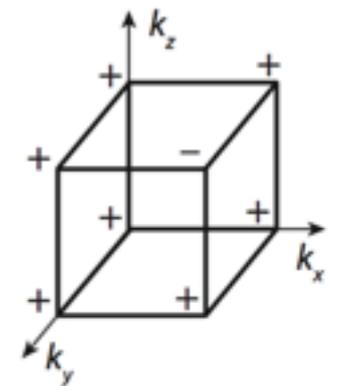
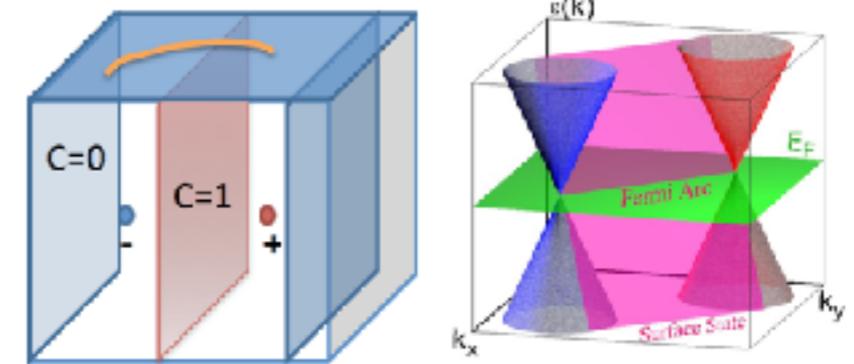


# Example 4: Representation-enforced Semimetal

Inversion symmetric but TR broken 3D system (SG2)

$$X = Z_2 \times Z_2 \times Z_2 \times \textcircled{Z_4}$$

A. Turner, ..., A. Vishwanath (2010) Weyl SM



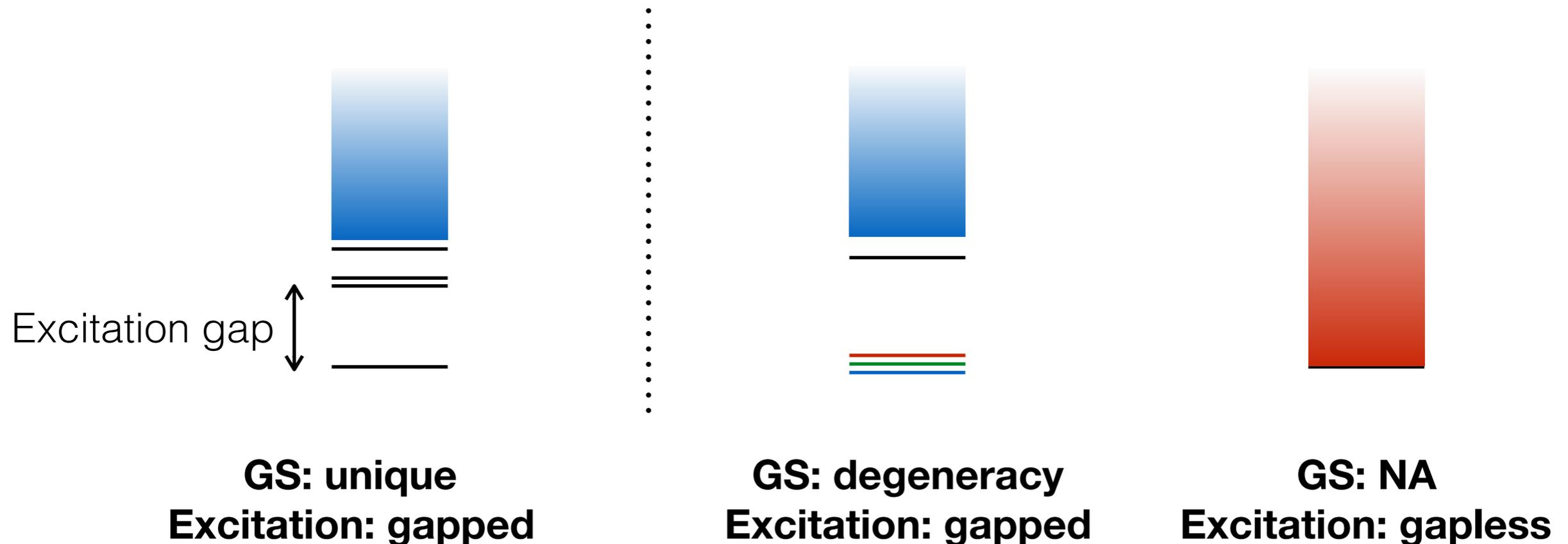
{BS}: “band structure” can be *semimetal*  
(*band touching at generic points in BZ*)

(We demanded band gap only at high-symmetric momenta)

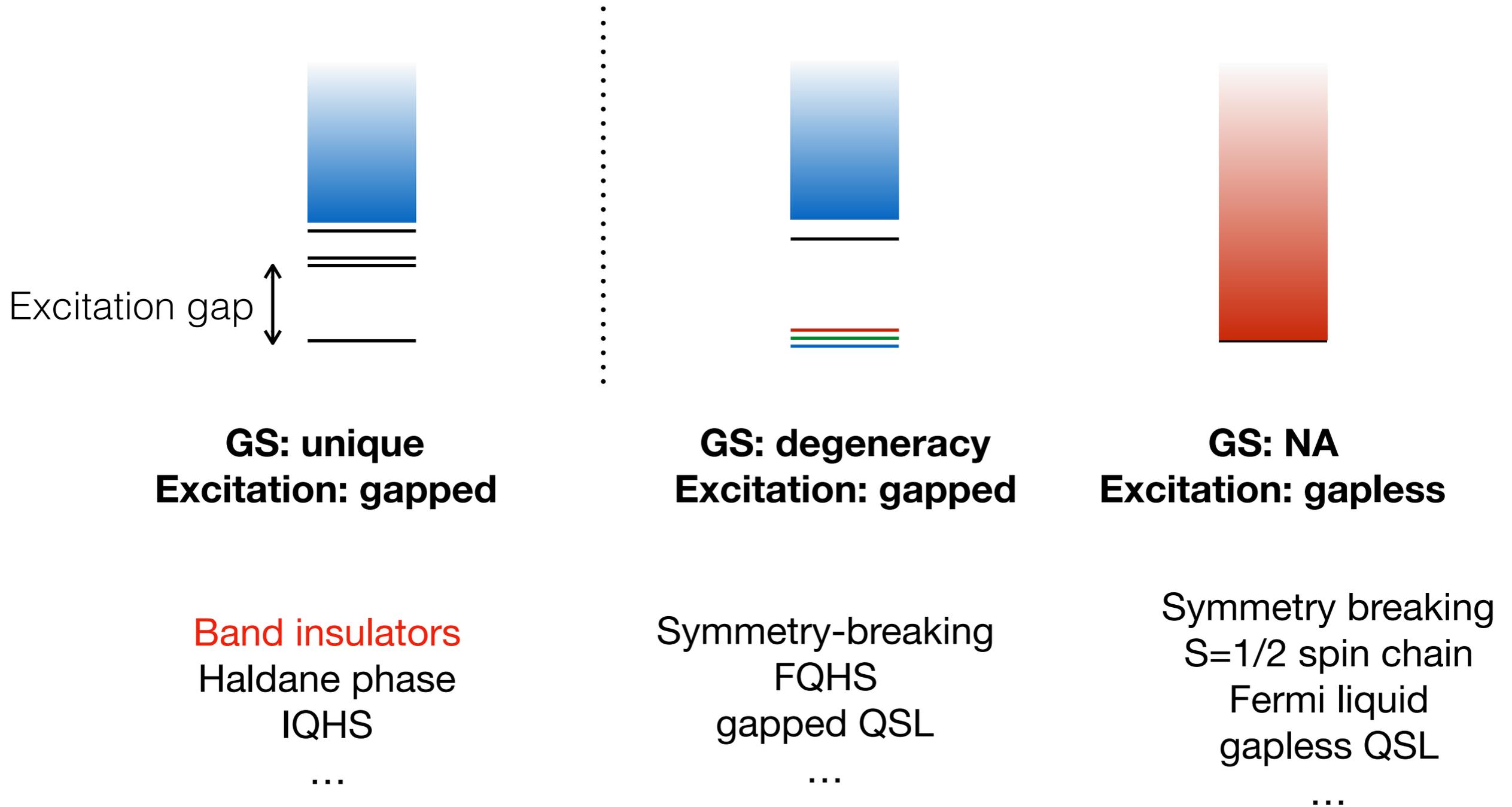
**Interaction effect**

# Three possibilities of Low energy spectrum

- Exact diagonalization under the periodic boundary condition
- Neglect finite size effect



# Three possibilities of Low energy spectrum



# Filling constraints in interacting systems

# Lieb-Schultz-Mattis theorem

LSM (1961)

## Unique Gapped GS $\rightarrow$ filling $\nu$ is even

- Assume  $U(1)$  & translation symmetry
- filling  $\nu =$  average number of particles per uc
- Extension to general class of  $H$ , higher  $D$

Affleck-Lieb (1988)

Yamanaka-Oshikawa-Affleck (1997)

Oshikawa (2000)

Hastings (2004)

# Refinement of Lieb-Schultz-Mattis for nonsymmorphic SGs

- Assume  $U(1)$  & **space group symmetry**
- Unique Gapped GS  $\rightarrow$  filling  $\nu$  is an integer multiple of  $m$
- $m = 2, 3, 4, 6$  depending on SG

Sid et al, (2013)  
PNAS (2015)

# Refinement of Lieb-Schultz-Mattis for spin-orbit coupled electrons

- If  $S_z$  is conserved  $v = v_{\uparrow} + v_{\downarrow}$

Apply LSM for  $v_{\uparrow}$  and  $v_{\downarrow}$  separately

$v = v_{\uparrow} + v_{\downarrow}$  ( $v_{\uparrow}=v_{\downarrow}$ ) must be even for unique gapped GS

- Even when  $S_z$  is not conserved

TRS is sufficient to prove  $v$  must be even

$v$  must be an integer multiple of  $2m$

PNAS (2015)

No.	No.	No.	No.	No.	No.	No.							
4	4n	39	4n	66	4n	100	4n	129	4n	165	4n	201	4n
7	4n	40	4n	67	4n	101	4n	130	8n	167	4n	203	4n
9	4n	41	4n	68	4n	102	4n	131	4n	169	12n	205	8n
11	4n	43	4n	70	4n	103	4n	132	4n	170	12n	206	4n <sup>†</sup>
13	4n	45	4n	72	4n	104	4n	133	4n <sup>†</sup>	171	6n	208	4n
14	4n	46	4n	73	4n <sup>†a</sup>	105	4n	134	4n	172	6n	210	4n
15	4n	48	4n	74	4n	106	4n <sup>†</sup>	135	4n <sup>†</sup>	173	4n	212	8n
17	4n	49	4n	76	8n	108	4n	136	4n	176	4n	213	8n
18	4n	50	4n	77	4n	109	4n	137	4n	178	12n	214	4n
19	8n	51	4n	78	8n	110	4n <sup>†</sup>	138	8n	179	12n	218	4n
20	4n	52	8n	80	4n	112	4n	140	4n	180	6n	219	4n
24	4n	53	4n	84	4n	113	4n	141	4n	181	6n	220	4n <sup>b</sup>
26	4n	54	8n	85	4n	114	4n	142	4n <sup>†</sup>	182	4n	222	4n
27	4n	55	4n	86	4n	116	4n	144	6n	184	4n	223	4n
28	4n	56	8n	88	4n	117	4n	145	6n	185	4n	224	4n
29	8n	57	8n	90	4n	118	4n	151	6n	186	4n	226	4n
30	4n	58	4n	91	8n	120	4n	152	6n	188	4n	227	4n
31	4n	59	4n	92	8n	122	4n	153	6n	190	4n	228	4n <sup>†</sup>
32	4n	60	8n	93	4n	124	4n	154	6n	192	4n	230	4n <sup>†</sup>
33	8n	61	8n	94	4n	125	4n	158	4n	193	4n		
34	4n	62	8n	95	8n	126	4n	159	4n	194	4n		
36	4n	63	4n	96	8n	127	4n	161	4n	198	8n		
37	4n	64	4n	98	4n	128	4n	163	4n	199	4n		

## Classification of all 230 space groups

Name of flat manifold

ITC No. (symbol) of elementary group  $\Gamma$  / condition on  $\nu$ .

List of space groups whose maximal elementary  $t$ -subgroup is  $\Gamma$ .  
The **bold italic** indicates that the most symmetric Wyckoff position of the space group corresponds to a lattice with more than  $\nu_{\text{min}}/2$  sites in each unit cell, implying that  $\nu_{\text{min}}$  cannot be realized by any atomic insulator.

### Symmorphic

#### Torus

No. 1 ( $P1$ )  $\nu \in 2\mathbb{Z}$

1, 2, 3, 5, 6, 8, 10, 12, 16, 21, 22, 23, 25, 35, 38, 42, 44, 47, 65, 69, 71, 75, 79, 81, 82, 83, 87, 89, 99, 107, 111, 115, 119, 121, 123, 139, 143, 146, 147, 148, 149, 150, 155, 156, 157, 160, 162, 164, 166, 168, 174, 175, 177, 183, 187, 189, 191, 195, 196, 197, 200, 202, 204, 207, 209, 211, 215, 216, 217, 221, 225, 229.

### Non-symmorphic

#### Dicosm

No. 4 ( $P2_1$ )  $\nu \in 4\mathbb{Z}$

4, 11, 14, 17, 18, 20, 26, 31, 36, 51, 53, 55, 58, 59, 63, 64, 90, 94, 113, 114, 127, 128, 129, **135**, 136, 137, 173, 176, 182, 185, 186, 193, 194.

#### Tetracosm

No. 76, 78 ( $P4_1, P4_2$ )  $\nu \in 8\mathbb{Z}$

76, 78, 91, 92, 95, 96, 212, 213.

No. 77 ( $P4_1$ )  $\nu \in 4\mathbb{Z}$

77, 84, 86, 93, 94, 101, 102, 105, **106**, 131, 132, **133**, 134, **135**, 136, 137, 208, 223, 224.

#### Tricosm

No. 144, 145 ( $P3_1, P3_2$ )  $\nu \in 6\mathbb{Z}$

144, 145, 151, 152, 153, 154, 171, 172, 180, 181.

#### Hexacosm

No. 169, 170 ( $P6_1, P6_2$ )  $\nu \in 12\mathbb{Z}$

169, 170, 178, 179.

No. 171, 172 ( $P6_3, P6_6$ )  $\nu \in 6\mathbb{Z}$

171, 172, 180, 181.

No. 173 ( $P6_3$ )  $\nu \in 4\mathbb{Z}$

173, 176, 182, 185, 186, 193, 194.

#### Didicosm

No. 19 ( $P2_1 2_1 2_1$ )  $\nu \in 8\mathbb{Z}$

19, 61, 62, 92, 96, 198, 205, 212, 213.

No. 24 ( $I2_1 2_1 2_1$ )  $\nu \in 4\mathbb{Z}$

24, 73, 74, 98, 122, 141, **142**, **199**, **206**, 210, **214**, 220, 227, 228, 230.

No. 80 ( $I4_1$ )  $\nu \in 4\mathbb{Z}$

80, 88, 98, 109, **110**, 141, **142**, 210, **214**, 227, 228, 230.

#### 2nd Amphicosm

No. 9 ( $Cc$ )  $\nu \in 4\mathbb{Z}$

9, 15, 36, 37, 40, 41, 43, 45, 46, 63, 64, 66, 68, 70, 72, **73**, 74, 88, 103, 104, 105, **106**, 108, 109, **110**, 112, 114, 120, 122, 124, 126, 128, 131, **133**, **135**, 137, 140, 141, **142**, 158, 159, 161, 163, 165, 167, 184, 185, 186, 188, 190, 192, 193, 194, 203, **206**, 218, 219, **220**, 222, 223, 226, 227, **228**, **230**.

#### 1st Amphicosm

No. 7 ( $Pc$ )  $\nu \in 4\mathbb{Z}$

7, 13, 14, 26, 27, 28, 30, 31, 32, 34, 39, 41, 48, 49, 50, 51, 53, 55, 58, 59, 64, 67, 68, 85, 86, 100, 101, 102, 103, 104, **106**, 116, 117, 118, 124, 125, 126, 127, 128, 129, 132, **133**, 134, **135**, 136, 137, 201, 222, 224.

#### 1st Amphidicosm

No. 29 ( $Pca2_1$ )  $\nu \in 8\mathbb{Z}$

29, 54, 57, 60, 61, 205.

#### 2nd Amphidicosm

No. 33 ( $Pa2_1$ )  $\nu \in 8\mathbb{Z}$

33, 52, 56, 60, 62, 130, 138.

# Refinement of Lieb-Schultz-Mattis for spin models with $Z_2 \times Z_2$

PRL 119, 127202 (2017)

PHYSICAL REVIEW LETTERS

week ending  
22 SEPTEMBER 2017

## Lattice Homotopy Constraints on Phases of Quantum Magnets

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The Lieb-Schultz-Mattis (LSM) theorem and its extensions forbid trivial phases from arising in certain quantum magnets. Constraining infrared behavior with the ultraviolet data encoded in the microscopic lattice of spins, these theorems tie the absence of spontaneous symmetry breaking to the emergence of exotic phases like quantum spin liquids. In this work, we take a new topological perspective on these theorems, by arguing they originate from an obstruction to “trivializing” the lattice under smooth, symmetric deformations, which we call the “lattice homotopy problem.” We conjecture that all LSM-like theorems for quantum magnets (many previously unknown) can be understood from lattice homotopy, which automatically incorporates the full spatial symmetry group of the lattice, including all its point-group symmetries. One consequence is that any spin-symmetric magnet with a half-integer moment on a site with even-order rotational symmetry must be a spin liquid. To substantiate the claim, we prove the conjecture in two dimensions for some physically relevant settings.

# Symmetry-based indicators of Chern numbers

TABLE XII. Symmetry-based indicators of band topology for systems of spinless fermions without time-reversal symmetry.

$X_{BS}$	Space groups
$\mathbb{Z}_2$	3, 11, 14, 27, 37, 45, 48, 49, 50, 52, 53, 54, 56, 58, 60, 61, 66, 68, 70, 73, 77, 79, 103, 104, 106, 110, 112, 114, 116, 117, 118, 120, 122, 126, 130, 133, 142, 162, 163, 164, 165, 166, 167, 171, 172, 184, 201, 203, 205, 206, 218, 219, 220, 222, 228, 230
$\mathbb{Z}_3$	143, 173, 188, 190
$\mathbb{Z}_4$	75, 124, 128
$\mathbb{Z}_6$	168, 192
$\mathbb{Z}_2 \times \mathbb{Z}_2$	12, 13, 15, 86, 88
$\mathbb{Z}_2 \times \mathbb{Z}_4$	84, 85, 148
$\mathbb{Z}_2 \times \mathbb{Z}_{12}$	147
$\mathbb{Z}_3 \times \mathbb{Z}_6$	176
$\mathbb{Z}_4 \times \mathbb{Z}_4$	87
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	10, 82
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	81
$\mathbb{Z}_3 \times \mathbb{Z}_3 \times \mathbb{Z}_3$	174
$\mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4$	83
$\mathbb{Z}_6 \times \mathbb{Z}_6 \times \mathbb{Z}_6$	175
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	2

$X_{BS}$ : the quotient group between the group of band structures and atomic insulators.

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$\mathbb{Z}_2$	P2 (3), 11, 14, 27, 37, 45, 48, 49, 50, 52, 53, 54, 56, 58, 60, 61, 66, 68, 70, 73, 77, 79, 103, 104, 106, 110, 112, 114, 116, 117, 118, 120, 122, 126, 130, 133, 142, 162, 163, 164, 165, 166, 167, 171, 172, 184, 201, 203, 205, 206, 218, 219, 220, 222, 228, 230
$\mathbb{Z}_3$	P3 (143), 173, 188, 190
$\mathbb{Z}_4$	P4 (75), 124, 128
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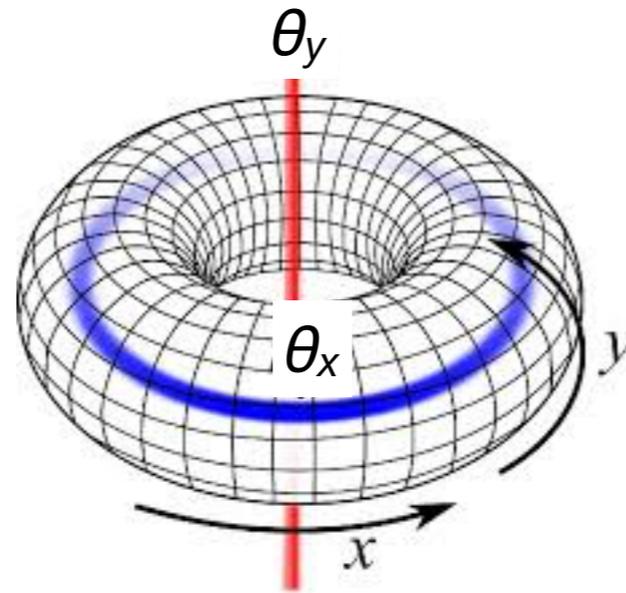
Cn rotation eigenvalues → Chern number modulo n

Chen Fang, Matthew J. Gilbert, B. Andrei Bernevig  
Phys. Rev. B 86, 115112 (2012)

$$i^C = \prod_{i \in occ.} (-1)^{F_i} \xi_i(\Gamma) \xi_i(M) \zeta_i(Y).$$

$X_{BS}$ : the quotient group between the group of band structures and atomic insulators.

# Symmetry-based indicators of **many-body** Chern number

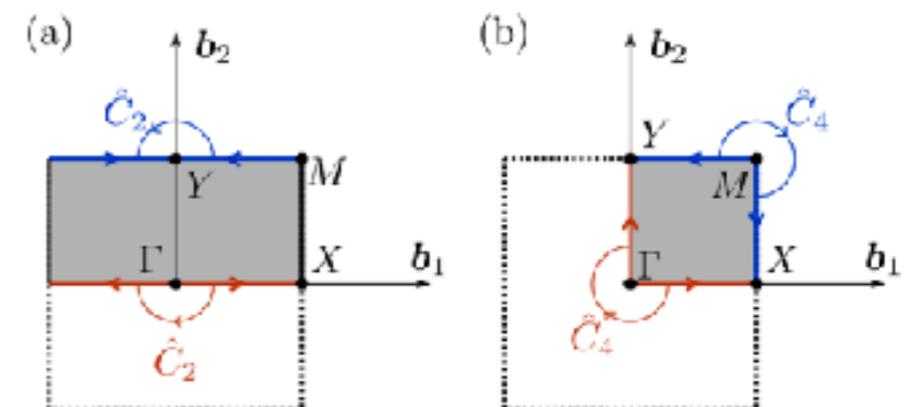


$$e^{\pi i C} = (-1)^C = \frac{w_{C_2}^X w_{C_2}^Y}{w_{C_2}^\Gamma w_{C_2}^M},$$

$$e^{\frac{-2\pi i C}{3}} = (-1)^{NS} w_{C_3}^\Gamma w_{C_3}^K w_{C_3}^{K'},$$

$$e^{\frac{-2\pi i C}{4}} = (-1)^{NS} w_{C_4}^\Gamma w_{C_4}^M w_{C_2}^X,$$

$$e^{\frac{-2\pi i C}{6}} = (-1)^{NS} w_{C_6}^\Gamma w_{C_3}^K w_{C_2}^M,$$



# New filling-constraints on **many-body** Chern number under external magnetic field

- Very nice work by Y.-M. Lu, Y. Ran, and M. Oshikawa (arXiv:1705.09298)

**Theorem 1. Filling-enforced constraint on  $\sigma_{xy}$  for IQHE:**

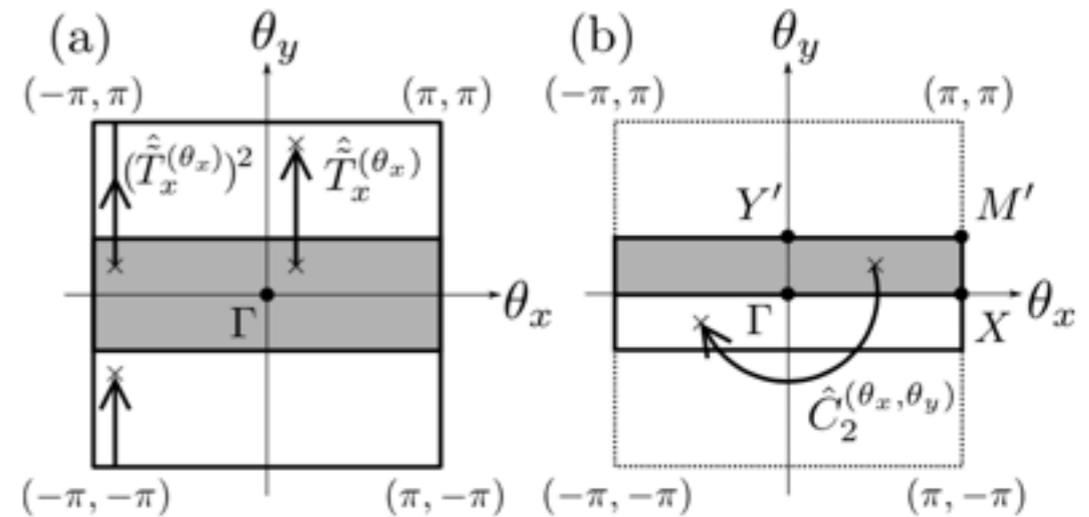
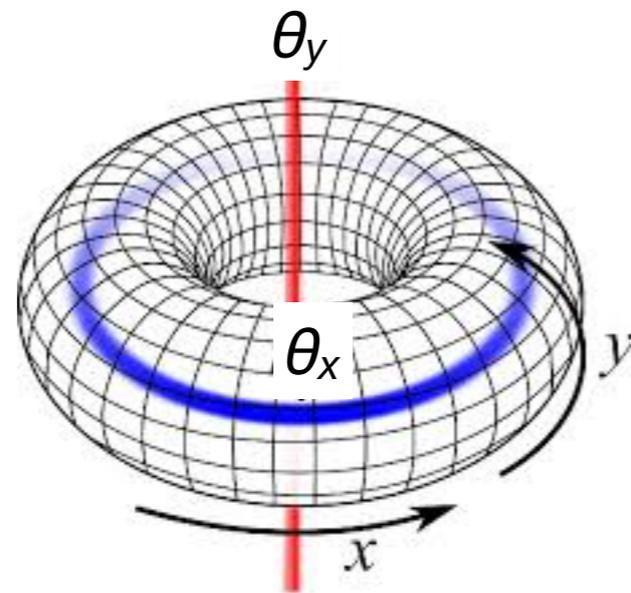
*In a generic two-dimensional (2d) system of bosons and/or fermions preserving magnetic translation symmetry  $(\bar{\rho})$  and  $U(1)$  charge conservation, if it has a unique gapped ground state on torus, its Hall conductivity must satisfy the following condition:*

$$\tilde{\sigma}_{xy} \cdot \phi = \bar{\rho} \pmod{1}, \quad (25)$$

*where  $\tilde{\sigma}_{xy} = \sigma_{xy} \cdot h/e^2$  is the Hall conductivity in the unit of  $e^2/h$ , and  $\bar{\rho}$  is the number of particles (or the charge in unit of fundamental charge  $e$ ) per unit cell.*

$$e^{2\pi i C} = 1. \quad \rightarrow \quad e^{2\pi i (\frac{p}{q} C - \bar{\rho})} = 1.$$

# filling and symmetry-based indicator of **many-body** Chern number under external magnetic field



$$e^{\pi i C} = (-1)^C = \frac{w_{C_2}^X w_{C_2}^Y}{w_{C_2}^\Gamma w_{C_2}^M},$$

$$\rightarrow e^{\pi i (\frac{p}{q} C - \bar{\rho})} = (-1)^{\frac{p}{q} C - \bar{\rho}} = \frac{w_{C_2}^X w_{T_x C_2}^{Y'}}{w_{C_2}^\Gamma w_{T_x C_2}^{M'}},$$

# Summary

- Symmetry enrich symmetry-protected topological phases
- Symmetry puts constraints on possible topological phases
- There must be more relations between symmetry and topology