Symmetry Indicators of Band Topology

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HCP, Vishwanath & Watanabe, 1703.00911; Nat. Commun. 2017
Watanabe*, HCP* & Vishwanath, 1707.01903; Sci. Adv. 2018

Ashvin Vishwanath
(Harvard)

Haruki Watanabe
(U of Tokyo)

Also: Eslam Khalaf (Harvard), Feng Tang & Xiangang Wan (Nanjing U)
A light, lightning recap
Atomic insulators
(aka band representations)
[Zak, 1980; Zak, Bacry, Michel, ~2000]

- Real-space construction/ description
- Manifestly symmetric and insulating

Particle-like electrons

Sym. rep: s,p,d… + crystal field
Band insulators

[Image: Diagram of energy bands with labels for symmetrical representations and wave-like patterns.]

Sym. rep

Wave-like

[Hemstreet & Fong (1974)]
Classical vs Quantum insulators

Particle-like

Wave-like
Classical vs Quantum insulators

Particle-like

Wave-like

Always
Classical vs Quantum insulators

Particle-like

Always

Wave-like

Sometimes
Classical vs Quantum insulators

Atomic (Particle-like)  Topo. (Wave-like)

Band insulators
Boundary: Classical
Boundary: Classical
Boundary: Classical

Safe trip!
Boundary: Quantum
Boundary: Quantum
“Necessarily quantum” insulators (aka topological insulators)

[HCP, Watanabe, Zaletel, Vishwanath, 1506.03816]

- Band insulators without any classical (real-space, symmetric and localized) description
- “Wannier obstructions”
- Nontrivial band topology forbidding smooth symmetric deformation to any atomic insulator
Main Goal

HCP, Vishwanath & Watanabe, 1703.00911
Bradlyn et al, 1703.02050

Efficient way(s) to tell trivial $\approx$ atomic $\approx$ classical from topological $\approx$ quantum

Applications:
large-scale materials discovery

Tang, HCP, Vishwanath, Wan, 1805.07314, 1806.04128, 1807.09744
Zhang, ..., Weng, Fang, 1807.08756
Vergniory, ..., Bernevig, Wang, 1807.10271
Main Goal

HCP, Vishwanath & Watanabe, 1703.00911
Bradlyn et al, 1703.02050

Efficient way(s) to tell trivial $\simeq$ atomic $\simeq$ classical from topological $\simeq$ quantum
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Efficient way(s) to tell trivial $\approx$ atomic $\approx$ classical from topological $\approx$ quantum
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Efficient way(s) to tell trivial $\approx$ atomic $\approx$ classical from topological $\approx$ quantum
How to compare?

Real space

- Lattice sites
- Reps of site-sym. groups

Momentum space

- Energy bands
- Bloch wave functions
- Reps at high-sym. momenta
How to compare?

Real space
- Lattice sites
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Momentum space
- Energy bands
- Bloch wave functions
  - Reps at high-sym. momenta

Fourier Trans.
How to compare?

Real space
- Lattice sites
- Reps of site-sym. groups

Momentum space
- Energy bands
- Bloch wave functions
  - Reps at high-sym. momenta

Wannier Fns. (if exist)

Fourier Trans.
How to compare?

Real space  
Momentum space

Fourier Trans.  
Straight-forward

Wannier Fns. (if exist)

Hard—requires knowing the Bloch wave functions over the BZ
How to compare?

Real space       Momentum space

Straight-forward

Wannier Fns.  Fourier Trans.
(if exist)

Hard—requires knowing the Bloch wave functions over the BZ

Simplification
- Symmetry-data in *the momentum space*
- Partial information, i.e., incomplete knowledge
Connaissance incomplète

With only momentum-space symmetry data…

• Generally, impossible to tell if a set of bands is trivial (i.e., if it is a band representation)

• But, possible to diagnose some band topology
  • i.e., not necessary, but sufficient, conditions on the existence of band topology
Clarification

Do not confuse sym. reps. in real vs. momentum spaces
Specifying sym. reps in...  

Real space  

- **Full knowledge** on a **restricted set** of band insulators (i.e., trivial)  

Momentum space  

- **Restricted knowledge** on the **full set** of band insulators
“Bootstrapping” from the trivial

Real space

- Full knowledge on a restricted set of band insulators (i.e., trivial)

I’ve computed everything about the trivial states!
"Bootstrapping" from the trivial

Real space

- Full knowledge on a restricted set of band insulators (i.e., trivial)

I’ve computed everything about the trivial states!

Uh...I thought we were interested in the nontrivial ones?
“Bootstrapping” from the trivial

Here comes the magic!
“Bootstrapping” from the trivial

Claim:

*Insofar as momentum-space symmetry representations are concerned,* knowledge on the trivial insulators, defined in the real space, allows one to map out the “space” of band insulators, including the topological ones.

HCP, Vishwanath & Watanabe, 1703.00911
Watanabe*, HCP* & Vishwanath, 1707.01903
Outline aka Take-homes

• A more modern way to solve the ancient problem of band symmetries
  ➡ By viewing band structures as a “vector space”

• Comparing momentum vs real space
  ➡ symmetry-based indicators of band topology

• Applications
  ➡ High throughput materials prediction
Outline aka Take-homes

- A more modern way to solve the ancient problem of band symmetries
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  - High throughput materials prediction
Band structures form a “vector space”

\[-\vec{b}_1 + 3\vec{b}_2\]
“Vector space”? 
(More accurately, $\mathbb{Z}^d$)

1. What does “addition” mean?

2. What does “subtraction” mean???

3. What are the bases and how to expand?

4. (Expert) Aren’t there some torsions?

Ans: Natural from a symmetry perspective
Sym. reps of band structures

A symmetry either
(i) Leaves a momentum invariant
   - (Degenerate) Bloch wave functions furnish (irreducible) representations
(ii) Relates two momenta
    - Energies identical
    - Wave functions symmetry-related
Sym. reps of band structures

[Hemstreet & Fong (1974)]
Sym. reps of band structures

Bands can cross only when they carry different symmetry labels

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Bands can cross only when they carry different symmetry labels.

Dimensions of the irreps determine how the bands are “stuck.”

[Hemstreet & Fong (1974)]
Sym. reps of band structures

Bands can cross only when they carry different symmetry labels.

Dimensions of the irreps determine how the bands are “stuck.”

Irreps follow rules under symmetry lowering:

\[ \Gamma_1 \rightarrow \Delta_1 \]
\[ \Gamma_{12} \rightarrow \Delta_1 \oplus \Delta_2 \]
\[ \Gamma_{15} \rightarrow \Delta_1 \oplus \Delta_{3,4} \]

[Hemstreet & Fong (1974)]
Topology meets band symmetries

- Topological properties: forget energetics within a set of bands
- Labels become simple counting
- Gaps above and below ensure counting is well-defined
- Finite list of high-symmetry momenta & reps

\[
(n_{\Gamma_1}, n_{\Gamma_{12}}, n_{\Gamma_{15}}, n_{\Sigma_1}, \ldots, \nu) = (0, 0, 1, 2, \ldots, 3) \in \mathbb{Z}^D
\]
Adding = stacking

- Counts of symmetry labels simply add
- Addition has the physical meaning of “stacking”, i.e., interlacing systems

[Hemstreet & Fong (1974)]
Imposing Compatibility Relations

- But these counts are not independent: “Compatibility Relations”

\[
\begin{align*}
\Gamma_1 & \rightarrow \Delta_1 \\
\Gamma_{12} & \rightarrow \Delta_1 \oplus \Delta_2 \\
\Gamma_{15} & \rightarrow \Delta_1 \oplus \Delta_{3,4}
\end{align*}
\]

\[
\begin{align*}
n_{\Delta_1} &= n_{\Gamma_1} + n_{\Gamma_{12}} + n_{\Gamma_{15}} \\
n_{\Delta_2} &= n_{\Gamma_{12}} \\
n_{\Delta_{3,4}} &= n_{\Gamma_{15}}
\end{align*}
\]
The group \{BS\}

- Generally, integer-valued linear equations

\[
\begin{pmatrix}
1 & 1 & 1 & -1 & 0 & 0 \\
0 & 1 & 0 & 0 & -1 & 0 \\
0 & 0 & 1 & 0 & 0 & -1
\end{pmatrix}
\begin{pmatrix}
n_{\Gamma_1} \\
n_{\Gamma_{12}} \\
n_{\Gamma_{15}} \\
n_{\Delta_1} \\
n_{\Delta_2} \\
n_{\Delta_{3,4}}
\end{pmatrix} = 0
\]

- Gapped band structure = solutions to \( C \vec{n} = \vec{0} \)

\( \{BS\} \equiv \ker C \cap \mathbb{Z}^D \cong \mathbb{Z}^{d_{BS}} \)

\( d_{BS} \): dimension of solution space

\( \mathbb{Z}^{d_{BS}} \) is an abelian group with \( d_{BS} \) generators
{Band structures} as a “vector space”

\[ \vec{n} \in \{\text{BS}\} \Rightarrow \vec{n} = \sum_{i=1}^{d_{BS}} m_i \vec{b}_i; \quad m_i \in \mathbb{Z} \]
Example: 1D w/ inversion


- 2 special momenta
- 2 types of irreps per momentum
- Total number of bands
- 5 symmetry labels

\[ \vec{n} = (n_0^+, n_0^-, n_\pi^+, n_\pi^-, \nu) \]

- 2 constraints
  \[ n_0^+ + n_0^- = \nu \]
  \[ n_\pi^+ + n_\pi^- = \nu \]

- 3 independent labels
  \[ \{\text{BS}\} = \mathbb{Z}^3 \]
Interlude: What have we done?

1. Forget about energetics within a set of bands isolated by band gaps above and below

2. Allow for negative “counts”
   - Inclusion of the negatives allows us to get a group
   - Similar spirit as K-theory-based discussions
     - Kitaev (2009); Freed & Moore (2013); Kruthoff et al (2016)
   - Circumvent the nightmare of permutations!
     - cf, eg, Bouckaert, Smoluchowski & Wigner (1936)
A more modern way to solve the ancient problem of band symmetries

- By viewing band structures as a “vector space”

- Comparing momentum vs real space
  - symmetry-based indicators of band topology

- Applications
  - High throughput materials prediction
Real-space (atomic) pictures contain all band-symmetry solutions
Trivial $\equiv$ Atomic insulators

Trivial band structures: those with a real-space description

Lattice Points + Orbitals $\rightarrow$ Fourier

Tight-binding orbitals fix momentum-space sym. reps.
Trivial = Atomic insulators

Trivial band structures: those with a real-space description

Lattice Points + Orbitals → \( \vec{a} \in \{BS\} \)

Fourier
Trivial = Atomic insulators

Trivial band structures: those with a real-space description
Trivial = Atomic insulators

Trivial band structures: those with a real-space description

\[
\{ \tilde{a} \} \leq \{ \text{BS} \}
\]

Lattice Points + Orbitals

Fourier
Trivial = Atomic insulators

Trivial band structures: those with a real-space description

Lattice Points + Orbitals \rightarrow \text{Subgroup from trivial BSs}

\{\vec{a}\} \leq \{\text{BS}\}
\|\{\text{AI}\} \leq \{\text{BS}\}
{BS} vs {AI}

Atomic
{BS} vs {AI}

Non-atomic = topological

Atomic
{BS} vs {AI}

Non-atomic = topological

Band topology indicated by

\[ X_{BS} \equiv \frac{\{BS\}}{\{AI\}} \]

(e.g., \( \mathbb{Z}_2 \times \mathbb{Z}_2 \))
\{\text{BS}\} \text{ vs } \{\text{AI}\}

Non-atomic = topological

Band topology indicated by

\[ X_{\text{BS}} \equiv \frac{\{\text{BS}\}}{\{\text{AI}\}} \]

(e.g., \( \mathbb{Z}_2 \times \mathbb{Z}_2 \))
“Bootstrapping” from the trivial

HCP, Vishwanath & Watanabe, 1703.00911
Watanabe*, HCP* & Vishwanath, 1707.01903

For all 1,651 magnetic space groups, with or without spin-orbit coupling,

\[ X_{BS} \equiv \frac{\{BS\}}{\{AI\}} \]

is a finite abelian group.

⇒ as “vector spaces,” the dimensions \( d_{BS} = d_{AI} \)

⇒ Basis for \( \{BS\} \) constructible from that of \( \{AI\} \)
Let \( \{ a_i \mid i = 1, \ldots, d_{AI} \} \) be a complete basis for \( \{ AI \} \).

Let \( \mathbf{b} \) be the sym. rep. vector of a band insulator, then

\[
\mathbf{b} = \sum_{i=1}^{d_{AI}} q_i a_i
\]

for some rational coefficients \( q_i \); in addition

- Any \( q_i \) is fractional \( \Rightarrow \) \( \mathbf{b} \) is topological
- All \( q_i \) are integers \( \Rightarrow \) \( \mathbf{b} \) can be trivial
Example: Time-reversal & Inversion

• The Fu-Kane parity criterion:

  Combinations of products of parities determine all the strong and weak $\mathbb{Z}_2$ indices

  [Fu & Kane, PRB 76, 045302 (2007)]

• This guarantees $X_{BS}$ is nontrivial whenever inversion is a symmetry
TR & inversion symmetric systems

- For 2D, $X_{BS} = \mathbb{Z}_2$
  - simply the quantum spin Hall index
- For 3D,

$$X_{BS} = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$
TR & inversion symmetric systems

• For 2D, \( X_{\text{BS}} = \mathbb{Z}_2 \)
  - simply the quantum spin Hall index

• For 3D,

\[
X_{\text{BS}} = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4
\]

\[\underline{\text{Weak TIs}}\]
TR & inversion symmetric systems

- For 2D, $X_{BS} = \mathbb{Z}_2$
  - simply the quantum spin Hall index

- For 3D,

\[
X_{BS} = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4
\]

Weak TIs \quad Strong TI
& something more,
protected by TR & inversion

[HCP, Vishwanath & Watanabe, 1703.00911]
“Something more”: Doubled Strong TI

- Two copies of the strong TI, no magnetoelectric response
- Entanglement signature [Alexandradinata et al (2014); HCP et al (2017)]
- Do not expect surface Dirac cone(s)
Physical surface signature?

Inversion-symmetric open-boundary conditions

1D Helical mode
~ quantum spin Hall edge

⇒ Stable against small inversion-breaking perturbation
⇒ “Hinge” modes

Song, Fang & Fang, 1708.02952;
Schindler et al., 1708.03636
Langbehn et al., 1708.03640
Benalcazar, Bernevig & Hughes, 1708.04230
Fang & Fu, 1709.01929
Good news: One group done!

Done: 1

1650 magnetic space groups left
All 1,651 magnetic space groups (spinful or spinless)

[Watanabe*, HCP* & Vishwanath, 1707.01903]

### TABLE III. Characterization of magnetic space groups (MSGs) in the triclinic family for spinful electrons.

<table>
<thead>
<tr>
<th>MSG</th>
<th>$d$</th>
<th>$X_{BIS}$</th>
<th>$\nu_{BIS}$</th>
<th>MSG</th>
<th>$d$</th>
<th>$X_{BIS}$</th>
<th>$\nu_{BIS}$</th>
<th>MSG</th>
<th>$d$</th>
<th>$X_{BIS}$</th>
<th>$\nu_{BIS}$</th>
<th>MSG</th>
<th>$d$</th>
<th>$X_{BIS}$</th>
<th>$\nu_{BIS}$</th>
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<td>1</td>
<td>(1)</td>
<td>1.3</td>
<td>IV</td>
<td>1</td>
<td>(1)</td>
<td>2.5</td>
<td>II</td>
<td>9</td>
<td>(2,2,2,4)</td>
<td>2.74</td>
<td>II</td>
<td>5</td>
<td>(2)</td>
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<tr>
<td>1.2</td>
<td>1</td>
<td>2</td>
<td></td>
<td>2.4</td>
<td>I</td>
<td>9</td>
<td>(2,2,2,4)</td>
<td>1.3</td>
<td>IV</td>
<td>1</td>
<td>(1)</td>
<td>2.6</td>
<td>III</td>
<td>1</td>
<td>(1)</td>
</tr>
</tbody>
</table>

$d$: Rank of the band structure group [BIS]

$X_{BIS}$: Symmetry-based indicators of band topology

$\nu_{BIS}$: Set of $\nu$ bands are symmetry-forbidden from being isolated by band gaps if $\nu \not\in \nu_{BIS}$.

### TABLE IV. Characterization of magnetic space groups (MSGs) in the monoclinic family for spinful electrons.

<table>
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<tr>
<th>MSG</th>
<th>$d$</th>
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<th>$\nu_{BIS}$</th>
<th>MSG</th>
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$d$: Rank of the band structure group [BIS]

$X_{BIS}$: Symmetry-based indicators of band topology

$\nu_{BIS}$: Set of $\nu$ bands are symmetry-forbidden from being isolated by band gaps if $\nu \not\in \nu_{BIS}$.

& ~20 more pages
In class AII (spin-orbit coupled with time-reversal $\mathcal{T}^2=-1$), nontrivial $X_{BS}$ implies (up to energetics):

- Strong topological insulator; or
- Topological crystalline insulator
- Weak TI
- Mirror Chern
- Hourglass
- Higher-order
- …

Khalaf, HCP, et al, 1711.11589
(also, Song, Zhang et al, 1711.11049)
Class All $X_{BS}$: Surface States

“Doubled strong TI”:

- Under spatial symmetry $g$
  \[ m(g \cdot \mathbf{r}) = \pm m(\mathbf{r}) \]

- Sign determined by the band topology of the bulk
- “-ve signature”: surface cannot be gapped everywhere
- Precise form of gaplessness determined by the symmetries at play
Some cautions

1. Why “band structures” instead of “band insulators”?
   - Gap condition *only* imposed at high-symmetry momenta; could have *irremovable* gapless points at generic momenta
     Hughes *et al*., PRB 83, 245132 (2011); Turner *et al*., PRB 85, 165120 (2012)

2. A full classification?
   - NO: connaissance incomplète!
   - Certain topological phases are not detected (e.g. no symmetry other than translations)
   - Symmetry *indicators* of band topology
Outline aka Take-homes

✓ A more modern way to solve the ancient problem of band symmetries
  ➡ By viewing band structures as a “vector space”

✓ Comparing momentum vs real space
  ➡ symmetry-based indicators of band topology

• Applications
  ➡ High throughput materials prediction
Ideally…

X-BS nontrivial materials

Google Search  I'm Feeling Lucky
Materials analysis flow

Chemistry data

compute/ guess

k-space irreps

Expand over \{BS\}

Integral

Expand over \{AI\}

Integral

(semi-)metallic

Guaranteed nontrivial

ab initio & wave function analysis

ab initio energetics
Non-magnetic materials search

[Tang, HCP, Vishwanath & Wan, 1805.07314, 1806.04128, 1807.09744]
[Also: Zhang et al., 1807.08756, Vergniory et al., 1807.10271]

Strong TIs Higher-order TCIs

\(\beta\)-MoTe\(_2\)

MgBi\(_2\)O\(_6\)

\(\text{Ba}_{11}\text{Bi}_{14}\text{Cd}_8\)

\(\text{PdO}\)

\(\text{Ag}_2\text{Zr}\)
Non-magnetic materials search

[1807.10271]

Tang, HCP, Vishwanath & Wan, 1805.07314, 1806.04128, 1807.09744

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Strong TIs, Higher-order TCIs

$\beta$-MoTe$_2$, PdO, MgBi$_2$O$_6$, Dirac SM

Also: Zhang et al., 1807.08756, Vergniory et al., 1807.10271
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Thanks!