Structure and Topology of Band Structures in the 1651 Magnetic Space Groups



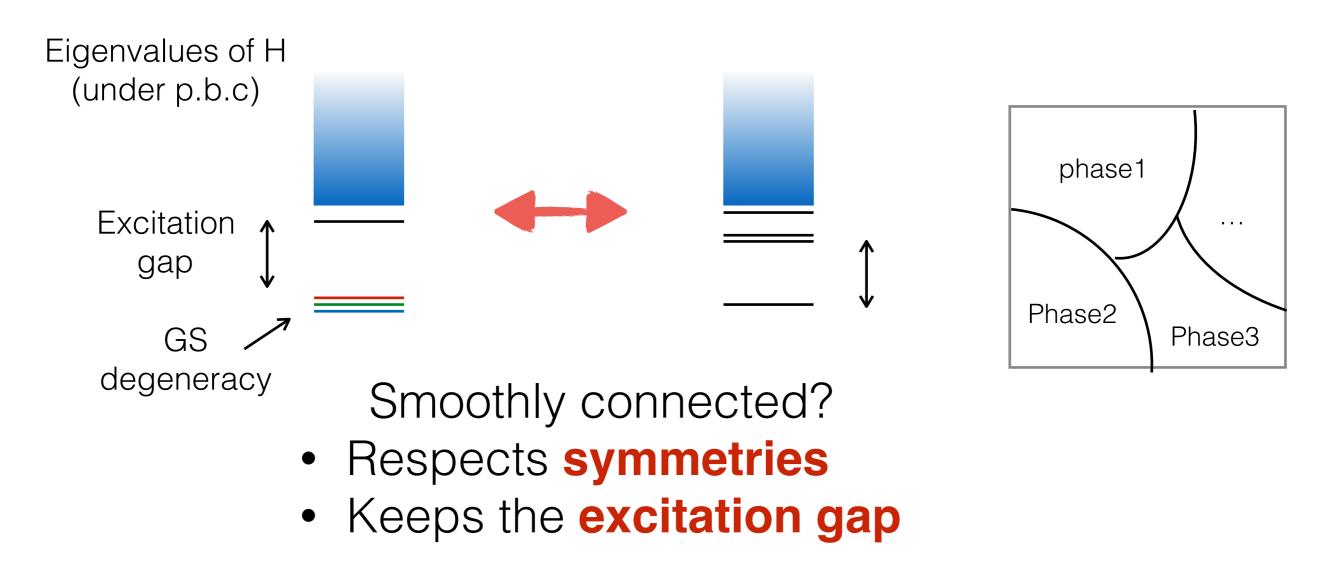
Haruki Watanabe University of Tokyo



[Noninteracting] Sci Adv (2016) PRL (2016) Nat Commun (2017) (New) arXiv:1707.01903 [Interacting] PNAS (2015) arXiv:1703.06882 Introduction 1: Symmetry & Quantum Phases

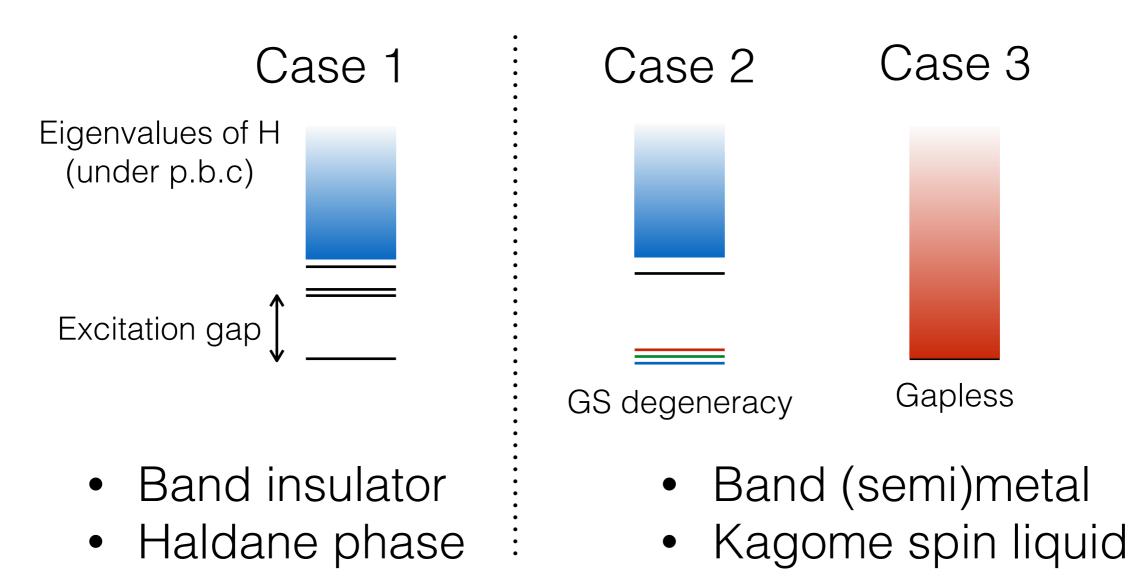
Quantum Phases distinguished by symmetries

- 1. Symmetry breaking
- 2. Symmetry Protected Topological phases (SPTs)



Constraints on possible / allowed phases: Lieb-Schultz-Mattis theorem

- Generalization of "Haldane conjecture"
- Constraints based on "Symmetries" + "filling"



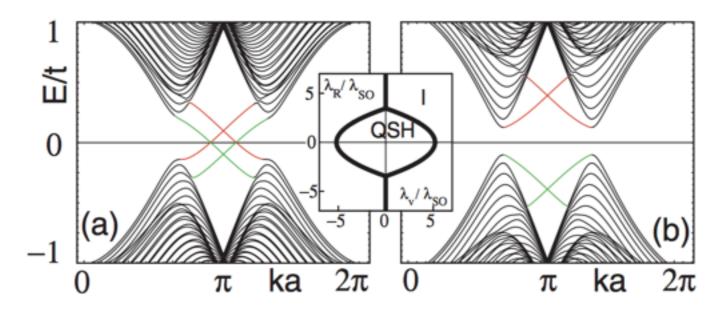
Recent refinement of Lieb-Schultz-Mattis theorem

- Original LSM: Lattice translation + U(1) symmetry LSM (1961), Affleck-Lieb (1986), Oshikawa (2000), ...
- Stronger constraints nonsymmprhic space groups Parameswaran et al (2013)
 1,651 Magnetic
- Extended to all 230 SPACE GROUPS space groups? HW, H. C. Po, A. Vishwanath & M.P. Zaletel, PNAS (2015)
- Stronger constraints in spin models H. C. Po, HW, C.-M, Jian & M. P. Zaletel, arXiv: 1703.06882

Introduction 2: Symmetries and Band Structure

Topological (crystalline) insulator

- Presence of surface / edge state
- Not smoothly connected to atomic limit



PRL 95, 146802 (2005)	PHYSICAL	REVIEW LETTERS	week ending 30 SEPTEMBER 200
Z_2 T	opological Order an	d the Quantum Spin Hall	Effect
	C. L. Ka	ne and E.J. Mele	
Department of Physic		y of Pennsylvania, Philadelphia, Pe 5; published 28 September 2005)	muyhenia 19104, USA
hand gap that support associated with a not elassification, which elassification of the	orts the transport of charge a swel Z_2 topological invariant his defined for time reversal quantum Hall effect. We o	e reversal invariant electronic state ind spin in gapless edge states. We s , which distinguishes it from an ordi- invariant Hamiltonians, is analogou stablish the Z_2 order of the QSH p t of the formalism applicable to mul-	how that this phase is nary insulator. The Z_2 s to the Chern number chase in the two band
DOI: 10.1103/PhysRe		PACS numbers: 7343-f, 72.251	1 - 73 - 1 - 1 - 1 - 1 - 1

Computing Z2 index?

The special subspaces can be identified by considering the matrix of overlaps, $\langle u_i(\mathbf{k}) | \Theta | u_j(\mathbf{k}) \rangle$. From the properties of Θ it is clear that this matrix is antisymmetric, and may be expressed in terms of a single complex number as $\epsilon_{ij}P(\mathbf{k})$. $P(\mathbf{k})$ is in fact equal to the *Pfaffian*

$$P(\mathbf{k}) = \Pr\left[\langle u_i(\mathbf{k}) | \Theta | u_j(\mathbf{k}) \rangle\right], \tag{4}$$

The Z_2 index can thus be determined by counting the number of pairs of complex zeros of P. This can be accomplished by evaluating the winding of the phase of $P(\mathbf{k})$ around a loop enclosing *half* the Brillouin zone (defined so that \mathbf{k} and $-\mathbf{k}$ are never both included).

$$I = \frac{1}{2\pi i} \oint_C d\mathbf{k} \cdot \nabla_{\mathbf{k}} \log[P(\mathbf{k}) + i\delta], \qquad (5)$$

... difficult

Fu-Kane formula for Inversion-symmetric TI

Strong index

 $v_0 = \Pi$ i, j, k = 0, π ξ (i, j, k)

- Weak indices
- $v_1 = \Pi_{j, k = 0, \pi} \xi_{(\pi, j, k)}$
- $v_2 = \Pi$ i, k = 0, π ξ (i, π , k)

Easy & Helpful for material search!

 $v_{3} = \prod_{i, j = 0, \pi} \xi_{(i, j, \pi)}$ irreps at high-sym momenta Combination of inversion eigenvalues indicates band insulator is TI protected by TR. nontrivial (not adiabatically connected to the atomic limit)

Band structures in momentum space

Typical band structure...

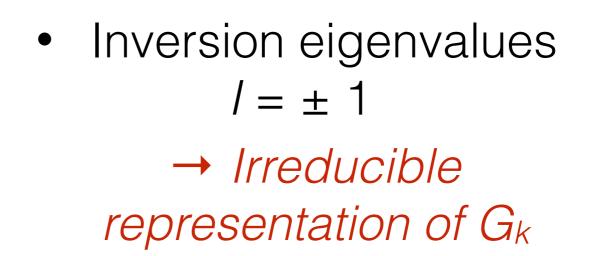
SiC Bands can cross only when different irreps Xe Dimensions of Хз -12 the irreps -16 \rightarrow degeneracy Σ А [Hemstreet & Fong (1974)]

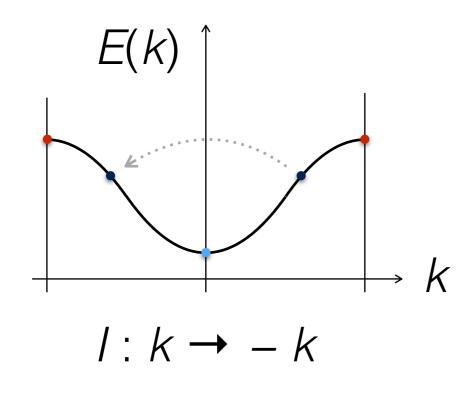
Relation among irreps upon symmetry lowering

Topological properties (i) Assume band gap at high sym momenta (ii) Forget energetics within a set of bands

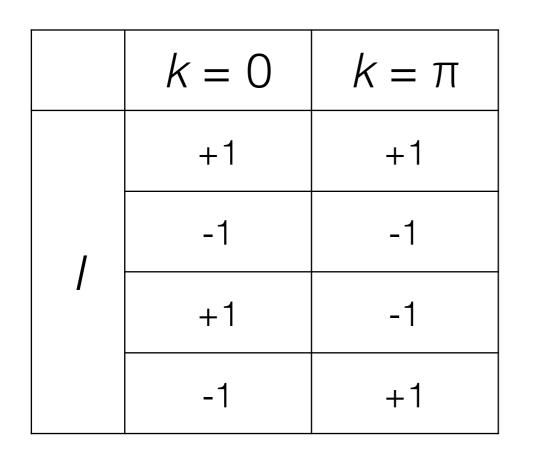
F

- Two invariant momenta $k = 0, \pi$
- → High-symmetry momenta Little group of k, G_k





 $n_{\mathbf{k}}^{\alpha}$: the number of times an irrep $u_{\mathbf{k}}^{\alpha}$ appears in BS $\mathbf{b} = (n_0^+, n_0^-, n_{\pi^+}, n_{\pi^-})$



Four possible combinations

$$b_1 = (1, 0, 1, 0)$$

$$b_2 = (0, 1, 0, 1)$$

$$b_3 = (1, 0, 0, 1)$$

$$b_4 = (0, 1, 1, 0)$$

$$b_1 + b_2 = b_3 + b_4$$

Only three are independent

Example:
Inversion-symmetric 1D chain
$$\boldsymbol{b} = (n_0^+, n_0^-, n_{\pi^+}, n_{\pi^-})$$

Relation among *n_ka*'s

$$n_0^+ + n_0^- = n_{\pi^+} + n_{\pi^-} = v (= \# \text{ of bands})$$

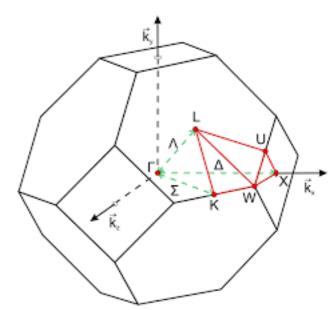
 $\boldsymbol{b} = n_0^+ (1, -1, 0, 0) + n_{\pi^+} (0, 0, 1, -1) + v (0, 1, 0, 1)$

$$\rightarrow$$
 {BS} = set of valid **b**'s = Z³

Note: we extended possible values of n to *all integers* (Classification stable against *subtracting* bands)

Group structure of Band structure

k : a high-sym mometum.
 Collect all different *types* of *k*



- G_{k} : the little group of **k**. i.e., { g in G | gk = k + G }
- $U_{\mathbf{k}}^{\alpha}$ ($\alpha = 1, 2, ...$): irreducible representation of $G_{\mathbf{k}}$ single rep for spinless electrons double reps for spinful electrons

Group structure of Band structure

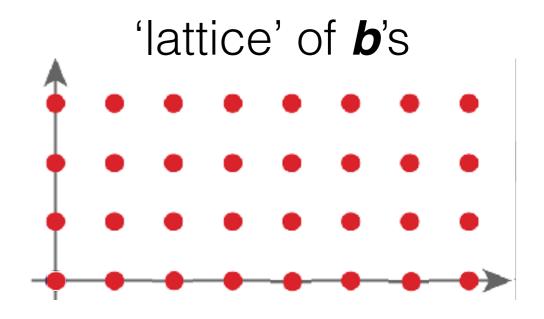
• $n_{\mathbf{k}}^{\alpha}$: the number of times $u_{\mathbf{k}}^{\alpha}$ appears in band structure

•
$$\boldsymbol{b} = (n_{\boldsymbol{k}1}^{1}, n_{\boldsymbol{k}1}^{2}, \dots n_{\boldsymbol{k}2}^{1}, n_{\boldsymbol{k}2}^{2}, \dots)$$

- Compatibility relations (+ TR sym) among $\{n_{\mathbf{k}}^{\alpha}\}$
- The set of valid \boldsymbol{b} 's : {BS} = $Z^{d_{BS}}$ $\Sigma_i m_i \boldsymbol{b}_i \in \{BS\}$

Kruthoff et al. arXiv:1703.09706

- spinless electrons in 2D
- K-theory calculation



Band structures in REAL space

Bloch vs Wannier

H. C. Po, HW, M.P. Zaletel & A. Vishwanath, Science Adv. 2(4), e1501782 (2016)

Momentum space picture

Representations of Gk

 $\boldsymbol{b} = (n_{\boldsymbol{k}1}^{1}, n_{\boldsymbol{k}1}^{2}, \dots n_{\boldsymbol{k}2}^{1}, n_{\boldsymbol{k}2}^{2}, \dots)$

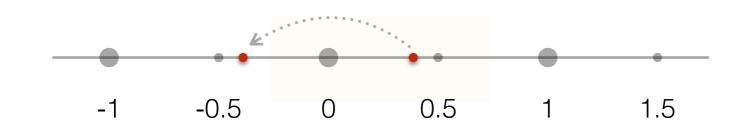
• Real space picture

Atomic Insulators (hopping → 0 limit. Product state)

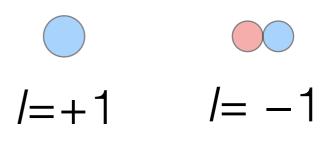
Wannier orbitals (symmetric, exponentially-localized)

Defines the trivial class of {BS}

Two symmetric positions (in UC) x = 0, 1/2

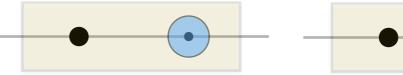


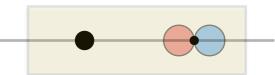
- Special position (Wyckoff position) Little group of x, G_X Parity even/odd orbital

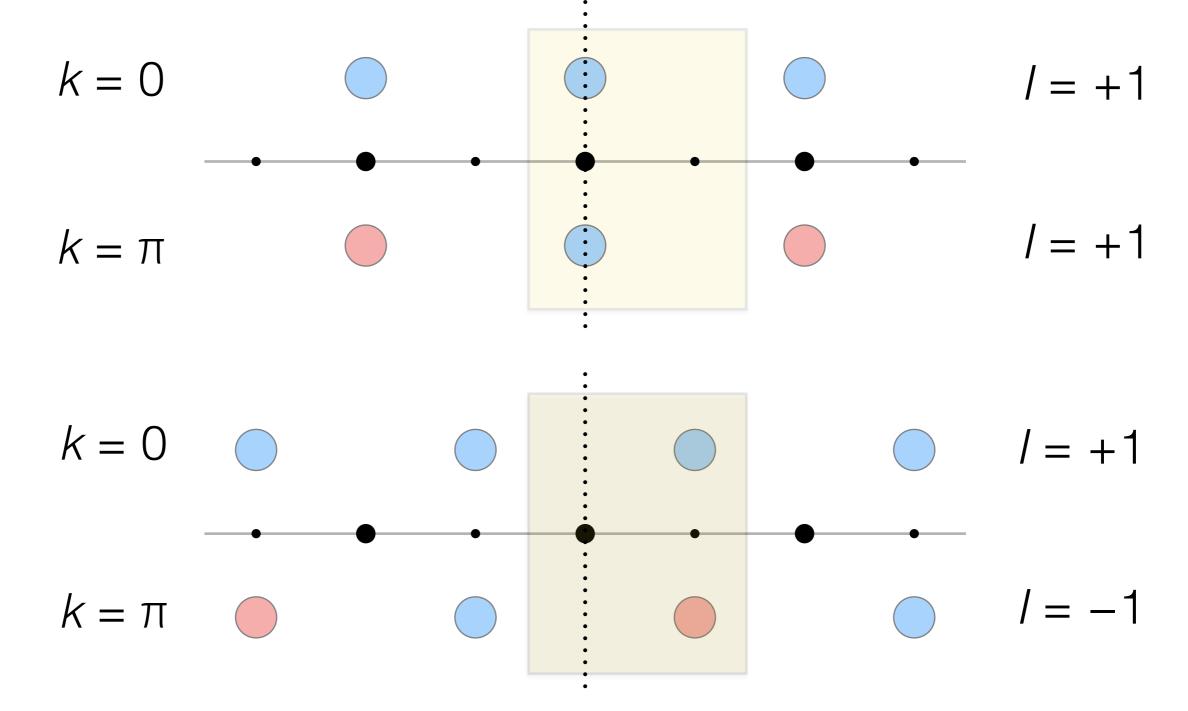


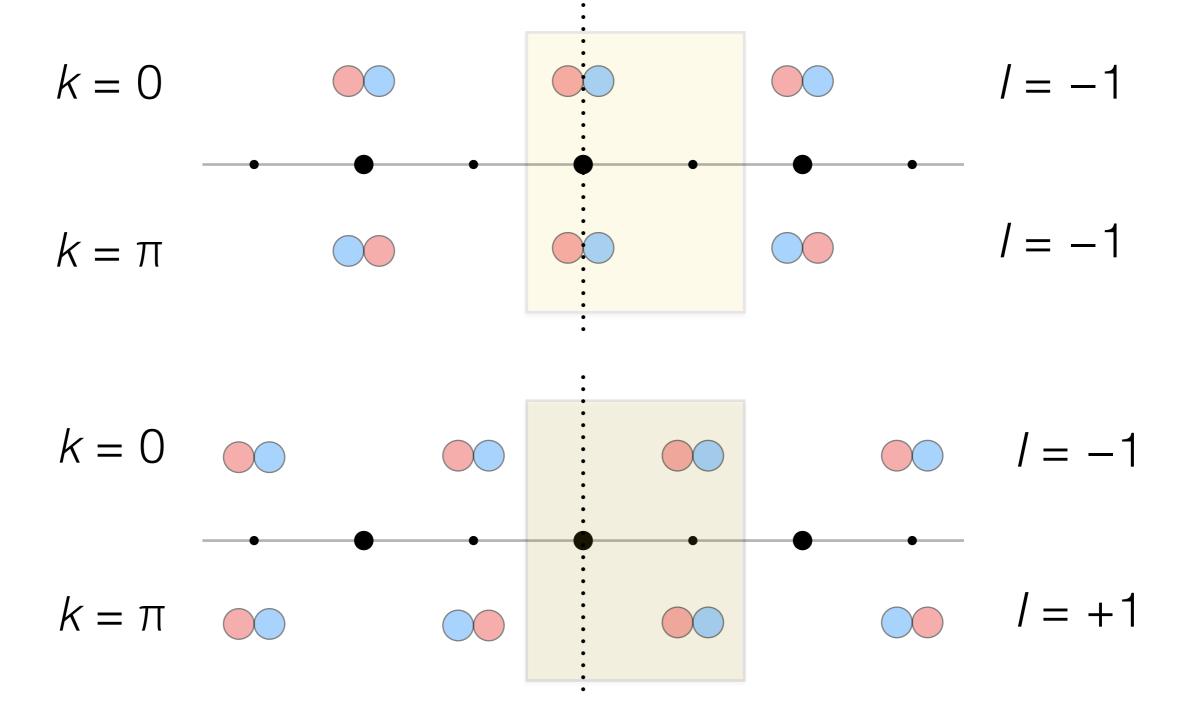
→ Irreducible representation of G_X

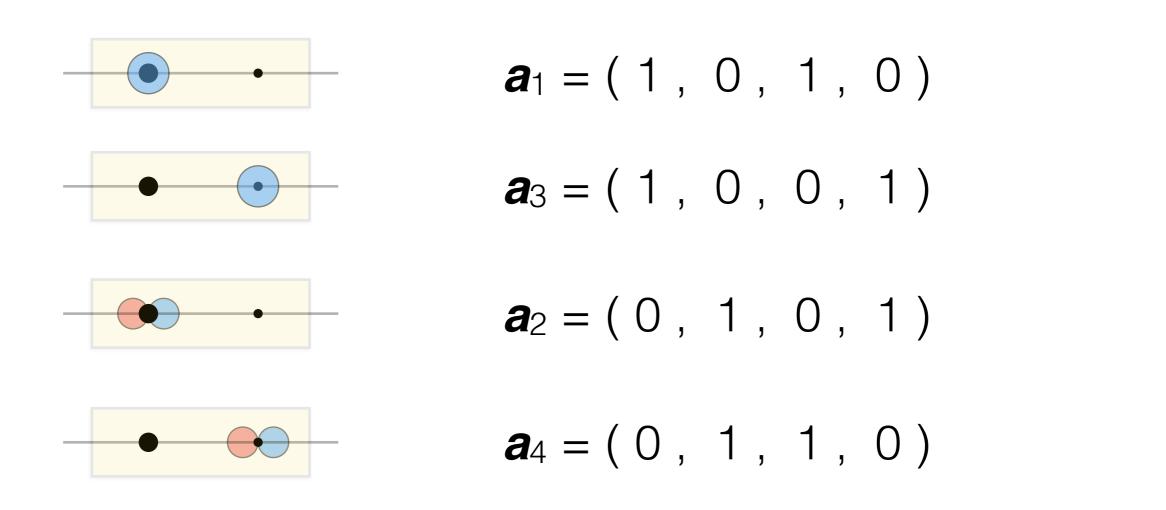












Set of all **b** corresponding to AI: $\{AI\} = Z^3$ = $a_3 + a_4$ In this example, $\{BS\} = \{AI\}$ (but not necessarily in general)

Listing up all atomic insulators

- **x**: chosen from a special Wyckoff position.
- $G_{\mathbf{x}}$: the little group of \mathbf{x} . i.e., { g in $G \mid g\mathbf{x} = \mathbf{x}$ }
- $u_{\mathbf{x}}^{\alpha}$ ($\alpha = 1, 2, ...$): irreducible representation of $G_{\mathbf{x}}$
- The combination (\mathbf{x} , $u_{\mathbf{x}}^{\alpha}$) determines AI and its \mathbf{b}

No. 199

12,3 $\sum_{i} m_{i} \boldsymbol{a}_{i} \in \{A\}$

• Set of all **a**'s corresponding to AI: $\{AI\} = Z^{d_{AI}}$

CONTINUED

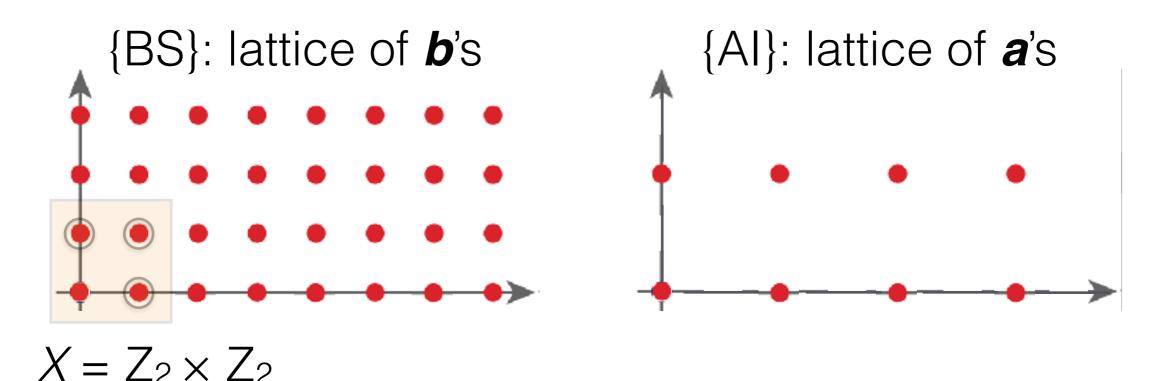


Position	ıs							
Multiplie			Coordinates					Reflection conditions
Wyckoff Site symr			(0,0,0)+ (1,1,	+(+)				k, k, l cyclically permutable General:
24 с	1	(1) x, y, z (5) z, x, y (9) y, z, x		$ \begin{array}{c} \frac{1}{2} & (3) \ \hat{v}, y + \\ \hat{y} & (7) \ \hat{v} + \frac{1}{4}, \\ \frac{1}{2} & (11) \ y + \frac{1}{2}, \end{array} $	$\bar{x}, y + \frac{1}{2}$	(8)	$ \begin{array}{c} x + \frac{1}{2}\bar{y} + \frac{1}{2}, \bar{z} \\ \bar{z}, x + \frac{1}{2}, \bar{y} + \frac{1}{2} \\ \bar{y} + \frac{1}{2}\bar{z}, x + \frac{1}{2} \end{array} $	kkl : a + k - l = 2n 0kl : k + l = 2n khl : i = 2n k00 : a = 2n
								Special: no extra conditions
12 b	2	x.0, 1	x+ 1,0,1 1,	.z,0 }, ī + ½,	0 0.	x	$0, \frac{3}{2}, \tilde{x} + \frac{1}{2}$	

Indicator of Band Topology Indicator of nontrivial band topology

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

Quotient space: $X = {BS}/{AI}$ {BS} > {AI}



Indicator of nontrivial band topology

$$X = \{BS\}/\{AI\} = Z \xrightarrow{OS} \xrightarrow{OAI} \times Z_{n1} \times Z_{n2} \times \ldots \times Z_{nN}$$

We found $d_{BS} = d_{AI}$ holds for all SGs

→ We can, in fact, compute {BS} from {AI} (easy to get) i.e., no need to list up / solve all compatibility relations (tough)

$$\boldsymbol{b} = \Sigma_i \ q_i \ \boldsymbol{a}_i \in \{BS\}$$

basis vectors of $\{AI\}$

Must be integer valued Can be fractional

If necessary, one can impose the "nonnegative" constraint at the end.

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

$X_{\rm BS}$	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	<i>188, 190</i>
\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	<i>128</i> , <i>225</i> , <i>226</i>
\mathbb{Z}_{12}	176, 192, 193, 194
$\mathbb{Z}_2 \times \mathbb{Z}_4$	14, 15, 48, 50, 53, 54, 55, 57, 59
	$63,\ 64,\ 66,\ 68,\ 71,\ 72,\ 73,\ 74,\ 84,\ 85$
	$m{86},\ m{125},\ m{129},\ m{131},\ m{132},\ m{134},\ m{147},\ m{148}$
	$162,\ 164,\ 166,\ 200,\ 201,\ 204,\ 206,\ 224$
$\mathbb{Z}_2 \times \mathbb{Z}_8$	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
$(Z_2)^2 \times \mathbb{Z}_4$	11, 12, 13, 49, 51, 65, 67, 69
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	<i>83</i> , <i>123</i>
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	2, 10, 47

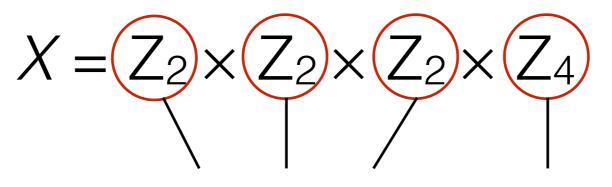
230 SGs x TRS without SOC

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	63
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	63
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	63
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	63
 6 11, 15, 35, 38, 54, 70, 73, 75, 88, 90, 103, 105, 10 113, 142, 149, 167, 168, 184, 195, 205, 219 7 13, 22, 23, 59, 64, 68, 82, 86, 117, 118, 120, 130, 1 165, 180, 181, 203, 206, 208, 209, 211, 218, 228, 2 8 21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217 	63
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	63
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
165, 180, 181, 203, 206, 208, 209, 211, 218, 228, 2 8 21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217	
8 21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217	
183, 190, 201, 217	30
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	

$X_{\rm BS}$	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
$(\mathbb{Z}_2)^2$	<i>12, 13, 15, 81, 84, 87</i>
$\mathbb{Z}_2 imes \mathbb{Z}_4$	147, 148
$(\mathbb{Z}_2)^3$	<i>10, 83, 175</i>
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	2

Example 1: *Representation-enforced* Quantum Band Insulator

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



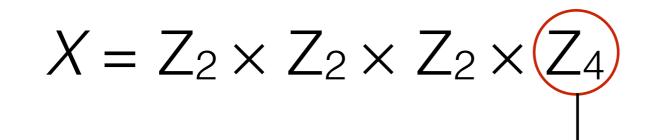
weak TI strong TI + α

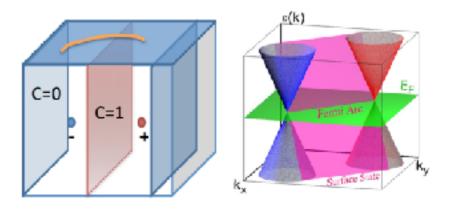
Two copies of TI No surface Dirac / no magnetoelectric response.

Still topologically nontrivial (residual entanglement) The experimental signatures are future work.

Example 2: Representation-enforced Semimetal

Inversion symmetric but TR broken 3D system (SG2)





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

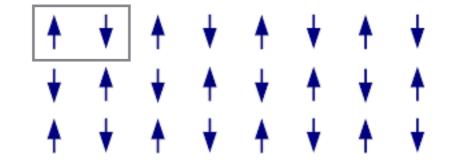
{BS}: "band structure" can be *band insulator* or *semimetal (band touching at generic points in BZ)*

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

Magnetic space groups

Magnetic space group

- In addition to an ordinary SG, we have additional anti-unitary operation T'= TR * g
- ex1: g = identity \rightarrow M = SG x {1, TRS}.
- ex2: $g = half translation \rightarrow AFM order$
- There are 1651 MSGs in 3D / 528 MLGs in 2D



Appendix A: Tables for spinful electrons

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Here we include the following tables for spinful electrons:

Tables EI-VIE: 4, X₂₂₁, and x₂₂₂ for MSGs.

Table IX: d. X11, and r11 for MLGs.

Table X: {r}₁₀₀ and {r}₁₀₁ for exceptional MSGs.

Instructions to how to read the tables can be found in Tables 1 and B. Not remark that the results on $d_i X_{inits}$ and w_{init} for types 1 and 11 MBGs, which accessed for 460 out of the 1651 entries, were already published in Ref. 14. For the readers' consensions, we reproduce them here alreagistic with the new results on the remaining 170 type 11 and 17 MBGs. Similarly, the data on exceptional filling publics among the type 11 MBGs (i.e., for time reversal symmetric systems) were reported in Refs. 1 and 9, but are also reproduced below.

MNO	4	X_{10}	1100	MBC	4	Xas	-	MNG	đ	X	100	MNG	4	X_{10}	-
111	ī	60	1	13.0	1	(1)	2	2.8 10	9	(2, 2, 2, 4)	2	2.7 IV	1	(20)	3
12 8	h	60		24.1	h	(2, 2, 2, 4)	1	2.6 10	1	(11)	2		Ľ		

of Rank of the band constant group (201) X_{Ref} (spacetary-based indicators of band topology w_{Ref} . Set of v bands are constrary-forbidden from being lashand by band gaps if $v \not\in w_{Ref}$. If

MHO I	(X_{2})	100	MK	2	4	X	HOR.	MN	2	×.	Xm	r 30	34560	1	X ₂₁₁	100
1. 1.	(2)	1	7.24	1	1	<pre>[1]</pre>	2	10.47	TV.	3	(2, 2)	2	13.70 EV	4	(2)	4
(2 m);	(1)	2	1.25	=	1	[1]	4	10.48	TV .	6	(2)	2	13.71 IV	2	(2)	4
0 mb	(1)	- 1	1.26	=	1	(I)		10.49	TV .	٠	(2)	2	13.72 IV	5	(2)	2
14 IV 2	(2)	2	3,27	DV.	1	[1]	4	11.50		6	(2)	2	13.73 DV	2	(2)	4
15 IV	(1)	2	1.28	DV.	1	[1]		11.51	=	5	(2, 2, 4)	4	13.74 DV	4	(2)	4
6 IV D	(1)	2	1.29	DV.	1	(1)	4	11.52	=	2	(20)	2	14,75 1	5	(2)	2
17 1	(1)	2	1,30	DV.	1	(1)	4	11.33	=	1	(20)	2	14.76 II	5.0	(2,4)	4
18 B)	(1)	4	2,31	DV.	1	(1)	2	11.54	==	5	(2, 2, 4)	2	14,77 12	1	(1)	4
(* m):	(1)	2	8.32	1	2	(1)	1	11.55	TV .	3	(2)	4	14.78 12	1	(1)	4
10 TV 1	(1)	4	8,33	=	1	(1)	2	11.56	TV .	5	(2)	2	14.79 12	5.0	(2,4)	2
at wijt	00	2	8,34		н.	(1)	1	11.57	N	к	(20)	4	14.80 EV	8	(2)	4
12 IV()	00	2	8,35	IN	×.	(11)	2	12.58		10	(3, 2)	1	14.81 IN	1	(2)	4
as 1 🏚	00	11	8.36	IN	×.	(1)	2	12.59		r	(3.2.4)	2	14.82 IN	1	10	4
34 B)	00		9,37	1	×.	(11)	2	12.60		1	00	2	14.83 (N	1.	(2)	2
15 M ()	00		9.38	н	×.	(11)	4	12.61		1	00	2	14.84 (N	1	(2)	4
36 IV 2	00		9.39		×.	(1)	2	12.62		1	(3.2.4)		15.85 T	1.1	1.11	2
ar wiji	00		5.40	IN	×.	(1)	2	12.60	N	s.	(20)	2	15.86 B	4.1	1.4	4
an 10	00	11	9.43	IN	к.	(1)	4	12.64	N	s.	(20)	2	6.87 10	1	00	2
19 B D	00		16.42	1	1.5	(2, 2, 2)	1	13.48		1	0.10	2	15.88 10	2	00	2
20 10	00	11	10.43	н		(2, 2, 2, 4)	2	13.66		s.	0.2.0	4	15.89 10	4.1	1.4	2
a N)	00		10.44		×.	(1)	2	13.67		1	00	2	15.90 IV	4	10	
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BA IN				a 1 (1)		29 104 75		10 154 TV		÷
16.5 DV				= 2 (I)		29 105 75		30 188 PV		÷
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C.H.IV				N 1 (1)		20 111 1		34 161 P		÷
17.12 IV				NI II		30 HZ B		34 162 TV		÷
(1.1) IV				NI II		20 112 10		34 163 P		÷
17.14 IV				NIO		20 114 10		34 164 PV		2
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18,36 1				11 0		20 116 P		15 IN6 E		2
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18.23 IV						38 123 1		36 173 1		-
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26.32 10				m a (2)		36 134 PK		37 181 E		5
26.33 ==				N 1 (1)		26 100 Pk		37 183 E		2
26.34 00				N 1 (1)		20 124 PM		77 184 P		2
20.35 EV				N 1 (1)		30 105 1		30 ING PK		1
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21.39 8				1 (1)		30 109 PA		26 189 11		1
21.40 11				2 (1)		32 340 FK		36 190 E		1
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21.42 IV				FN 4 [1]		32 HC P		36 192 IV		2
21.43 EV				N 2 (1)		32 1-0 P		36 193 P		2
21.44 IV				PV 1 (1)		20 144 1		36 194 P		4
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22.46 8				N 4 (1)		30 \$46 E		39 196 E		4
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22.48 IV				W 3 (1)		20 148 10		20108.00		2
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40 206 18 2		2 47 29			(4)	52,306										
40.207 10 2		2 48 25			(2)	52,347										
40.208 EV[3		2 49 25				52,308										2
40.209 EV 1		4 48 25			(1)	52,309									60	4
40230 EV[3		2 49 29			(2)	52,310										4
41211 1 2		2 48 26			(1)	52,311									(2)	4
41252 8 1		4 49 26			(2)	52.342									(2)	4
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41 296 EV 2					(2.2.4)										(4)	
41 217 EV 1		4 49 26			(1)	52.317									60	4
41 218 IV 2		2 49.26			(1)	52.318									(4)	
42 219 1 1		2 49.28				52,319									1, 2)	4
42 220 H 1		2 49 21			(2, 2)	52,320									(2)	4
42 221 10 2		1 49 21			(1)	53,321									(2)	4
42 222 88 3		1 0 21			(2)	53,322									(2)	*
42 223 EV 1		2 49 21			(2)	53.325									(2)	4
43 224 1 2		2 49 23			(2)	53,324									(2)	4
43 225 10 1		4 49 21			(2)	53.325									(2)	-
43 226 10 1		2 49 23			(2)	53,336									(2)	-
40.227 (0) 2		2 50 21		3	(2)	53,327									(2)	4
43 228 DV 1		4 50 21				53,328										*
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44 230 H 1		3 59 28			(1)	53,330									60	1
44 234 18 2		59.28			(8.8)	50,014									60	1
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49 238 1 1		2 59 28			(8)	53,318									60	1
49 236 8 1		4 59 29			(8)	53,336									(2)	1
49 297 88 1		3 59 26			(8)	54,337									(2)	4
49 234 10 3		2 59 28			(R)	54,338									(2)	-
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06 342 E 1		4 51 28			(1)	54.342										1
46 243 III 1		2 51 24			(1)	54,343									(2)	2
46 264 10 2		2 51 29				54,344									(4)	1
46 245 10 2		2 51 28			(2)	54,345									20	1
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46.348 EV 2		4 51 29				54,348									(2)	2
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TABLE I. Characterization of band structures (BSs) in a magnetic space group (MSG); excerpt from Tables III-VIII.

MSG ^a	d^{b}	$X_{\rm BS}{}^{\rm c}$	${\nu_{\mathrm{BS}}}^{d}$	$X = Z_2 \times Z_2 \times Z_2 \times Z_4$
2.5 II	9	(2,2,2,4)	2	$\mathcal{N} = \mathcal{L}_{\mathcal{L}} \mathcal{N} \mathcal{L}_{\mathcal{L}} \mathcal{N} \mathcal{L}_{\mathcal{L}} \mathcal{N} \mathcal{L}_{\mathcal{L}} \mathcal{L} \mathcal{L} \mathcal{L} \mathcal{L} \mathcal{L} \mathcal{L} L$
209.51 IV				X = trivial

- ^a MSG number in the Belov-Neronova-Smirnova notation, followed by a Roman numeral I, ..., IV indicating its type.
- ^b Number of linearly independent BSs.
- ^c Symmetry-based indicator of band topology, which takes the form
- $\prod_i \mathbb{Z}_{n_i}$; denoted by the collection of positive integers (n_1, n_2, \cdots) . ^d For most of the MSGs, the set of physical BS fillings $\{\nu\}_{BS}$ and the set of AI fillings $\{\nu\}_{AI}$ agree with each other, and they take the form $\{\nu\}_{BS} = \{\nu\}_{AI} = \nu_{BS} \mathbb{N}$. The asterisk indicates violation to this rule, detailed in Table \mathbf{X} .

Example 3: Representation-enforced Semimetal

Magnetic Layer Group (2D) MSG 3.4 (P_a 112) π rotation + TR * half translation.

$$X = Z_2$$

$$\eta = \prod_{n:\text{occupied } \mathbf{k} = (\pi, 0), (\pi, \pi)} \eta_{n, \mathbf{k}},$$

(a) $\begin{array}{c} -i\sigma_{0} + t_{J}\sigma_{1} \\ -J\sigma_{3} \\ +J\sigma_{3} \end{array}$ (b) $(J/t, t_{J}/t) = (1, 1/4)$ (c) $(J/t, t_{J}/t) = (1, 3/4)$ $\begin{array}{c} E_{\mathbf{k}} \\ f_{k} \\ F_$

Example 4: *Filling-enforced* Semimetal

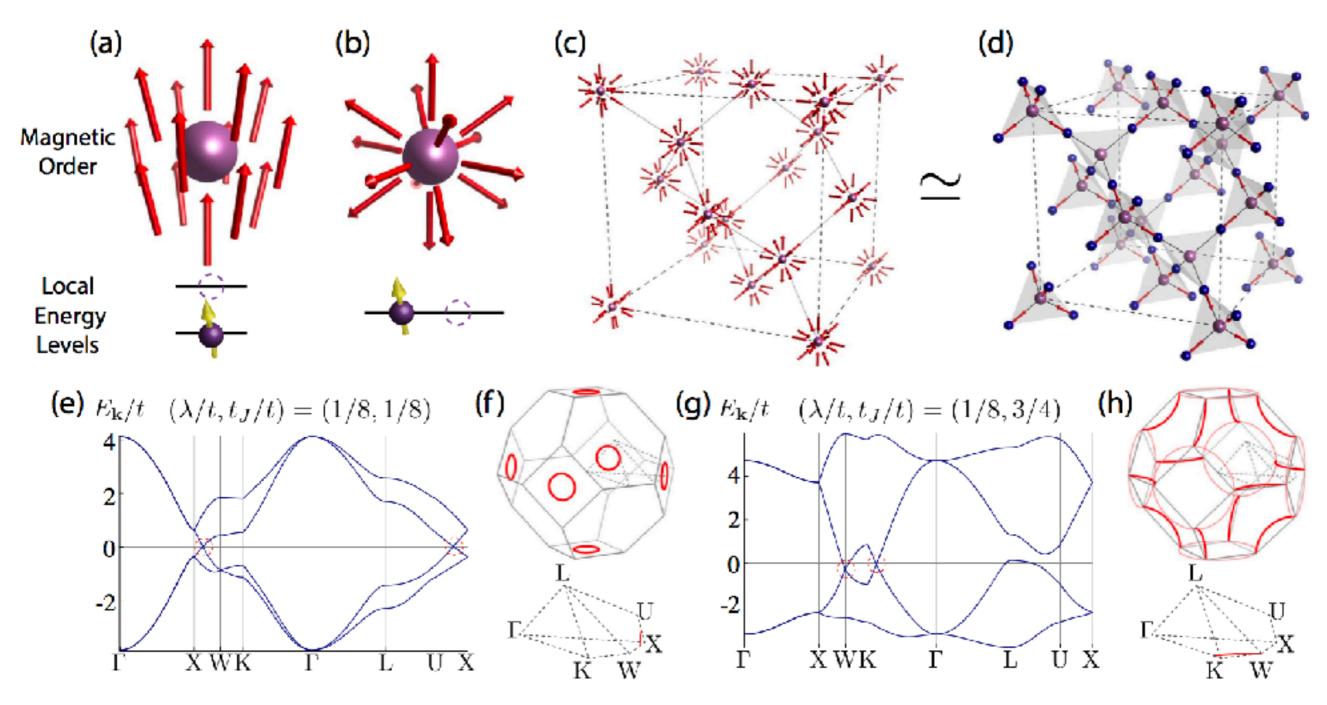


FIG. 2. Magnetic filling-enforced semimetals. (a,b) Symmetries of a magnetic order can prohibit atomic insulators (AIs) at odd site fillings.

Summary

- Higher symmetry → Richer phases & stronger constraints
- Our band topology indicator might accelerate new material search / screening process