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

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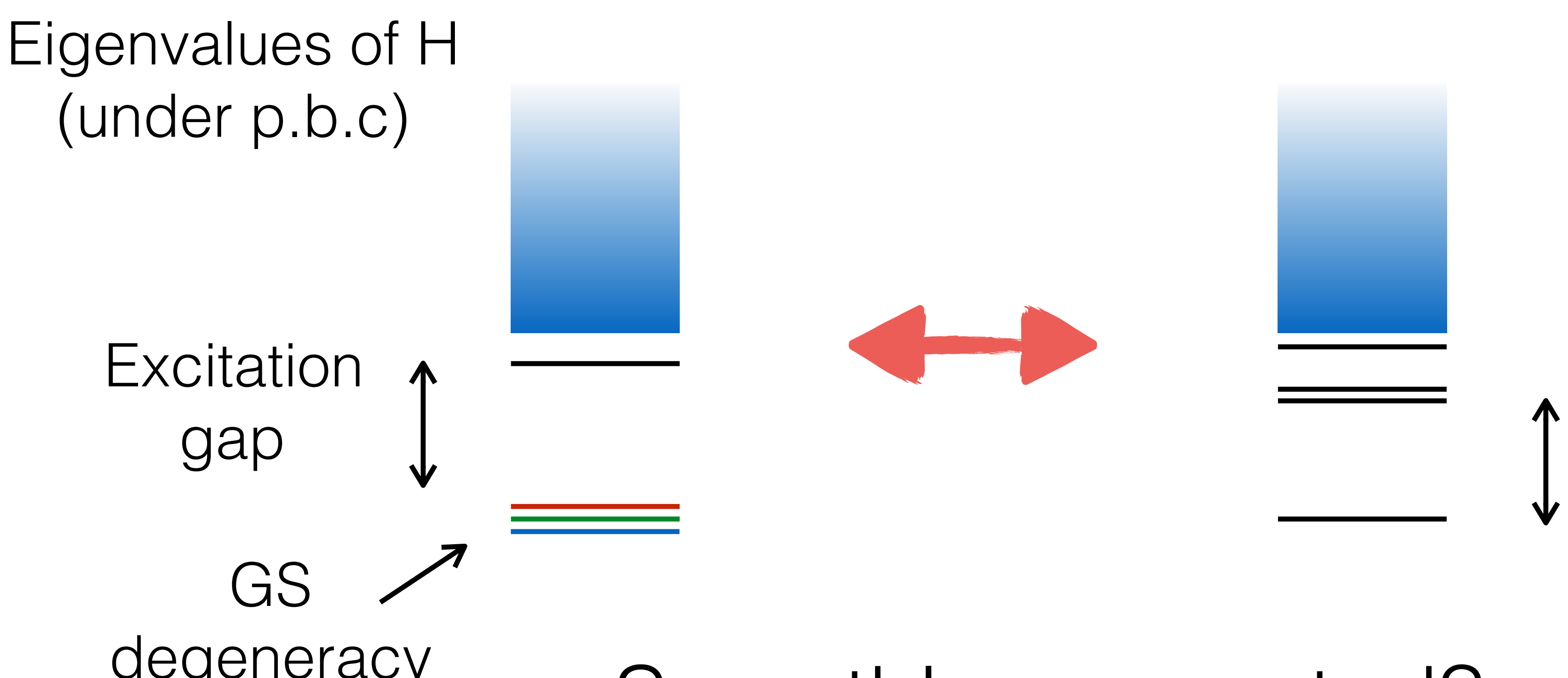
[Noninteracting]
Sci Adv (2016)
PRL (2016)
Nat Commun (2017)
(New) arXiv:1707.01903

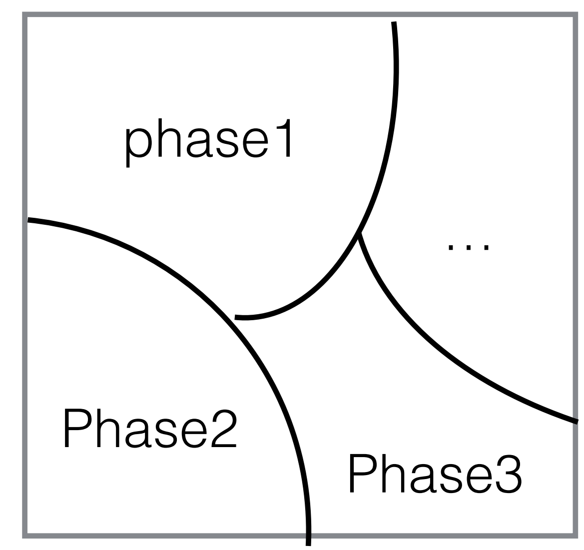
[Interacting]
PNAS (2015)
arXiv:1703.06882

# Introduction 1:
## Symmetry & Quantum Phases

# Quantum Phases distinguished by symmetries

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



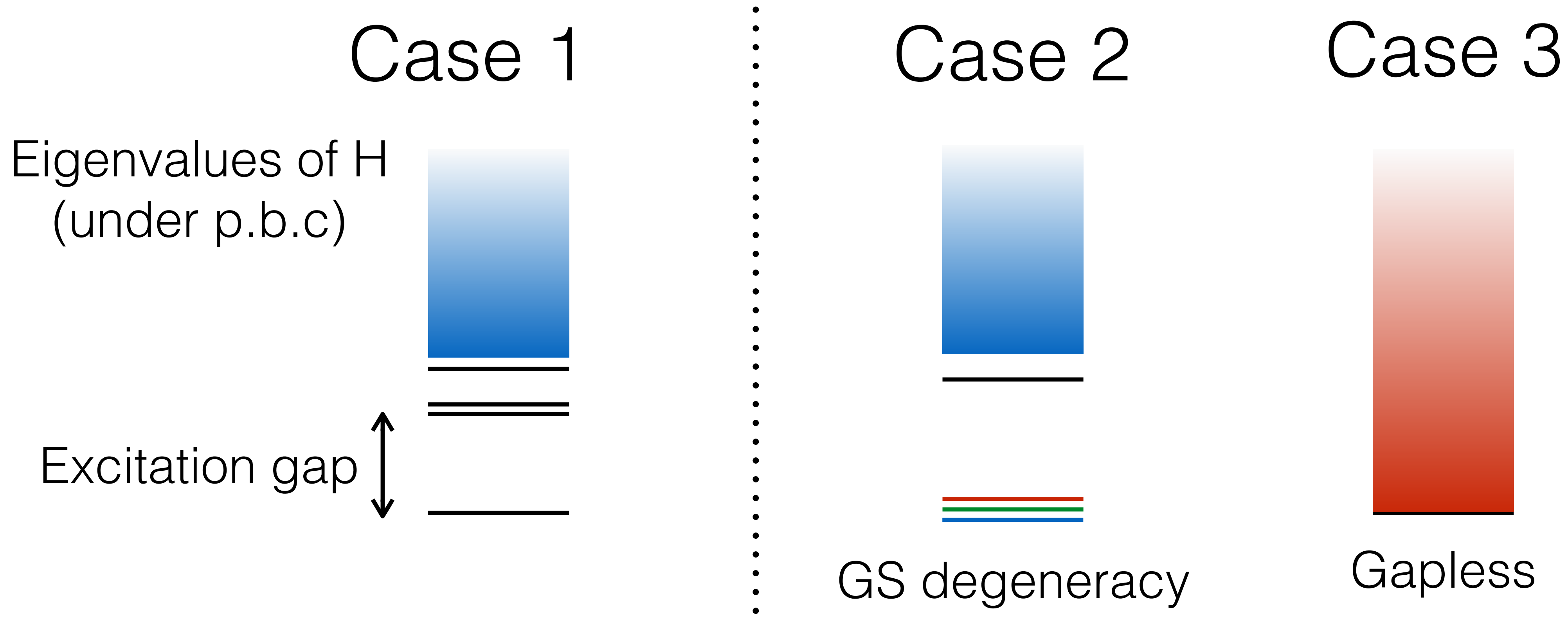




Smoothly connected?

- Respects **symmetries**
- Keeps the **excitation gap**

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

- Generalization of “Haldane conjecture”
- Constraints based on “Symmetries” + “filling”




- Band insulator
- Haldane phase

- Band (semi)metal
- Kagome spin liquid

# Recent refinement of Lieb-Schultz-Mattis theorem

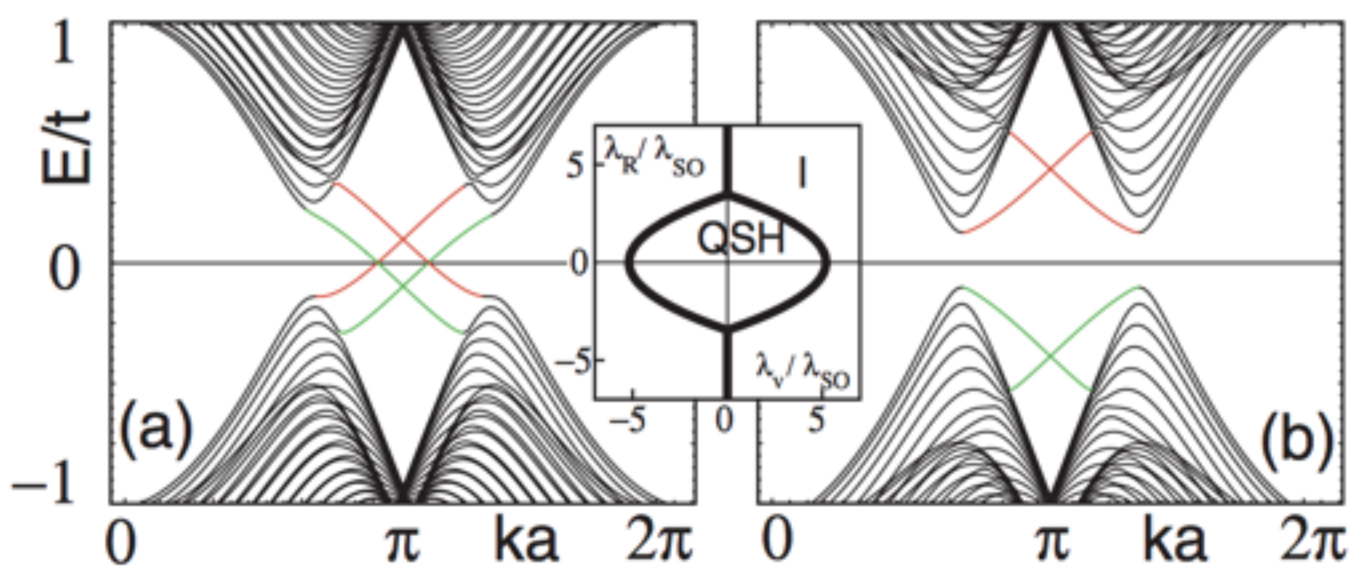
- Original LSM: Lattice translation + U(1) symmetry
  LSM (1961), Affleck-Lieb (1986), Oshikawa (2000), …
- Stronger constraints nonsymmprhic space groups
  Parameswaran et al (2013)
- Extended to all 230 SPACE GROUPS → 1,651 Magnetic space groups?
  HW, H. C. Po, A. Vishwanath & M.P. Zaletel, PNAS (2015)
- 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 2005

**$Z_2$ Topological Order and the Quantum Spin Hall Effect**

C. L. Kane and E. J. Mele

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(Received 22 June 2005; published 28 September 2005)

The quantum spin Hall (QSH) phase is a time reversal invariant electronic state with a bulk electronic band gap that supports the transport of charge and spin in gapless edge states. We show that this phase is associated with a novel $Z_2$ topological invariant, which distinguishes it from an ordinary insulator. The $Z_2$ classification, which is defined for time reversal invariant Hamiltonians, is analogous to the Chern number classification of the quantum Hall effect. We establish the $Z_2$ order of the QSH phase in the two band model of graphene and propose a generalization of the formalism applicable to multiband and interacting systems.

DOI: 10.1103/PhysRevLett.95.146802 PACS numbers: 73.43.−f, 72.25.Hg, 73.61.Wp, 85.75.−d

# 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 $\Theta$ 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*

$$P(\mathbf{k}) = \mathrm{Pf}\,[\langle u_i(\mathbf{k})|\Theta|u_j(\mathbf{k})\rangle], \qquad (4)$$

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

$$\nu_0 = \prod_{i,\, j\, ,k\, =\, 0,\, \pi} \xi_{(i,\, j,\, k)}$$

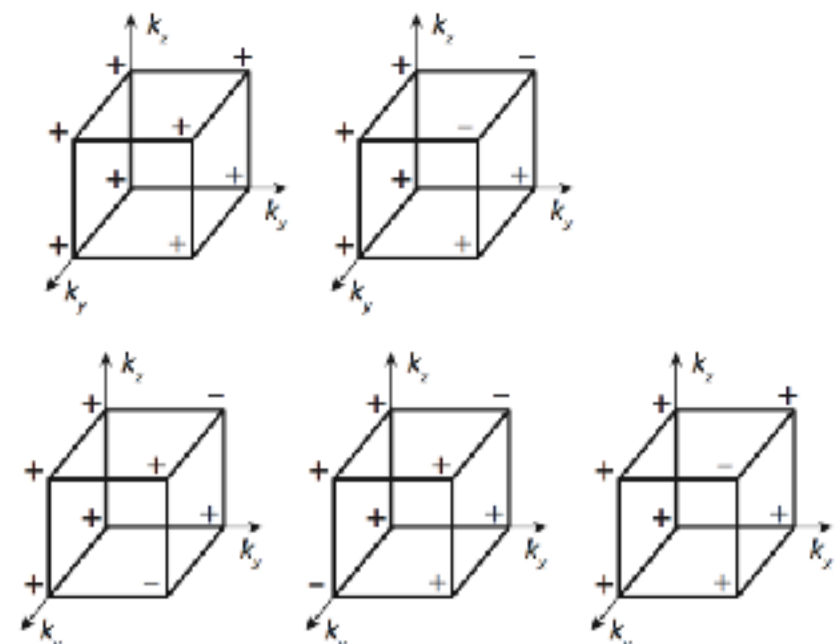
Easy & Helpful for material search!

- Weak indices

$$\nu_1 = \prod_{j,\, k\, =\, 0,\, \pi} \xi_{(\pi,\, j,\, k)}$$

$$\nu_2 = \prod_{i,\, k\, =\, 0,\, \pi} \xi_{(i,\, \pi,\, k)}$$

$$\nu_3 = \prod_{i,\, j\, =\, 0,\, \pi} \xi_{(i,\, j,\, \pi)}$$



irreps at high-sym momenta

Combination of ~~inversion eigenvalues~~ *indicates*

band insulator is ~~TI protected by TR~~.

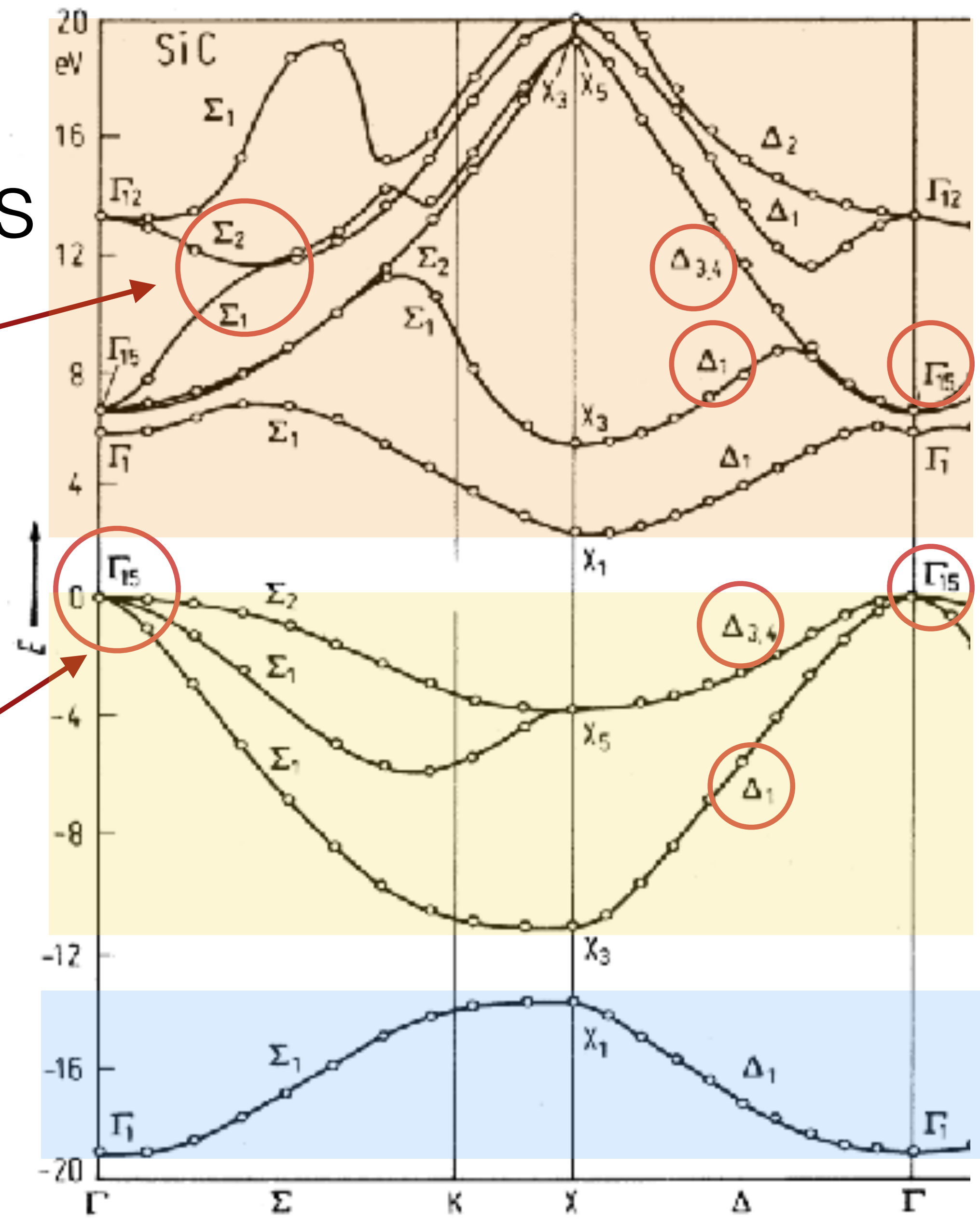
nontrivial (not adiabatically connected to the atomic limit)

# Band structures in momentum space

# Typical band structure…

Bands can cross only when different irreps

Dimensions of the irreps → degeneracy

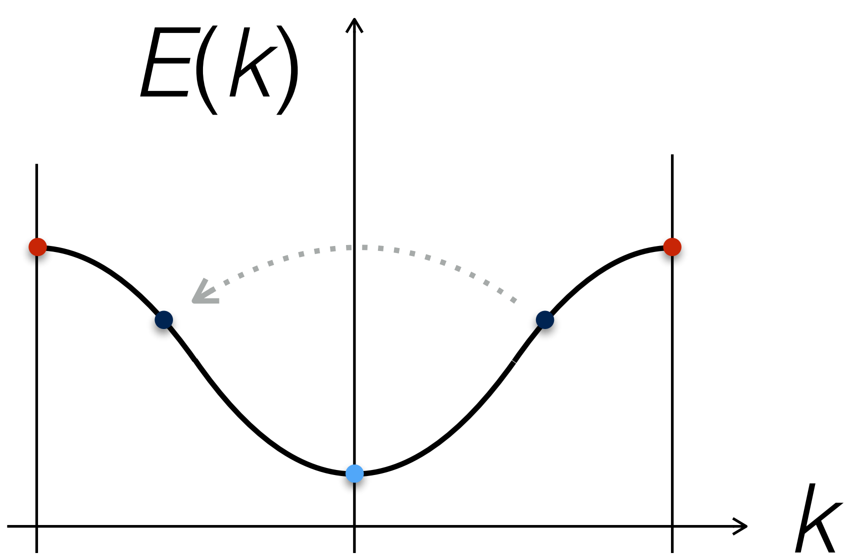



[Hemstreet & Fong (1974)]

Relation among irreps upon symmetry lowering

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

# Example: Inversion-symmetric 1D chain




$I : k \rightarrow -k$

- Two invariant momenta
  $k = 0, \pi$

  → *High-symmetry momenta*
  *Little group of k, $G_k$*

- Inversion eigenvalues
  $I = \pm 1$

  → *Irreducible representation of $G_k$*

# Example:
# Inversion-symmetric 1D chain

$n_{\boldsymbol{k}}^{\alpha}$ : the number of times an irrep $u_{\boldsymbol{k}}^{\alpha}$ appears in BS

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

| | $k = 0$ | $k = \pi$ |
|---|---|---|
| $I$ | +1 | +1 |
| | -1 | -1 |
| | +1 | -1 |
| | -1 | +1 |

$\leftrightarrow$

$$\boldsymbol{b}_1 = (\ 1\ ,\ \ 0\ ,\ \ 1\ ,\ \ 0\ )$$
$$\boldsymbol{b}_2 = (\ 0\ ,\ \ 1\ ,\ \ 0\ ,\ \ 1\ )$$
$$\boldsymbol{b}_3 = (\ 1\ ,\ \ 0\ ,\ \ 0\ ,\ \ 1\ )$$
$$\boldsymbol{b}_4 = (\ 0\ ,\ \ 1\ ,\ \ 1\ ,\ \ 0\ )$$
$$\boldsymbol{b}_1 + \boldsymbol{b}_2 = \boldsymbol{b}_3 + \boldsymbol{b}_4$$

Four possible combinations

Only three are independent

# Example: Inversion-symmetric 1D chain

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

Relation among $n_{\boldsymbol{k}}{}^\alpha$'s

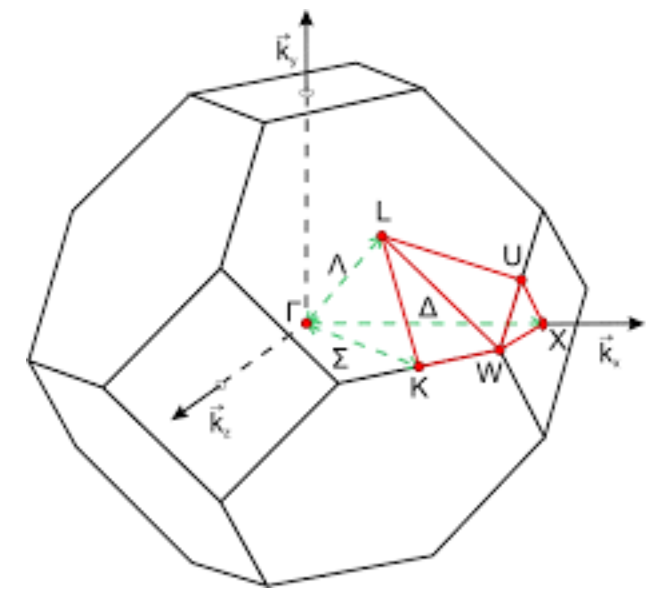
$$n_0{}^+ + n_0{}^- = n_\pi{}^+ + n_\pi{}^- = \mathrm{v}\ (= \#\ \text{of bands})$$

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

→ {BS} ≡ set of valid $\boldsymbol{b}$'s $= Z^3$

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

# Group structure of Band structure




- $\boldsymbol{k}$ : a high-sym mometum.

Collect all different *types* of $\boldsymbol{k}$

- $G_{\boldsymbol{k}}$ : the little group of $\boldsymbol{k}$. i.e., $\{\, g \text{ in } G \mid g\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{G} \,\}$

- $u_{\boldsymbol{k}}^{\alpha}$ ($\alpha = 1, 2, \ldots$): irreducible representation of $G_{\boldsymbol{k}}$

single rep for spinless electrons

double reps for spinful electrons

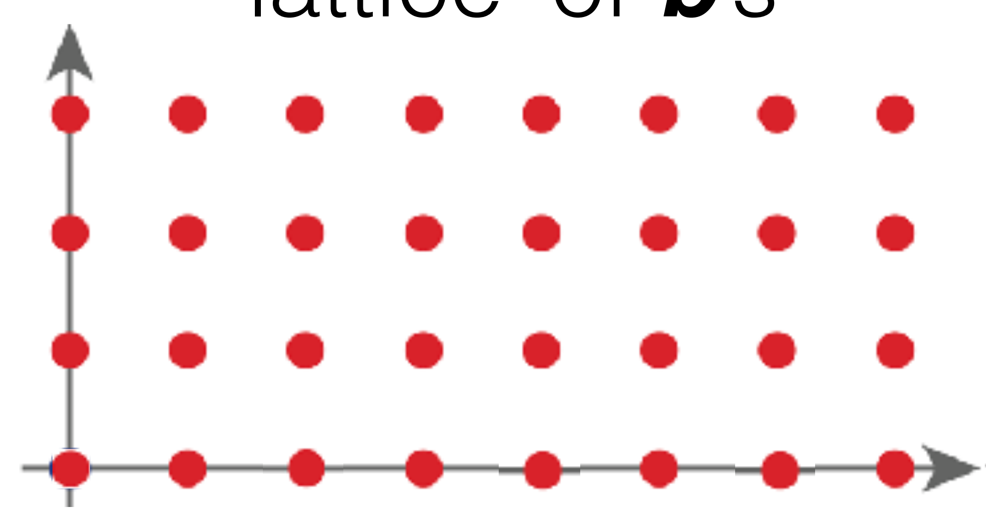
# Group structure of Band structure

- $n_{\boldsymbol{k}}^{\alpha}$ : the number of times $u_{\boldsymbol{k}}^{\alpha}$ appears in band structure
- $\boldsymbol{b} = (n_{\boldsymbol{k}_1}^{1}, n_{\boldsymbol{k}_1}^{2}, \ldots n_{\boldsymbol{k}_2}^{1}, n_{\boldsymbol{k}_2}^{2}, \ldots)$
- Compatibility relations (+ TR sym) among $\{n_{\boldsymbol{k}}^{\alpha}\}$
- The set of valid $\boldsymbol{b}$'s : $\{\mathrm{BS}\} = Z^{d_{\mathrm{BS}}}$

$$\Sigma_i\, m_i\, \boldsymbol{b}_i \in \{\mathrm{BS}\}$$

Kruthoff *et al.* arXiv:1703.09706
- spinless electrons in 2D
- K-theory calculation

'lattice' of $\boldsymbol{b}$'s



# 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 $G_{\boldsymbol{k}}$

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

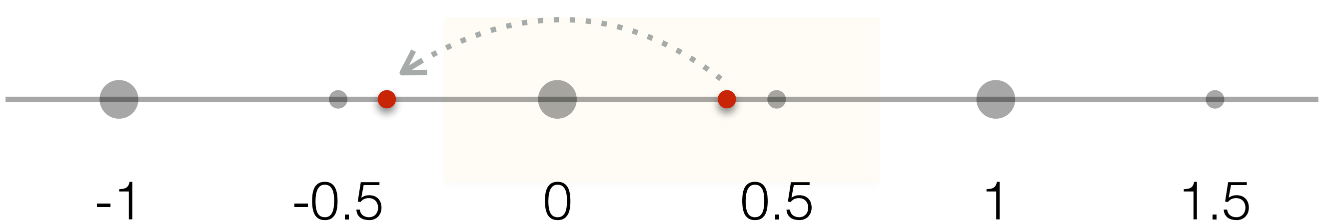
- Real space picture

Atomic Insulators (hopping → 0 limit. Product state) = Wannier orbitals (symmetric, exponentially-localized)

Defines the trivial class of {BS}

# Example:
# Inversion-symmetric 1D chain

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



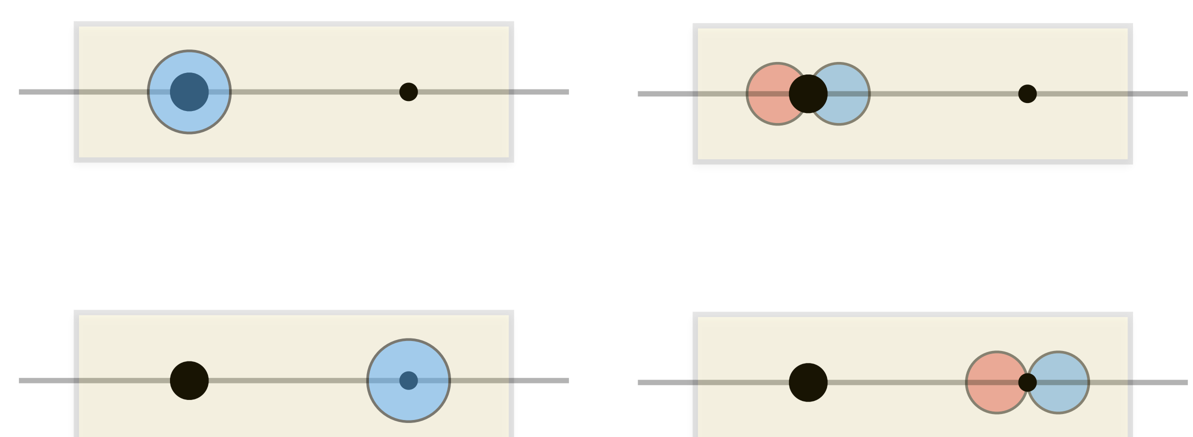

*→ Special position*
*(Wyckoff position)*

*Little group of x, $G_x$*

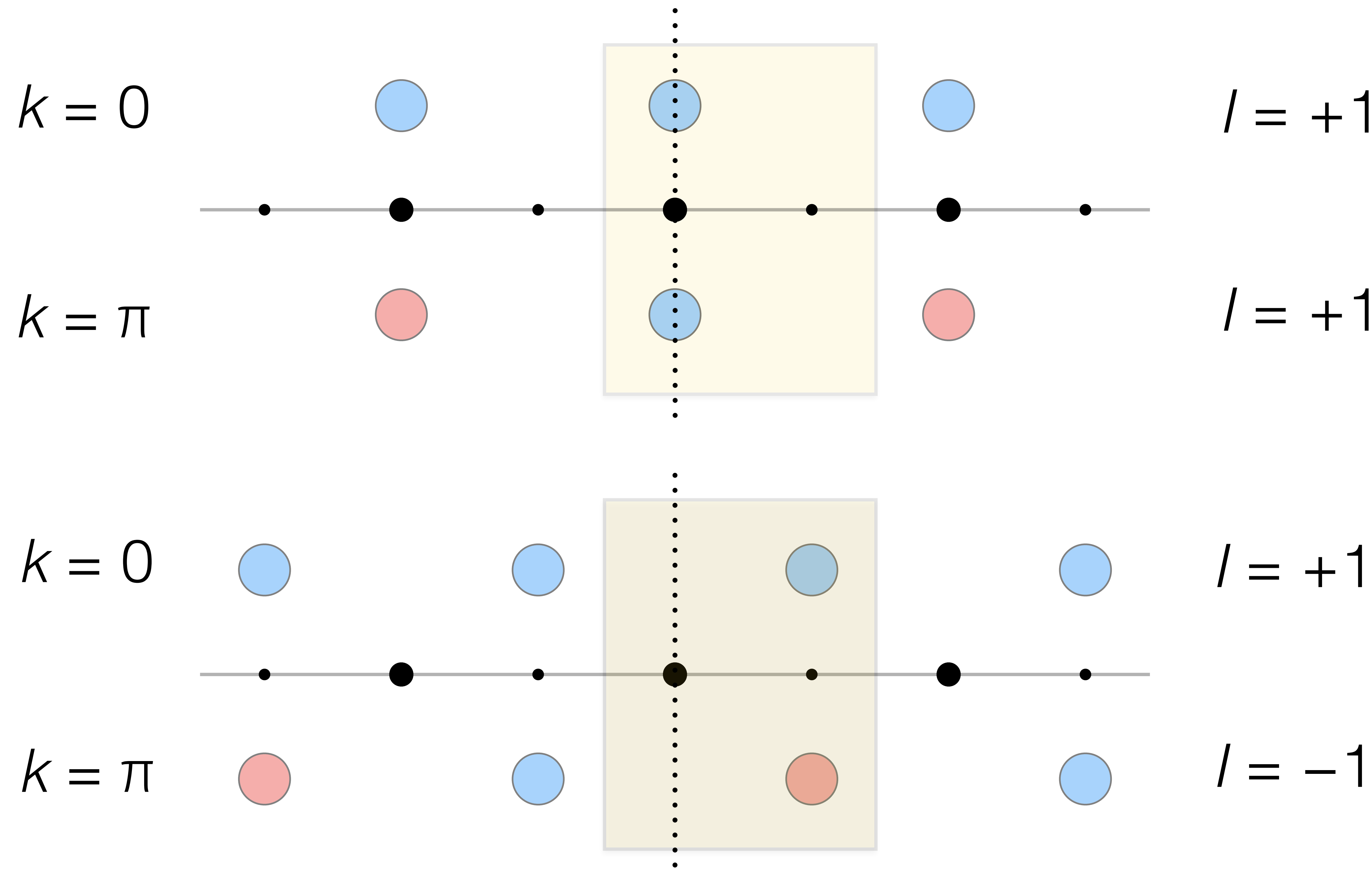
- Parity even/odd orbital

$I=+1$ $I=-1$

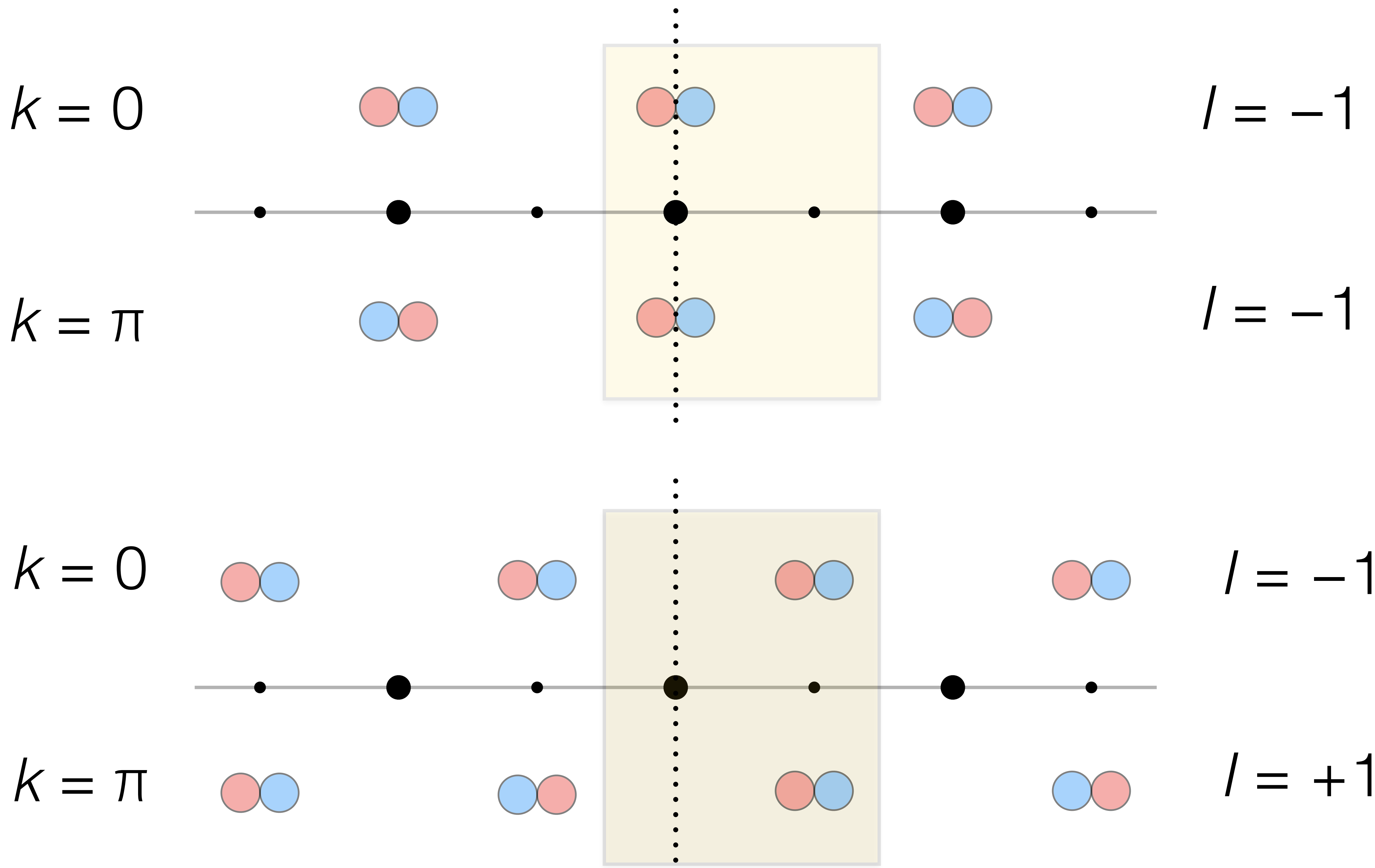
*→ Irreducible representation of $G_x$*



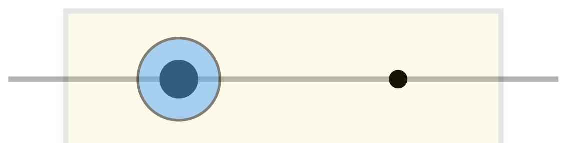
# Example:
# Inversion-symmetric 1D chain



# Example: Inversion-symmetric 1D chain

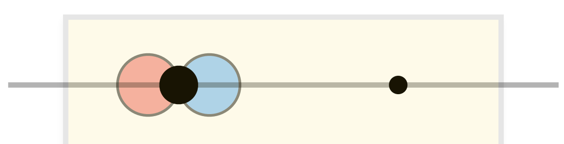


# Example:
# Inversion-symmetric 1D chain

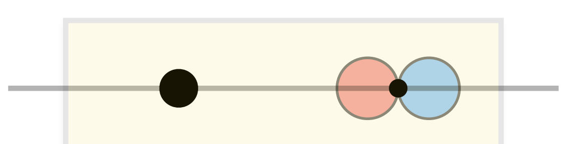


$\boldsymbol{a}_1 = (\,1\,,\;0\,,\;1\,,\;0\,)$

$\boldsymbol{a}_3 = (\,1\,,\;0\,,\;0\,,\;1\,)$



$\boldsymbol{a}_2 = (\,0\,,\;1\,,\;0\,,\;1\,)$



$\boldsymbol{a}_4 = (\,0\,,\;1\,,\;1\,,\;0\,)$

Set of all $\boldsymbol{b}$ corresponding to AI: $\{\mathrm{AI}\} = \mathbb{Z}^3$

$$\boldsymbol{a}_1 + \boldsymbol{a}_2 = \boldsymbol{a}_3 + \boldsymbol{a}_4$$

In this example, {BS} = {AI} (but not necessarily in general)

# Listing up all atomic insulators

- $\boldsymbol{x}$: chosen from a special Wyckoff position.
- $G_{\boldsymbol{x}}$ : the little group of $\boldsymbol{x}$. i.e., $\{\, g \text{ in } G \mid g\boldsymbol{x} = \boldsymbol{x} \,\}$
- $u_{\boldsymbol{x}}^{\alpha}$ ($\alpha$ = 1, 2, …): irreducible representation of $G_{\boldsymbol{x}}$
- The combination ($\boldsymbol{x}$, $u_{\boldsymbol{x}}^{\alpha}$) determines AI and its $\boldsymbol{b}$
- Set of all $\boldsymbol{a}$'s corresponding to AI: $\{\mathrm{AI}\} = \mathbb{Z}^{d_{\mathrm{AI}}}$

$$\textstyle\sum_i m_i\, \boldsymbol{a}_i \in \{\mathrm{AI}\}$$


CONTINUED     No. 199     $I2_13$

**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac12,\frac12,\frac12)$; (2); (3); (5)

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | | Coordinates $(0,0,0)+\ (\frac12,\frac12,\frac12)+$ | | | | | | Reflection conditions |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | h,k,l cyclically permutable<br>General: |
| 24 | c | 1 | (1) $x,y,z$ | (2) $\bar{x}+\frac12,\bar{y},z+\frac12$ | (3) $\bar{x},y+\frac12,\bar{z}+\frac12$ | (4) $x+\frac12,\bar{y}+\frac12,\bar{z}$ | | | $hkl$ : $h+k+l=2n$ |
| | | | (5) $z,x,y$ | (6) $z+\frac12,\bar{x}+\frac12,\bar{y}$ | (7) $\bar{z}+\frac12,\bar{x},y+\frac12$ | (8) $\bar{z},x+\frac12,\bar{y}+\frac12$ | | | $0kl$ : $k+l=2n$ |
| | | | (9) $y,z,x$ | (10) $\bar{y},z+\frac12,\bar{x}+\frac12$ | (11) $y+\frac12,\bar{z}+\frac12,\bar{x}$ | (12) $\bar{y}+\frac12,\bar{z},x+\frac12$ | | | $hhl$ : $l=2n$<br>$h00$ : $h=2n$ |
| | | | | | | | | | Special: no extra conditions |
| 12 | b | 2 . . | $x,0,\frac14$ | $\bar{x}+\frac12,0,\frac34$ | $\frac14,x,0$ | $\frac34,\bar{x}+\frac12,0$ | $0,\frac14,x$ | $0,\frac34,\bar{x}+\frac12$ | |
| 8 | a | . 3 . | $x,x,x$ | $\bar{x}+\frac12,\bar{x},x+\frac12$ | $\bar{x},x+\frac12,\bar{x}+\frac12$ | $x+\frac12,\bar{x}+\frac12,\bar{x}$ | | | |

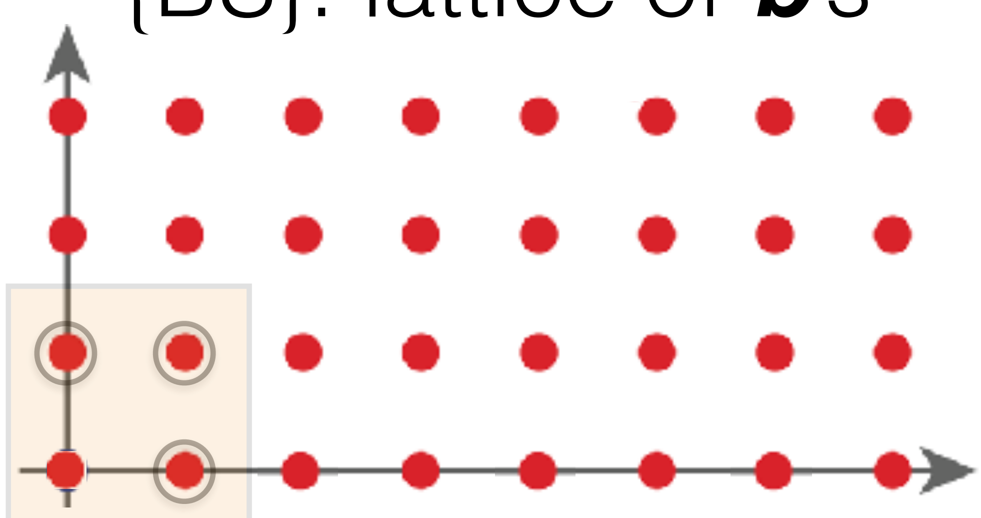
# Indicator of Band Topology

# Indicator of nontrivial band topology

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

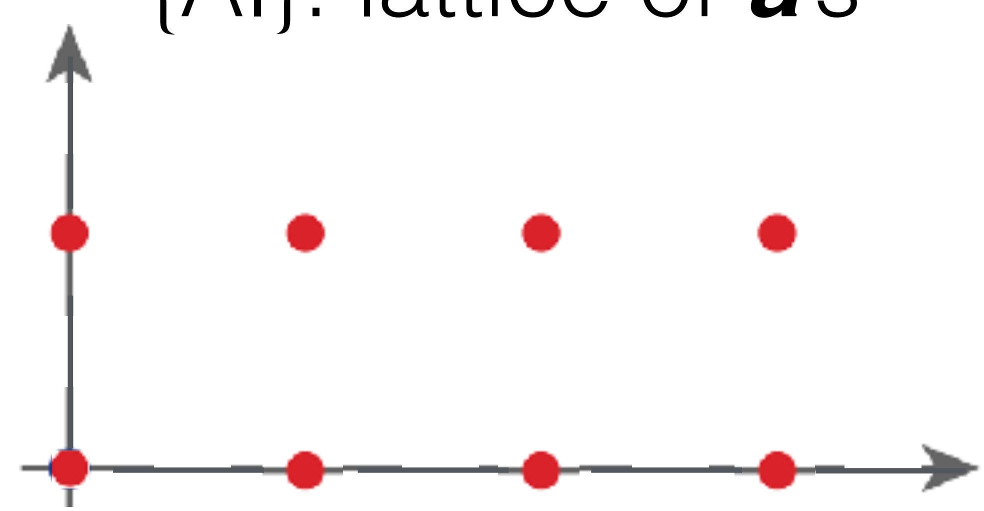
Quotient space: $X = \{BS\}/\{AI\}$ $\{BS\} > \{AI\}$

{BS}: lattice of ***b***’s



$X = Z_2 \times Z_2$

{AI}: lattice of ***a***’s



# Indicator of nontrivial band topology

$$X = \{\mathrm{BS}\}/\{\mathrm{AI}\} = \cancel{\mathbb{Z}^{d_{\mathrm{BS}}-d_{\mathrm{AI}}}} \times \mathbb{Z}_{n1} \times \mathbb{Z}_{n2} \times \ldots \times \mathbb{Z}_{n\mathrm{N}}$$

We found $d_{\mathrm{BS}} = d_{\mathrm{AI}}$ 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)

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

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* |

| $X_{BS}$ | 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 |

| $X_{\mathrm{BS}}$ | 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 1: *Representation-enforced* Quantum Band Insulator

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 + α

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

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

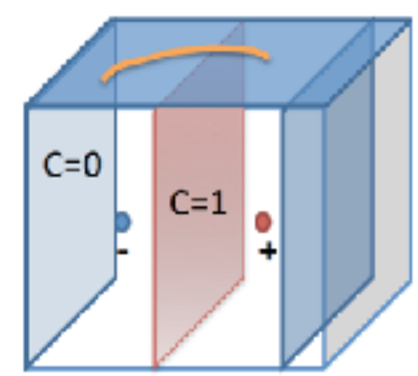
# Example 2:
# *Representation-enforced* Semimetal

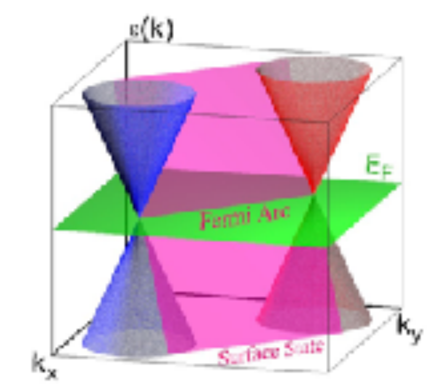
Inversion symmetric but TR broken 3D system (SG2)

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

Weyl SM

A. Turner, …, A. Vishwanath (2010)



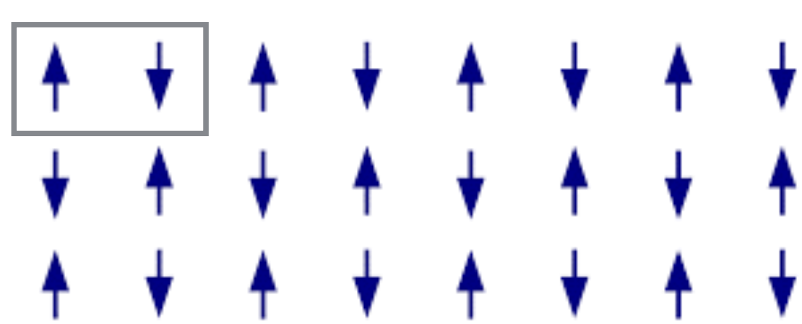

{BS}: "band structure" can be *band insulator*
or *semimetal (band touching at generic points in BZ)*

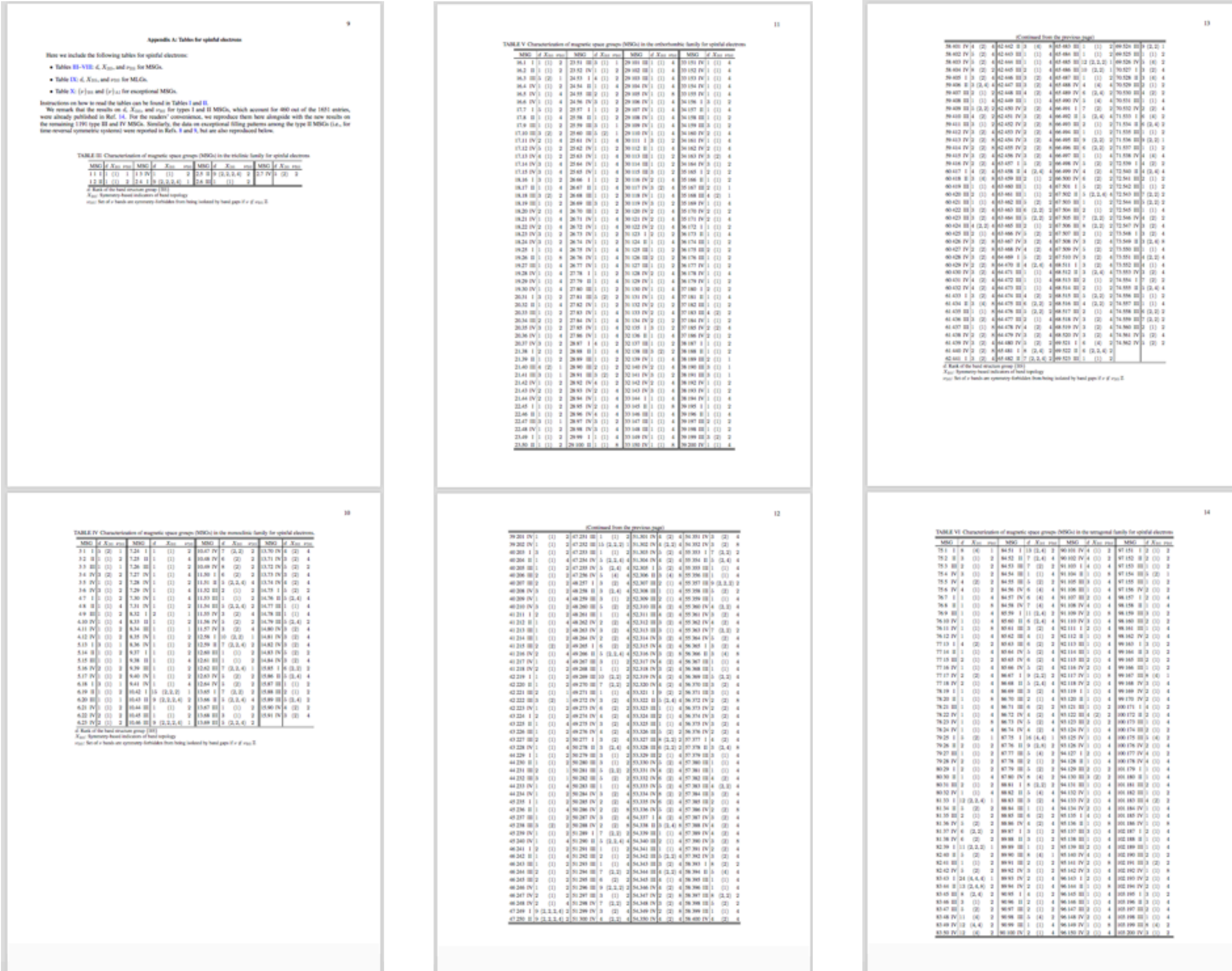
(We demanded band gap only at high-symmetric momenta)

# Magnetic space groups

# Magnetic space group

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

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Appendix A: Tables for spinful electrons
Here we include the following tables for spinful electrons:
Tables III–VIII: d, X_BS, and ν_BS for MSGs.
Table IX: d, X_BS, and ν_BS for MLGs.
Table X: {ν}_BS and {ν}_AI for exceptional MSGs.
Instructions on how to read the tables can be found in Tables I and II.
TABLE III: Characterization of magnetic space groups (MSGs) in the triclinic family for spinful electrons
10
11
12
13
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TABLE VII. Characterization of magnetic space groups (MSGs) in the hexagonal family for spinful electrons

TABLE VIII. Characterization of magnetic space groups (MSGs) in the cubic family for spinful electrons

$d$: Rank of the band structure group {BS}
$X_{BS}$: Symmetry-based indicators of band topology
$\nu_{BS}$: Set of $\nu$ bands are symmetry-forbidden from being isolated by band gaps if $\nu \notin \nu_{BS}\mathbb{Z}$
*: Exhibiting exceptional filling pattern; see Table X

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TABLE IX. Characterization of the projections of magnetic space groups (MSGs) which correspond to magnetic layer group, assumi[ng] ... electrons.

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$d$: Rank of the band structure group {BS}
$X_{BS}$: Symmetry-based indicators of band topology
$\nu_{BS}$: Set of $\nu$ bands can only be isolated by band gaps if $\nu \in \nu_{BS}\mathbb{Z}$

TABLE I. **Characterization of band structures (BSs) in a magnetic space group (MSG); excerpt from Tables III–VIII.**

| MSG[a] | | $d$[b] | $X_{\mathrm{BS}}$[c] | $\nu_{\mathrm{BS}}$[d] |
|---|---|---|---|---|
| 2.5 | II | 9 | $(2,2,2,4)$ | 2 |
| 209.51 | IV | 3 | $(1)$ | 2* |

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

$$X = \text{trivial}$$

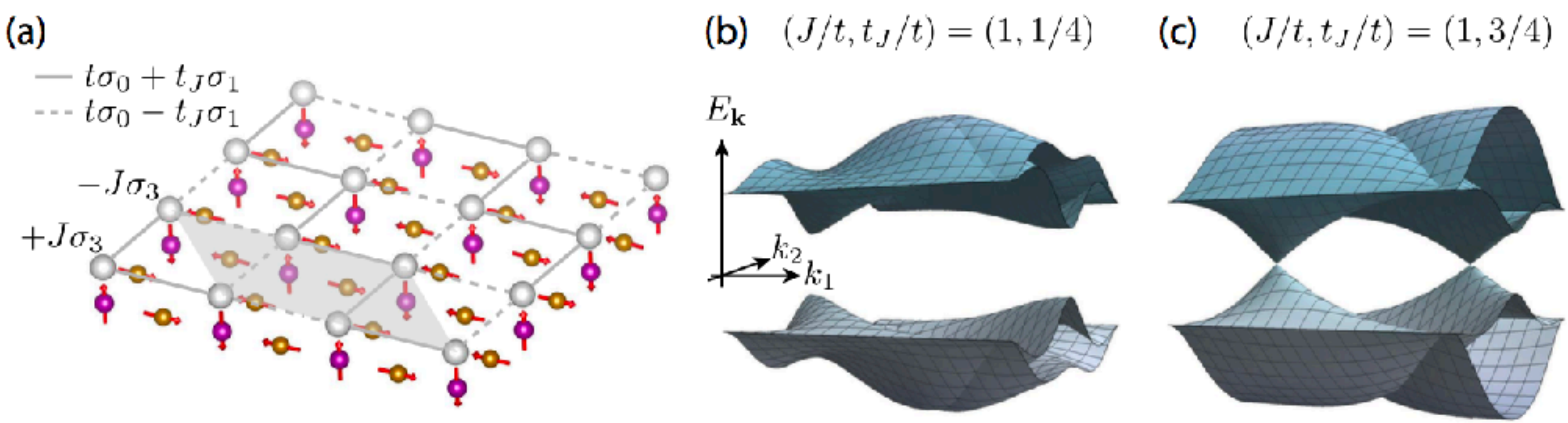
[a] MSG number in the Belov-Neronova-Smirnova notation, followed by a Roman numeral I, . . . , IV indicating its type.
[b] Number of linearly independent BSs.
[c] Symmetry-based indicator of band topology, which takes the form $\prod_i \mathbb{Z}_{n_i}$; denoted by the collection of positive integers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

# Example 3:
# *Representation-enforced* Semimetal

Magnetic Layer Group (2D)
MSG 3.4 ($P_a112$)
π rotation + TR * half translation.

X = $Z_2$

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




$$h(\boldsymbol{k}) = \sum_{i=0}^{2} g_i(\boldsymbol{k})\sigma_i,$$

# Example 4: *Filling-enforced* Semimetal

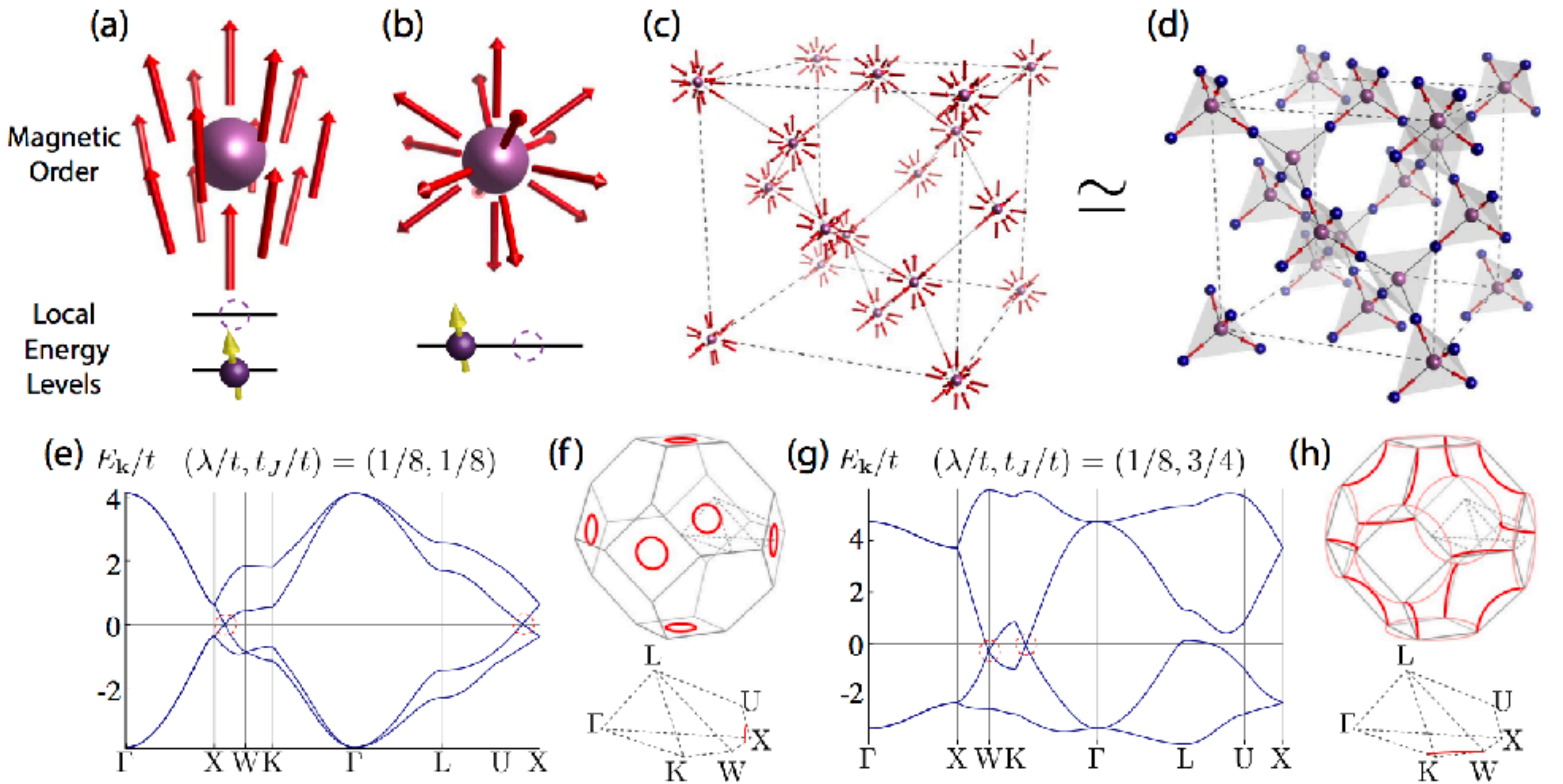



FIG. 2. **Magnetic filling-enforced semimetals.** (a,b) Symmetries of a magnetic order can prohibit atomic insulators (AIs) at odd site fillings.

# Summary

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