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)

Smoothly connected?
- Respects **symmetries**
- Keeps the **excitation gap**

Eigenvalues of $H$ (under p.b.c)

Excitation gap

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

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

**Case 1**
- Eigenvalues of $H$ (under p.b.c)
- Excitation gap
- Band insulator
- Haldane phase

**Case 2**
- GS degeneracy
- Band (semi)metal

**Case 3**
- Gapless
- 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 nonsymmetric space groups
  Parameswaran et al (2013)

- Extended to all 230 SPACE GROUPS

- Stronger constraints in spin models
Introduction 2:
Symmetries and Band Structure
Topological (crystalline) insulator

- Presence of surface / edge state
- Not smoothly connected to atomic limit
Computing Z2 index?

The special subspaces can be identified by considering the matrix of overlaps, $\langle u_i(k)|\Theta|u_j(k)\rangle$. 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 $\epsilon_{ij}P(k)$. $P(k)$ is in fact equal to the Pfaffian

$$P(k) = \text{Pf}[\langle u_i(k)|\Theta|u_j(k)\rangle],$$

(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 $P(k)$ around a loop enclosing half the Brillouin zone (defined so that $k$ and $-k$ are never both included).

$$I = \frac{1}{2\pi i} \oint_C dk \cdot \nabla_k \log[P(k) + i\delta],$$

(5)

... difficult
Fu-Kane formula for Inversion-symmetric TI

- **Strong index**
  \[ \nu_0 = \prod_{i, j, k = 0, \pi} \xi(i, j, k) \]

- **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)

Easy & Helpful for material search!
Band structures in momentum space
Typical band structure...

Bands can cross only when different irreps

Relation among irreps upon symmetry lowering

Dimensions of the irreps $\rightarrow$ degeneracy

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

[Hemstreet & Fong (1974)]
Example: Inversion-symmetric 1D chain

- Two invariant momenta
  \[ k = 0, \pi \]
  \[ \rightarrow \text{High-symmetry momenta} \]
  \[ \text{Little group of } k, G_k \]

- Inversion eigenvalues
  \[ l = \pm 1 \]
  \[ \rightarrow \text{Irreducible representation of } G_k \]
Example: Inversion-symmetric 1D chain

\( n_k^\alpha \): the number of times an irrep \( u_k^\alpha \) appears in BS

\[ b = (n_0^+, n_0^-, n_{\pi^+}, n_{\pi^-}) \]

<table>
<thead>
<tr>
<th>( l )</th>
<th>( k = 0 )</th>
<th>( k = \pi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>+1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>+1</td>
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<td>-1</td>
</tr>
<tr>
<td>-1</td>
<td>+1</td>
<td>+1</td>
</tr>
</tbody>
</table>

Four possible combinations

Only three are independent

\[ b_1 = (1, 0, 1, 0) \]
\[ b_2 = (0, 1, 0, 1) \]
\[ b_3 = (1, 0, 0, 1) \]
\[ b_4 = (0, 1, 1, 0) \]

\[ b_1 + b_2 = b_3 + b_4 \]
Example: Inversion-symmetric 1D chain

\[ b = (n_0^+, n_0^-, n_{\pi}^+, n_{\pi}^-) \]

Relation among \( n_k^\alpha \)'s

\[ n_0^+ + n_0^- = n_{\pi}^+ + n_{\pi}^- = \nu \quad (= \text{# of bands}) \]

\[ b = n_0^+ (1, -1, 0, 0) + n_{\pi}^+ (0, 0, 1, -1) + \nu (0, 1, 0, 1) \]

\[ \rightarrow \{ \text{BS} \} \equiv \text{set of valid } b \text{'s} = \mathbb{Z}^3 \]

Note: we extended possible values of \( n \) to all integers (Classification stable against subtracting bands)
Group structure of Band structure

- $\mathbf{k}$: a high-sym momentum.
  Collect all different types of $\mathbf{k}$

- $G_k$: the little group of $\mathbf{k}$. i.e., \{ $g$ in $G$ | $g\mathbf{k} = \mathbf{k} + G$ \}

- $u_{k}^{\alpha}$ ($\alpha = 1, 2, \ldots$): irreducible representation of $G_k$
  single rep for spinless electrons
  double reps for spinful electrons
Group structure of Band structure

- $n_{k^\alpha}$: the number of times $u_{k^\alpha}$ appears in band structure
- $b = (n_{k_1^1}, n_{k_1^2}, \ldots n_{k_2^1}, n_{k_2^2}, \ldots)$
- Compatibility relations (+ TR sym) among $\{n_{k^\alpha}\}$
- The set of valid $b$'s: $\{\text{BS}\} = \mathbb{Z}^{d_{\text{BS}}}$
  \[ \sum_i m_i \mathbf{b}_i \in \{\text{BS}\} \]

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

'\text{lattice}' of $b$'s
Band structures in REAL space
Bloch vs Wannier

- Momentum space picture
  
  Representations of $G_k$
  
  $b = (n_{k1}^1, n_{k1}^2, \ldots n_{k2}^1, n_{k2}^2, \ldots)$

- Real space picture

  Atomic Insulators
  
  (hopping $\to$ 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) $x = 0, 1/2$

- Parity even/odd orbital $l=+1$ $l=-1$

→ Irreducible representation of $G_x$

→ Special position (Wyckoff position)

Little group of $x$, $G_x$
Example:
Inversion-symmetric 1D chain

\[ k = 0 \]

\[ k = \pi \]

\[ l = +1 \]

\[ l = +1 \]

\[ l = +1 \]

\[ l = -1 \]
Example:
Inversion-symmetric 1D chain

\[ k = 0 \quad l = -1 \]

\[ k = \pi \quad l = -1 \]

\[ k = 0 \quad l = -1 \]

\[ k = \pi \quad l = +1 \]
Example:
Inversion-symmetric 1D chain

\[ a_1 = (1, 0, 1, 0) \]
\[ a_2 = (0, 1, 0, 1) \]
\[ a_3 = (1, 0, 0, 1) \]
\[ a_4 = (0, 1, 1, 0) \]

Set of all \( b \) corresponding to AI: \( \{AI\} = Z^3 \)

\[ a_1 + a_2 = a_3 + a_4 \]

In this example, \( \{BS\} = \{AI\} \) (but not necessarily in general)
Listing up all atomic insulators

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

\[
\sum_i m_i \mathbf{a}_i \in \{\text{AI}\}
\]
Indicator of Band Topology
Indicator of nontrivial band topology

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

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

$X = Z_2 \times Z_2$
Indicator of nontrivial band topology

\[ X = \frac{\{BS\}}{\{AI\}} = \mathbb{Z}^{d_{BS}-d_{AI}} \times \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \ldots \times \mathbb{Z}_{n_N} \]

We found \( d_{BS} = d_{AI} \) holds for all SGs

\[ \rightarrow \text{We can, in fact, compute } \{BS\} \text{ from } \{AI\} \text{ (easy to get)} \]

i.e., no need to list up / solve all compatibility relations (tough)

\[ b = \sum_i q_i a_i \in \{BS\} \]

Must be integer valued  Can be fractional

If necessary, one can impose the "nonnegative" constraint at the end.
230 SGs x TRS with SOC

<table>
<thead>
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<th>$d$</th>
<th>SGs</th>
</tr>
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<tr>
<td>6</td>
<td>69, 71, 85, 125, 129, 132, 163, 165, 190, 201, 203, 205, 206, 215, 216, 222</td>
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<tr>
<td>7</td>
<td>12, 65, 84, 128, 131, 140, 188, 189, 202, 204, 223</td>
</tr>
<tr>
<td>8</td>
<td>124, 127, 148, 166, 193, 200, 224, 225, 227</td>
</tr>
<tr>
<td>9</td>
<td>2, 10, 47, 87, 139, 147, 162, 164, 176, 192, 194, 174, 187</td>
</tr>
<tr>
<td>10</td>
<td>225, 229</td>
</tr>
<tr>
<td>11</td>
<td>83, 123</td>
</tr>
<tr>
<td>14</td>
<td>175, 191, 221</td>
</tr>
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<table>
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<tr>
<th>$X_{BS}$</th>
<th>SGs</th>
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<td>$\mathbb{Z}_3$</td>
<td>188, 190</td>
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<tr>
<td>$\mathbb{Z}_8$</td>
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<tr>
<td>$\mathbb{Z}_{12}$</td>
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<td>$\mathbb{Z}_3 \times \mathbb{Z}_3$</td>
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<tr>
<td>$\mathbb{Z}_4 \times \mathbb{Z}_8$</td>
<td>127, 221</td>
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<tr>
<td>$\mathbb{Z}<em>6 \times \mathbb{Z}</em>{12}$</td>
<td>175, 191</td>
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<td>$(\mathbb{Z}_2)^2 \times \mathbb{Z}_4$</td>
<td>11, 12, 13, 49, 51, 65, 67, 69</td>
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<tr>
<td>$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$</td>
<td>83, 123</td>
</tr>
<tr>
<td>$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$</td>
<td>2, 10, 47</td>
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230 SGs x TRS without SOC

<table>
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<th>SGs</th>
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<td>1, 4, 7, 9, 19, 29, 39, 76, 78, 144, 145, 169, 170</td>
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<td>8, 31, 36, 41, 43, 80, 92, 95, 110, 146, 161, 198</td>
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<td>24, 28, 37, 59, 60, 62, 77, 79, 91, 95, 102, 104, 143, 155, 157, 158, 185, 186, 196, 197, 210</td>
</tr>
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<td>5</td>
<td>3, 14, 17, 27, 42, 44, 52, 56, 57, 94, 98, 100, 101, 108, 114, 122, 150, 156, 182, 214, 220</td>
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<td>6</td>
<td>11, 15, 35, 38, 54, 70, 73, 75, 88, 90, 103, 105, 107, 113, 142, 149, 167, 168, 184, 195, 205, 219</td>
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<td>7</td>
<td>13, 23, 23, 59, 64, 68, 82, 86, 117, 118, 130, 130, 163, 165, 180, 181, 203, 206, 208, 209, 211, 218, 228, 230</td>
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<td>8</td>
<td>21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217</td>
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<td>2, 25, 48, 50, 53, 55, 72, 99, 121, 126, 138, 141, 147, 188, 207, 216, 222</td>
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<td>51, 87, 89, 115, 129, 134, 162, 164, 174, 189, 193, 222, 226</td>
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<td>49, 140, 192, 200</td>
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<td>15</td>
<td>10, 69, 71, 124, 127, 132, 187</td>
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<td>225, 229</td>
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<td>65, 83, 131, 139, 175</td>
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<td>221</td>
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<td>191</td>
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<tr>
<td>20</td>
<td>47, 123</td>
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<tr>
<th>$\mathbb{Z}_2$</th>
<th>SGs</th>
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| $\mathbb{Z}_2 \times \mathbb{Z}_4$ | 12, 13, 15, 81, 84, 87 |

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<th>$(\mathbb{Z}_2)^2$</th>
<th>SGs</th>
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| $\mathbb{Z}_2 \times \mathbb{Z}_4$ | 10, 83, 175 |

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<tbody>
<tr>
<td>$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$</td>
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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 + \( \alpha \)

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)

\[ X = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4 \]

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 $T' = TR \times g$

- ex1: $g = \text{identity} \rightarrow M = \text{SG} \times \{1, \text{TRS}\}$.

- ex2: $g = \text{half translation} \rightarrow \text{AFM order}$

- There are 1651 MSGs in 3D / 528 MLGs in 2D
Appendix E: Tables for spatial electrons

Here we include the following tables for spatial electrons:

- Table III: $\xi$, $\alpha_\sigma$, and $\nu_\sigma$ for MNOs.
- Table IV: $\xi$, $\alpha_\sigma$, and $\nu_\sigma$ for MNOs.
- Table V: $\xi$, $\alpha_\sigma$, and $\nu_\sigma$ for exceptional MNOs.

Instructions on how to read the tables can be found in Tables I and II.

**Table III: Characterization of magnetic mass groups (MNOs) for the sixfold family for spatial electrons**

<table>
<thead>
<tr>
<th>MNO</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.2</td>
<td>0.3</td>
<td>0.4</td>
<td>0.2</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>2</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
</tr>
<tr>
<td>4</td>
<td>0.8</td>
<td>0.9</td>
<td>1.0</td>
<td>0.8</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
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**Table IV: Characterization of magnetic mass groups (MNOs) for the sixfold family for spatial electrons**

<table>
<thead>
<tr>
<th>MNO</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
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<td>0.3</td>
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<tr>
<td>2</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
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<tr>
<td>3</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
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<tr>
<td>4</td>
<td>0.8</td>
<td>0.9</td>
<td>1.0</td>
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<td>0.9</td>
<td>1.0</td>
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<tr>
<td>5</td>
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<td>1.1</td>
<td>1.2</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
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**Table V: Characterization of magnetic mass groups (MNOs) for the exceptional family for spatial electrons**

<table>
<thead>
<tr>
<th>MNO</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
<th>$\xi$</th>
<th>$\alpha_\sigma$</th>
<th>$\nu_\sigma$</th>
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</thead>
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<td>0.3</td>
<td>0.4</td>
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<tr>
<td>2</td>
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<td>0.6</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
</tr>
<tr>
<td>4</td>
<td>0.8</td>
<td>0.9</td>
<td>1.0</td>
<td>0.8</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
</tr>
</tbody>
</table>
TABLE I. Characterization of band structures (BSs) in a magnetic space group (MSG); excerpt from Tables III–VIII.

<table>
<thead>
<tr>
<th>MSG(^a)</th>
<th>(d)^(b)</th>
<th>(X_{BS})^(c)</th>
<th>(\nu_{BS})^(d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5 II</td>
<td>9 ((2,2,2,4))</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>209.51 IV</td>
<td>3 ((1))</td>
<td>2(^*)</td>
<td></td>
</tr>
</tbody>
</table>

\(X = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4\)

\(X = \text{trivial}\)

\(^a\) 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 \((n_1, n_2, \ldots)\).

\(^d\) 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 X.
Example 3: 
Representation-enforced Semimetal

Magnetic Layer Group (2D)  
MSG 3.4 ($\text{Pa}_{112}$)  
$\pi$ rotation + TR * half translation.

\[ X = \mathbb{Z}_2 \]

\[ \eta = \prod_{n: \text{occupied}} \prod_{k=\left(\pi, 0\right), \left(\pi, \pi\right)} ^{n,k} \eta_{n,k}, \]

\[ \left( J/t, t_J/t \right) = \left( 1, 1/4 \right) \quad \left( J/t, t_J/t \right) = \left( 1, 3/4 \right) \]

\[ h(k) = \sum_{i=0}^{2} g_i(k) \sigma_i, \]
Example 4: Filling-enforced Semimetal

(a) Magnetic Order
(b) Local Energy Levels

(e) $E_k/t \ (\lambda/t, t_J/t) = (1/8, 1/8)$
(f) $E_k/t \ (\lambda/t, t_J/t) = (1/8, 3/4)$

FIG. 2. Magnetic filling-enforced semimetals. (a,b) Symmetries of a magnetic order can prohibit atomic insulators (AIs) at odd site fillings. (c) The magnetic point-group symmetries of a ferromagnetic arrangement is compatible with nondegenerate local energy levels. (b) These theoretical considerations can be employed to design and fabricate nontrivial semimetallic systems with desired topological properties. (h) A diagram illustrating the band structure of the system.
Summary

• Higher symmetry → Richer phases & stronger constraints

• Our band topology indicator might accelerate new material search / screening process