Symmetry Indicators of Band Topology

Adrian Po
(MIT)

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)

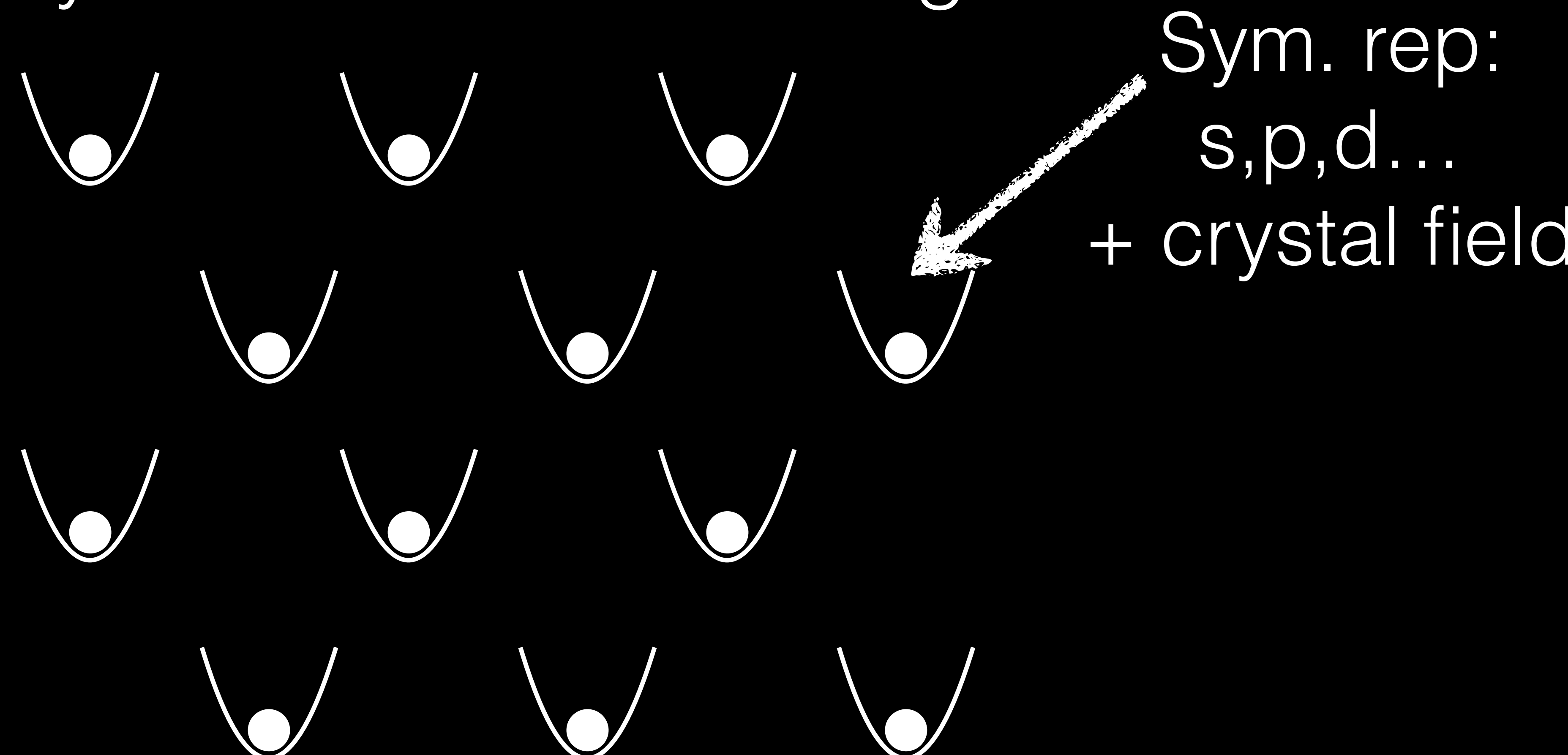
A light, lightning recap

Atomic insulators

(aka band representations)

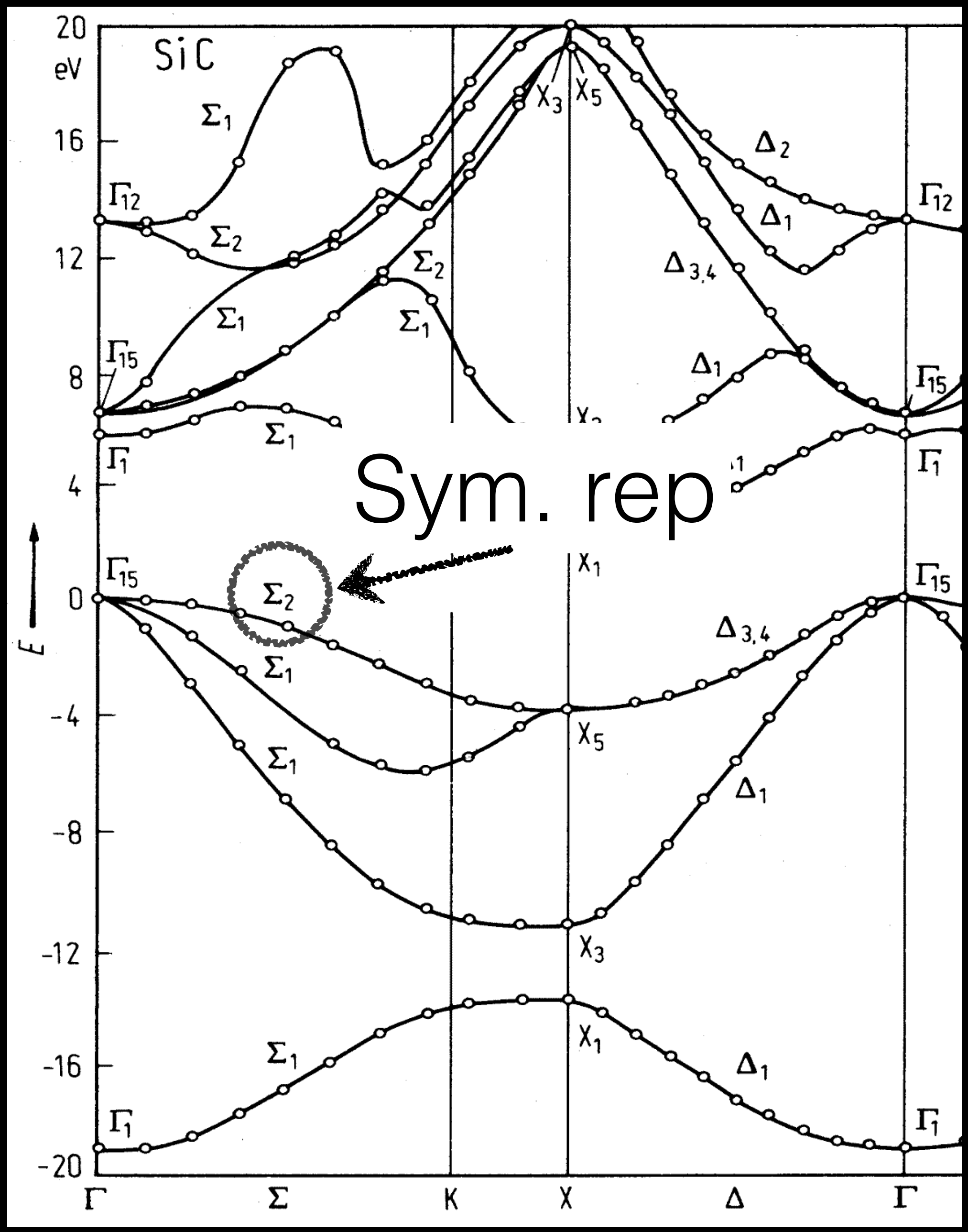
[Zak, 1980; Zak, Bacry, Michel, ~2000]

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

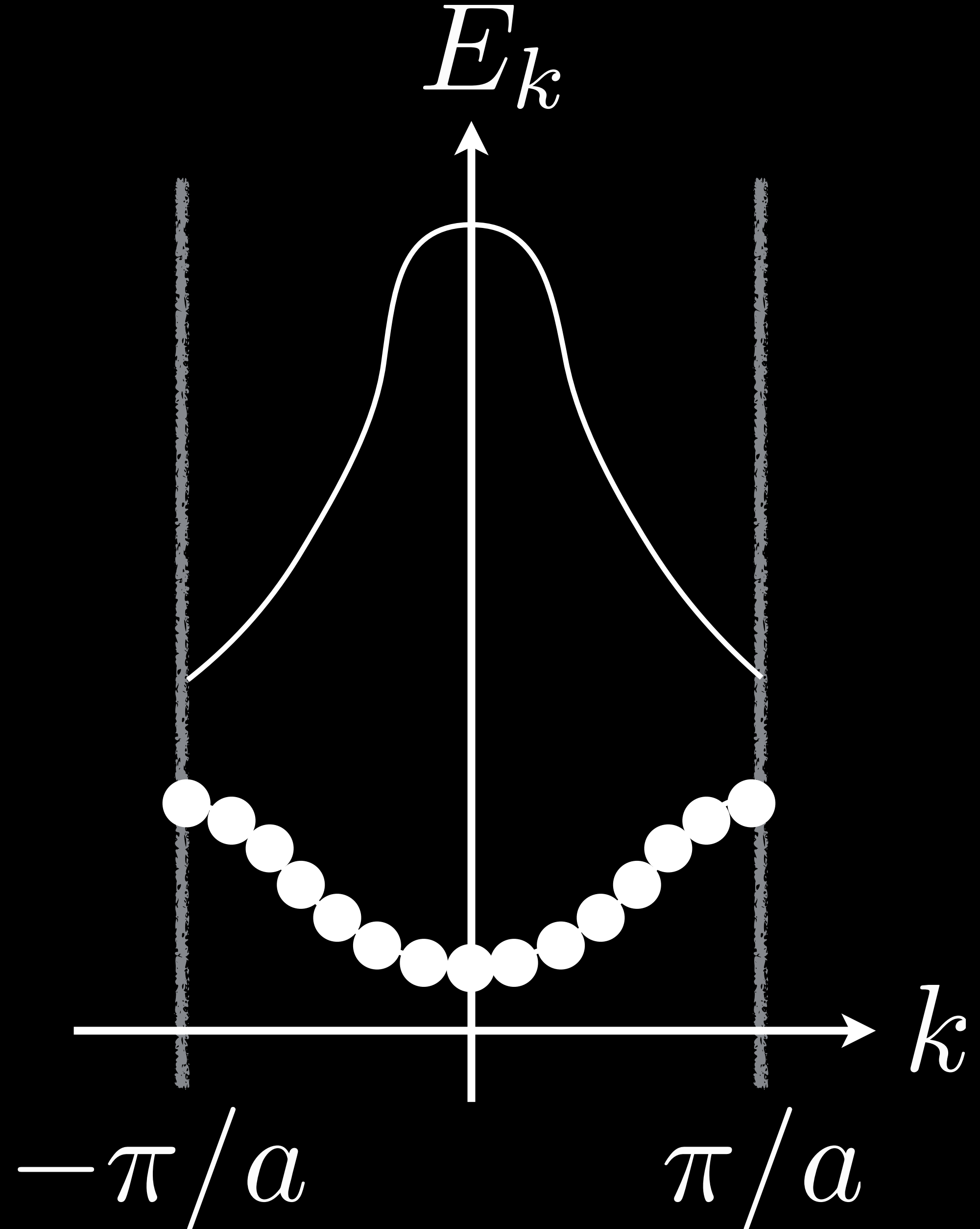


Particle-like electrons

Band insulators

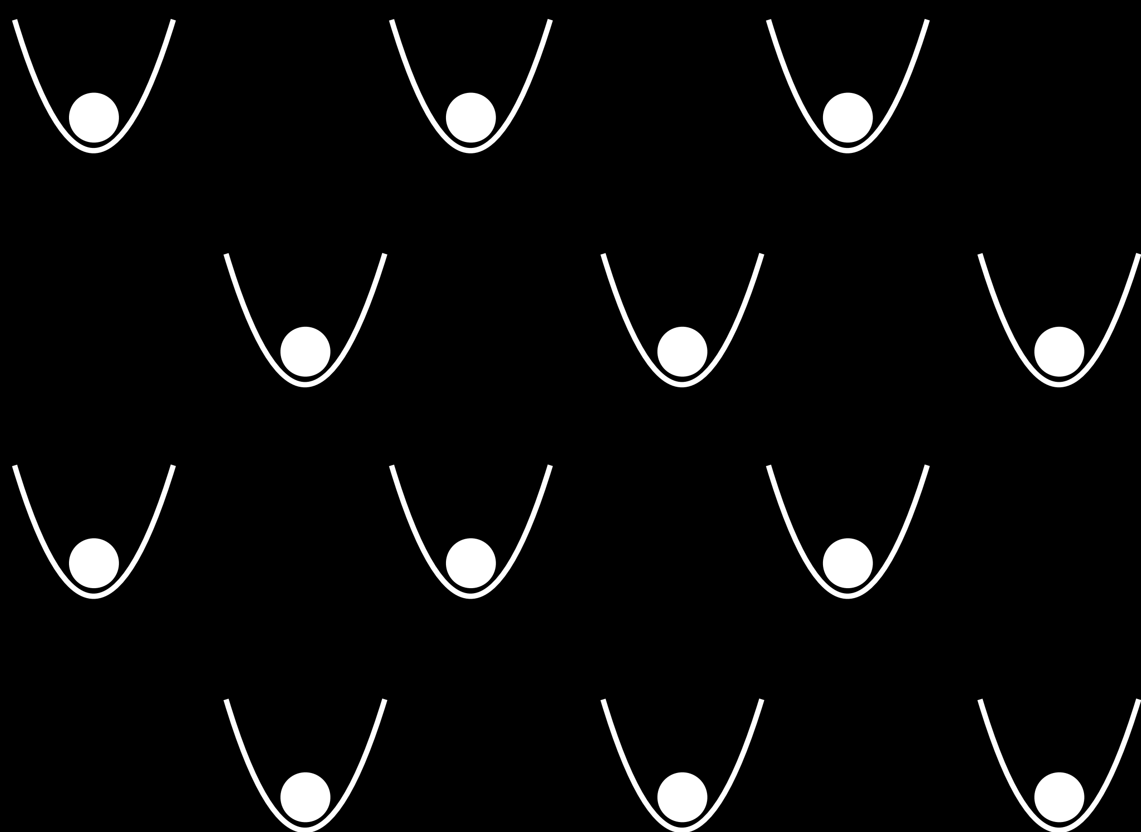


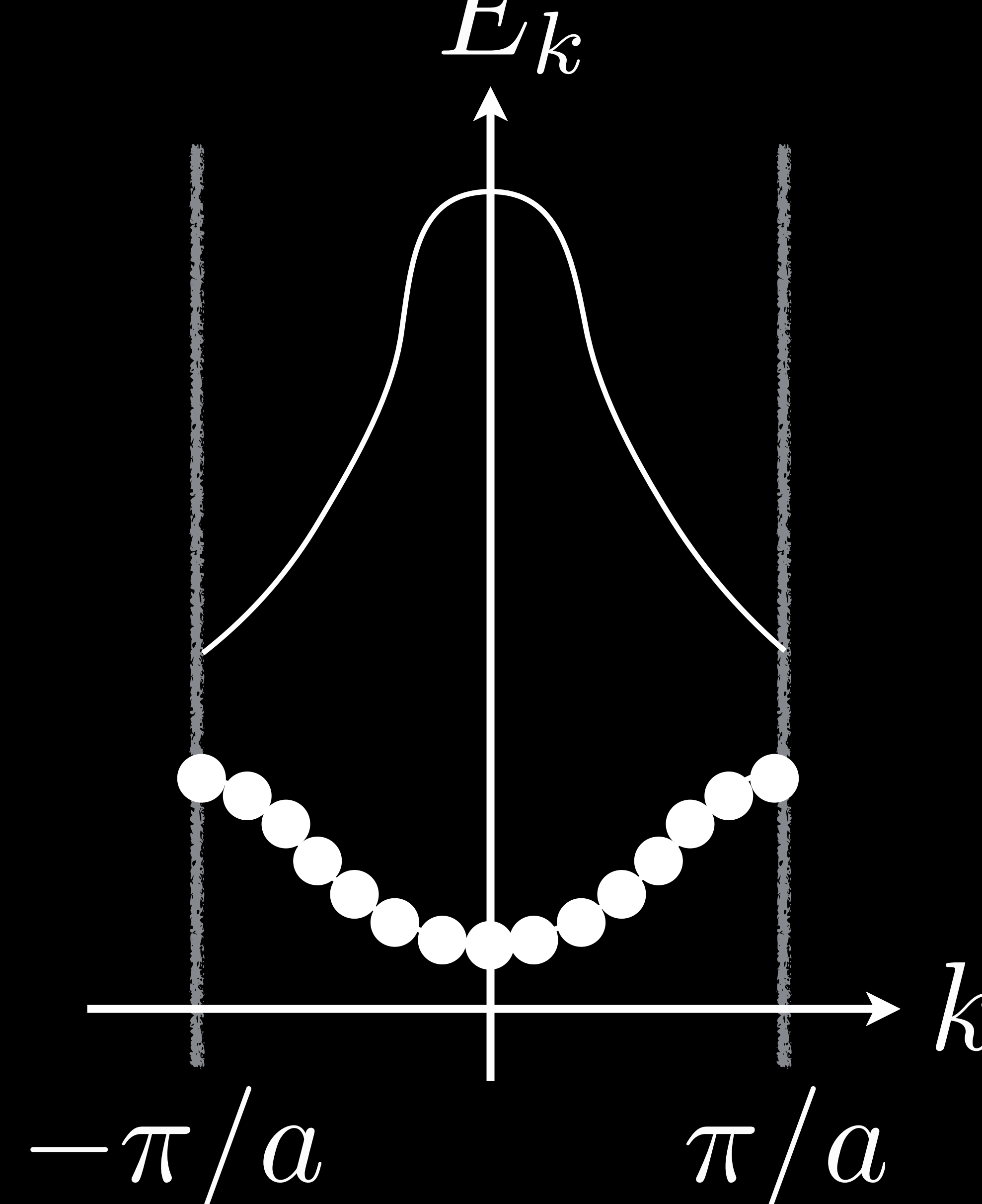
[Hemstreet & Fong (1974)]



Wave-like

Classical vs Quantum insulators

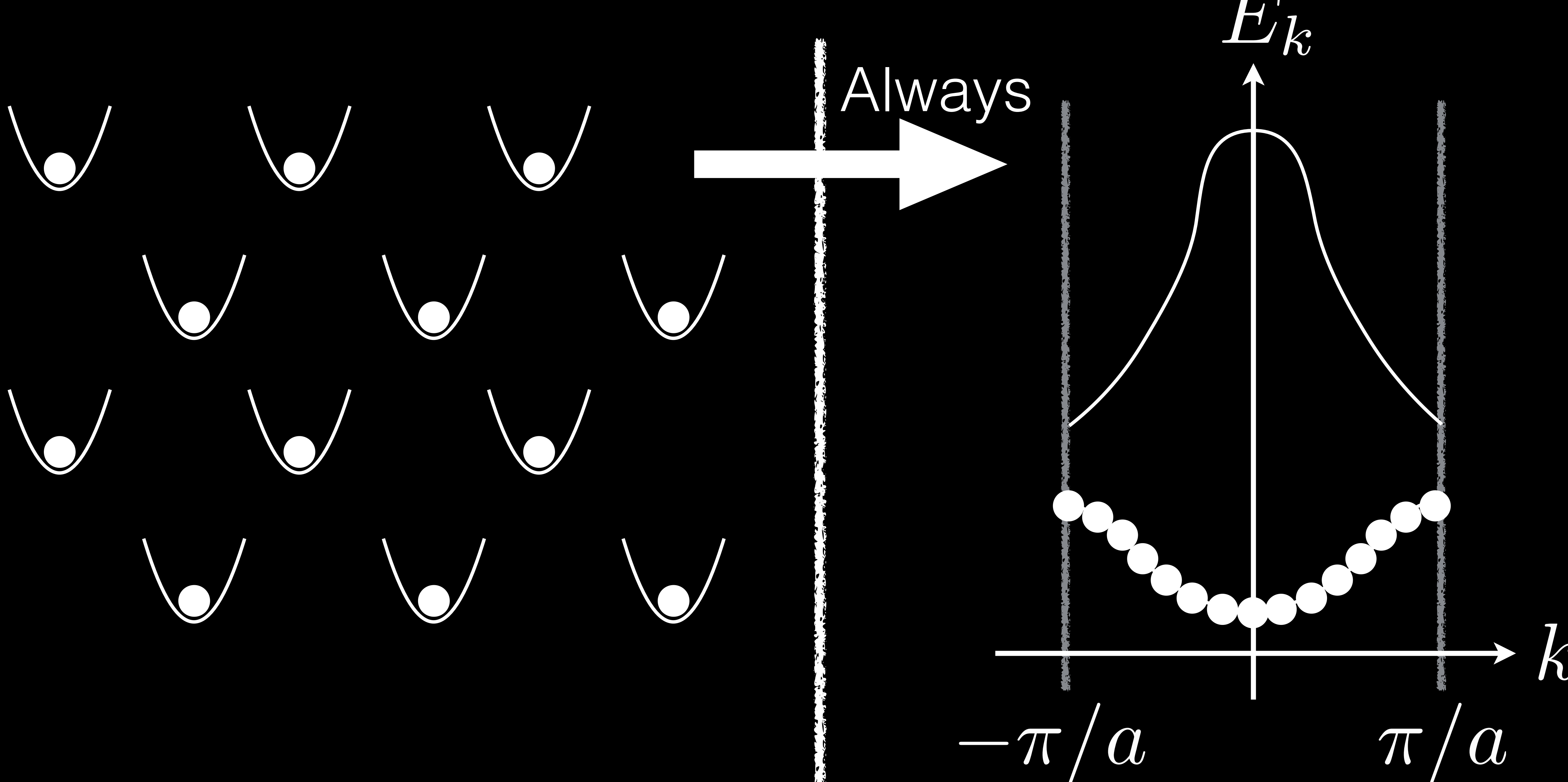




Particle-like

Wave-like

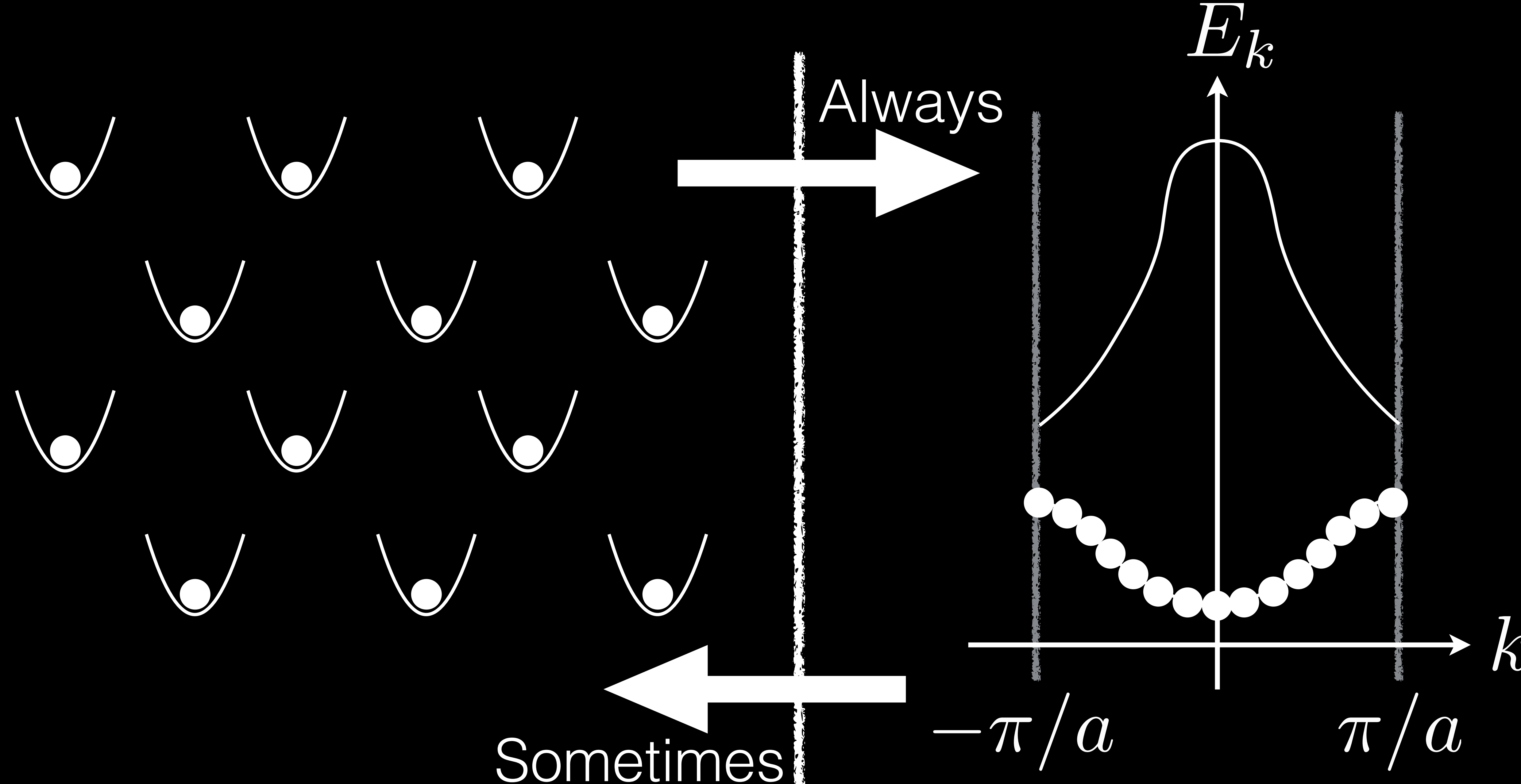
Classical vs Quantum insulators



Particle-like

Wave-like

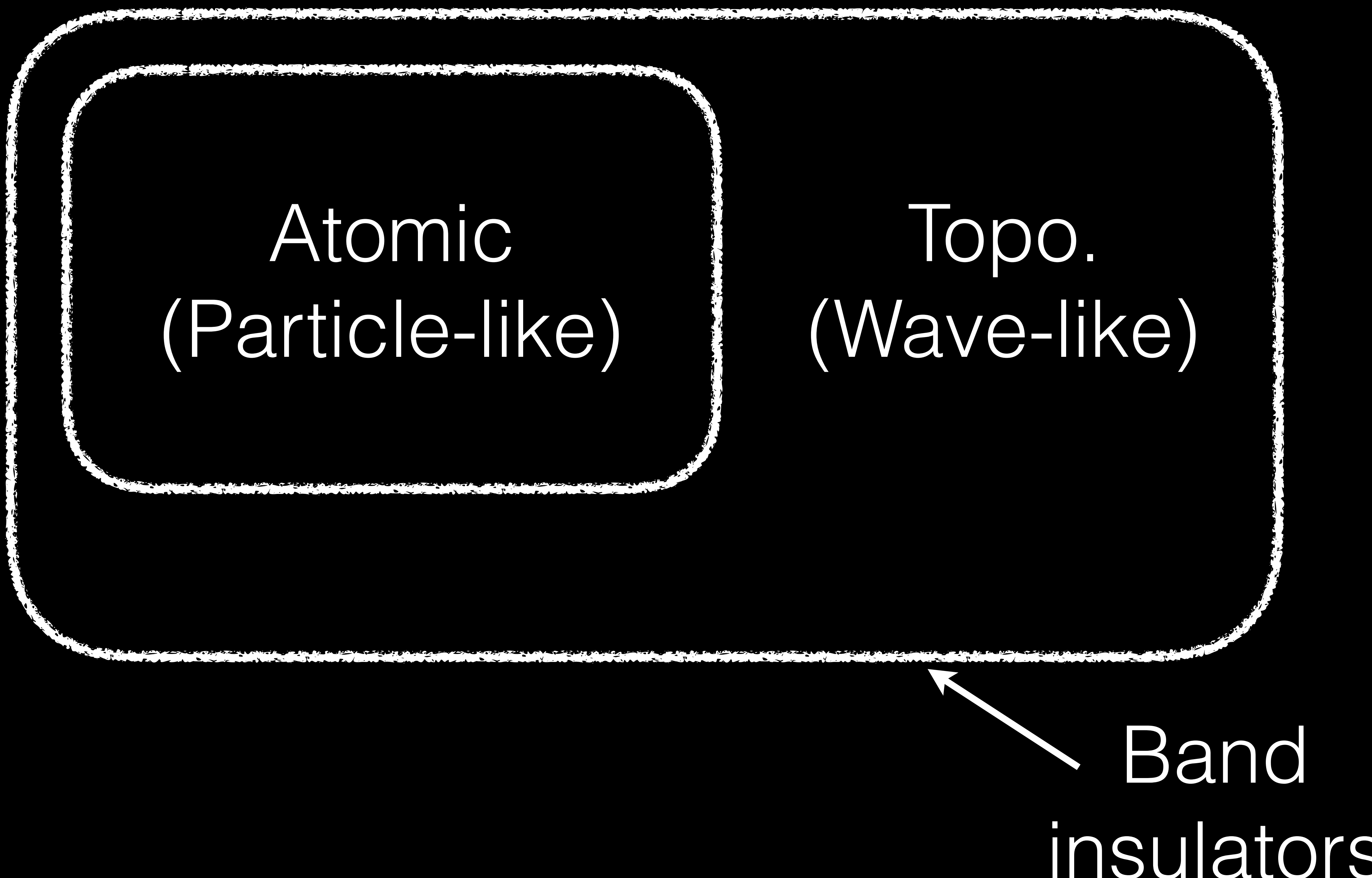
Classical vs Quantum insulators



Particle-like

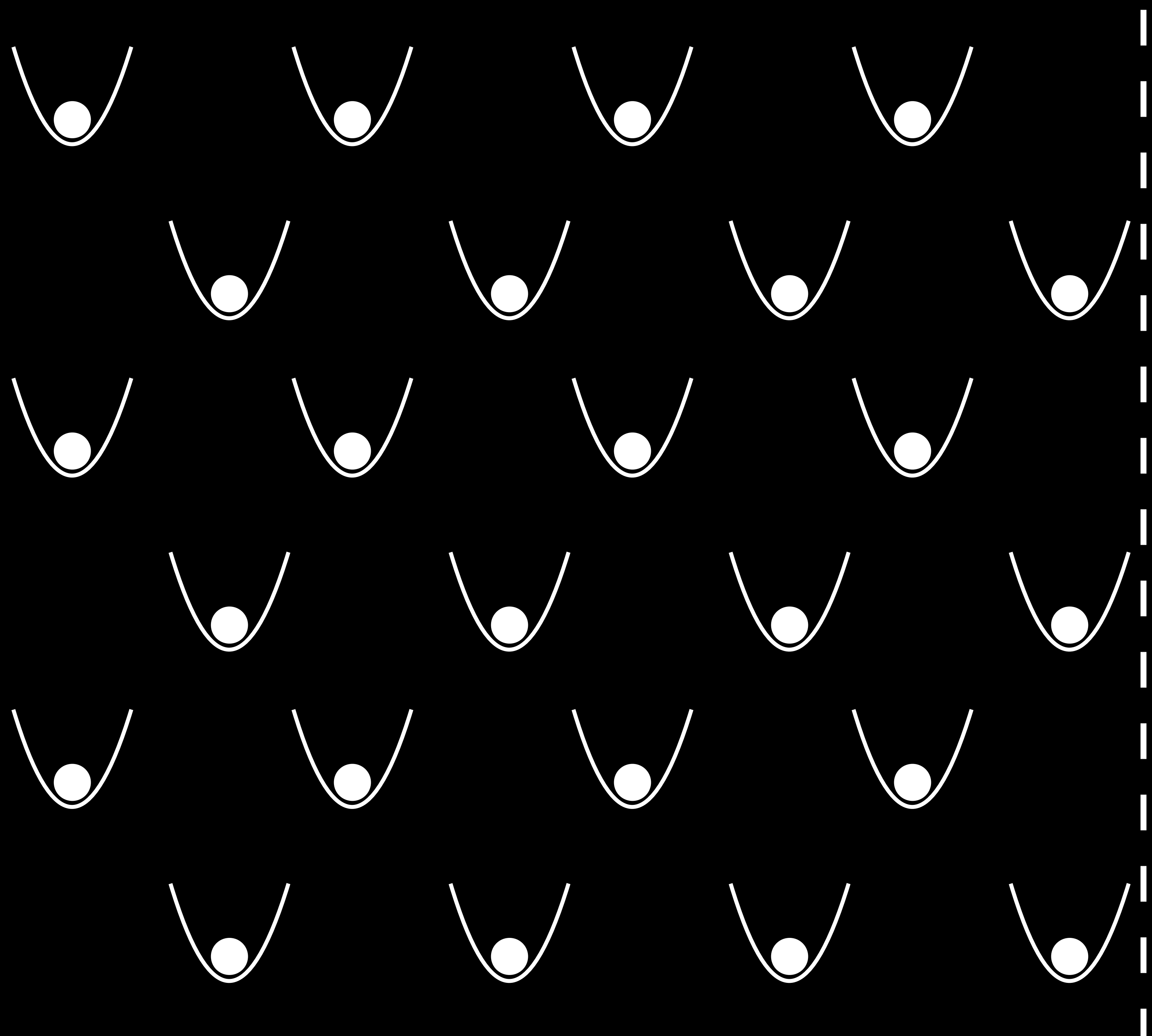
Wave-like

Classical vs Quantum insulators

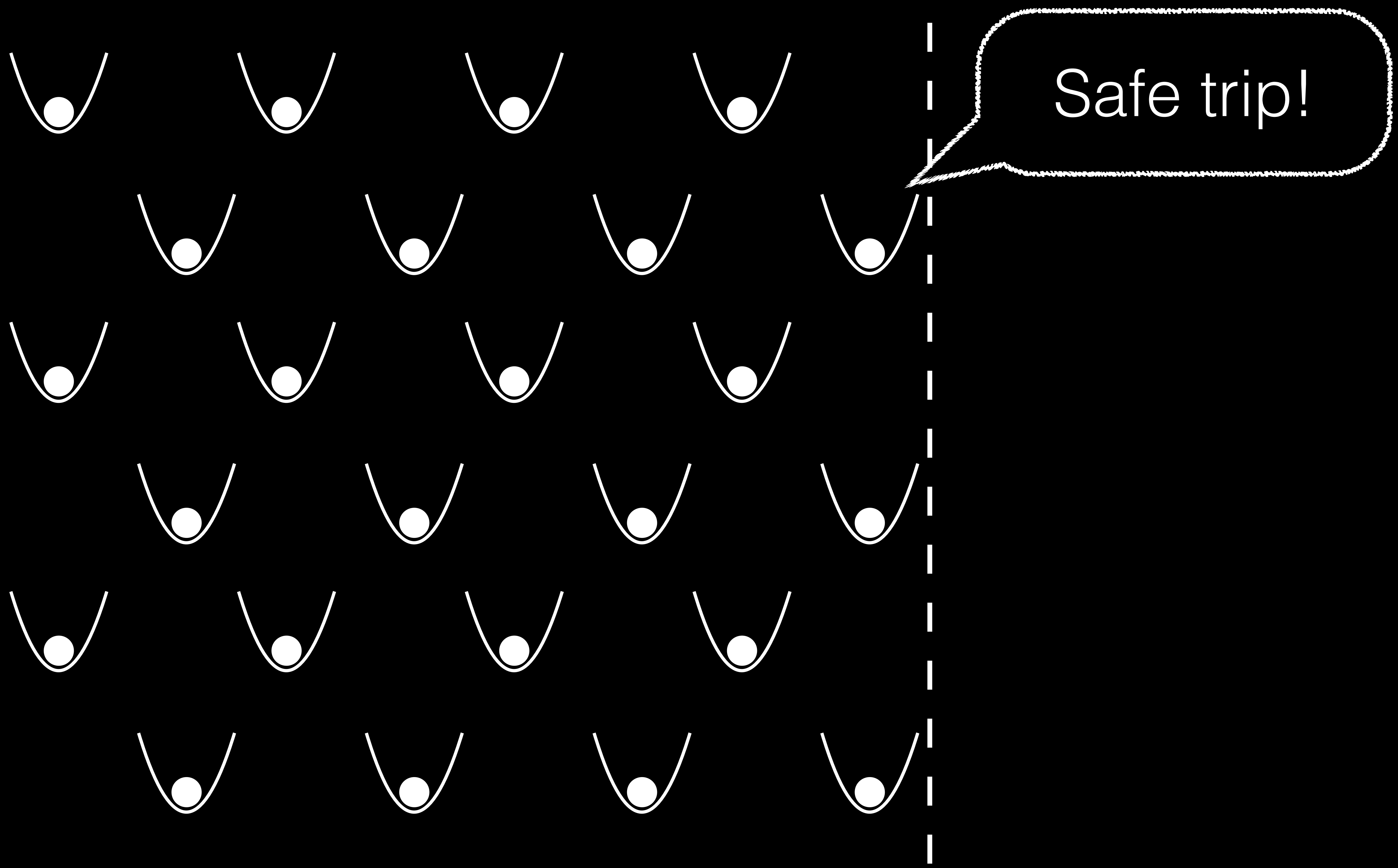


Boundary: Classical

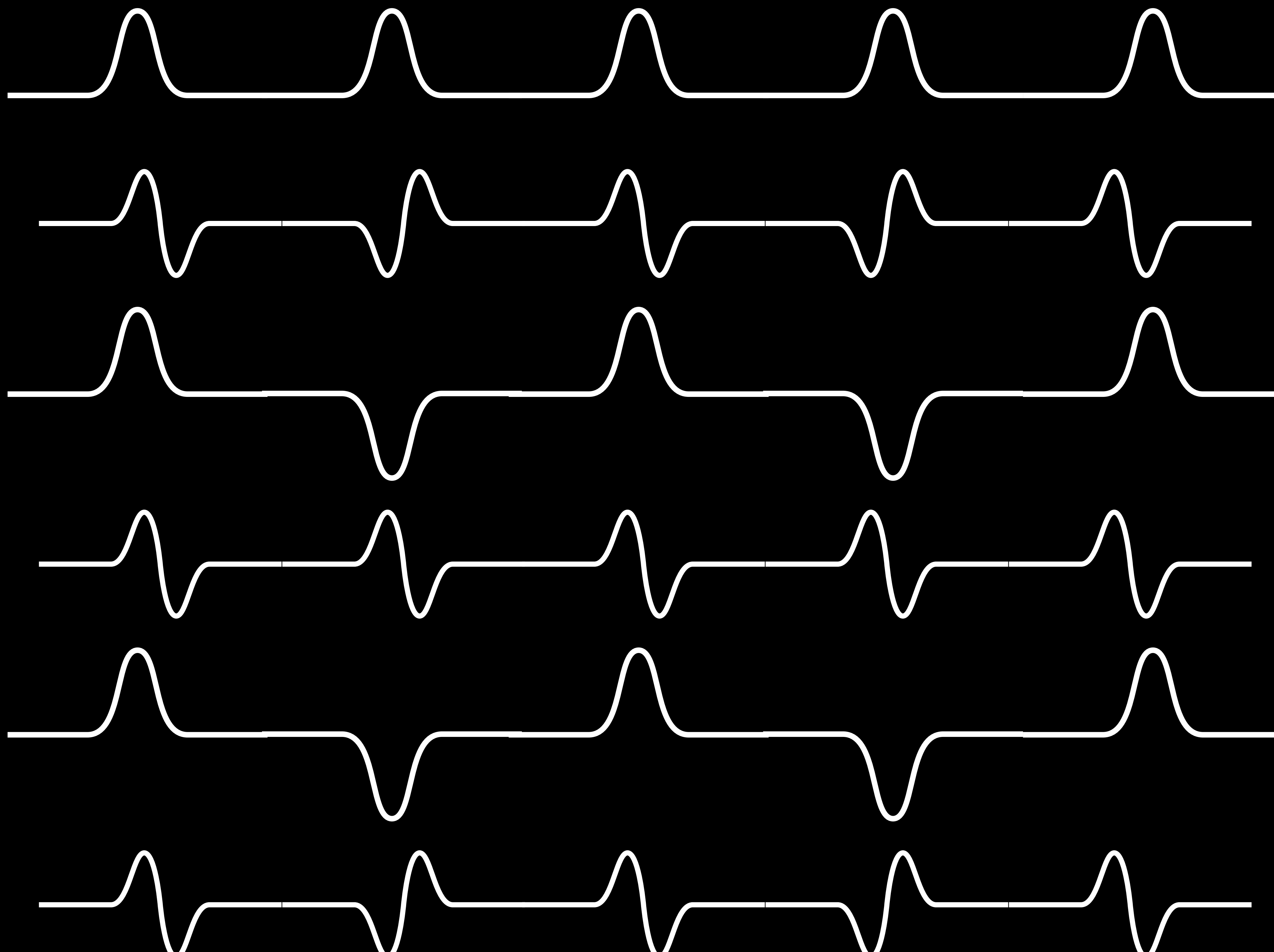
Boundary: Classical



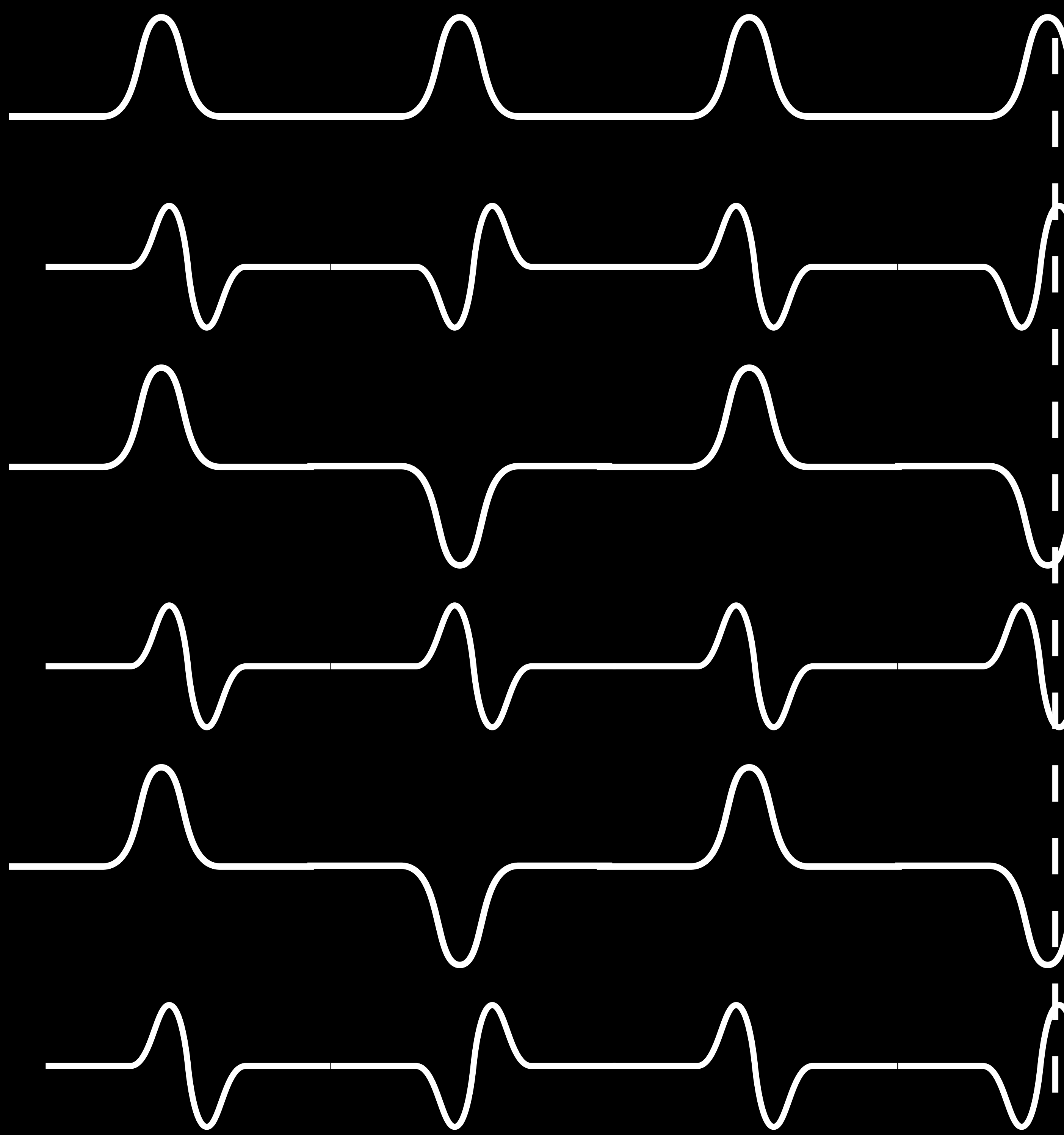
Boundary: Classical



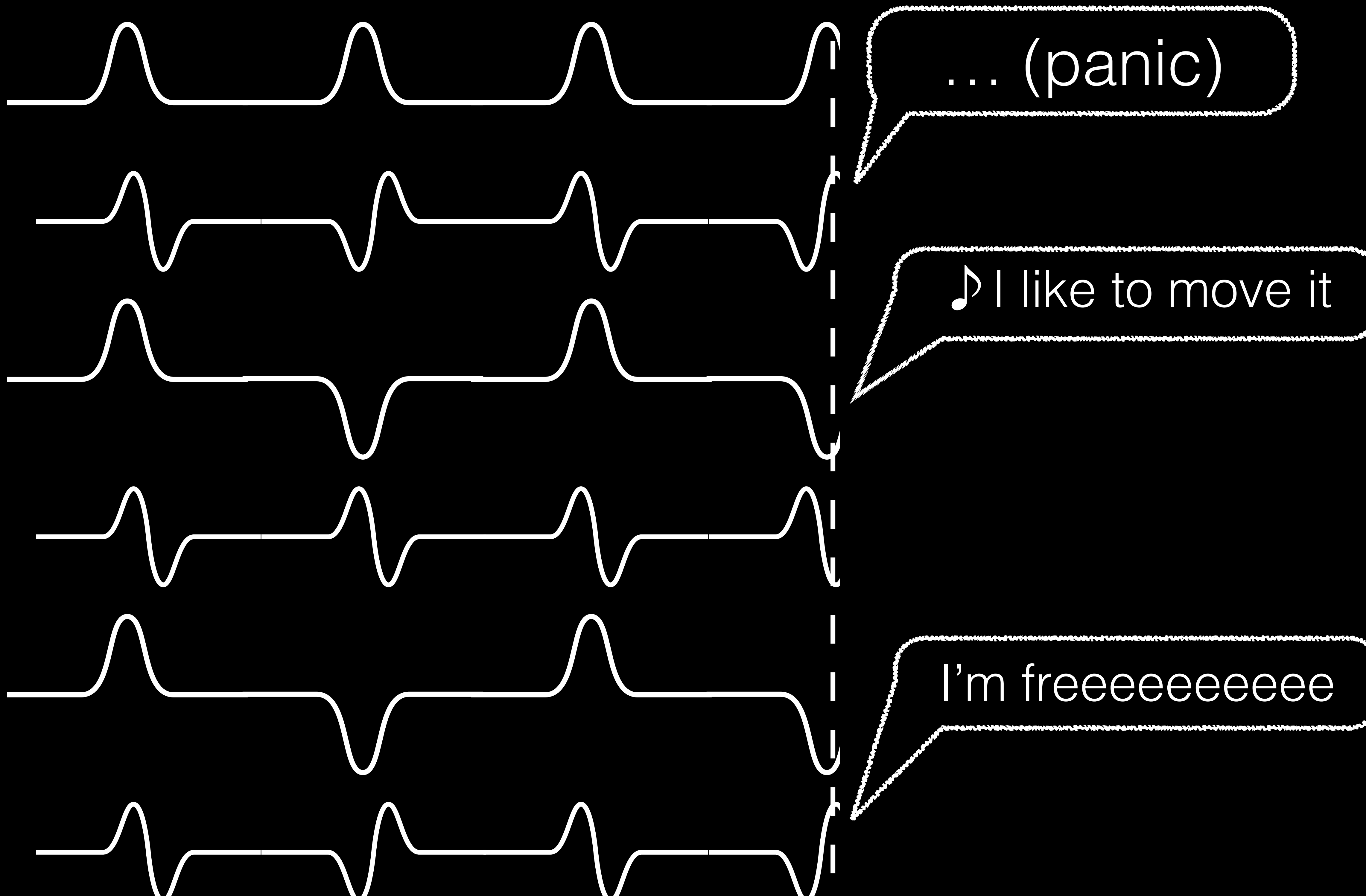
Boundary: Quantum



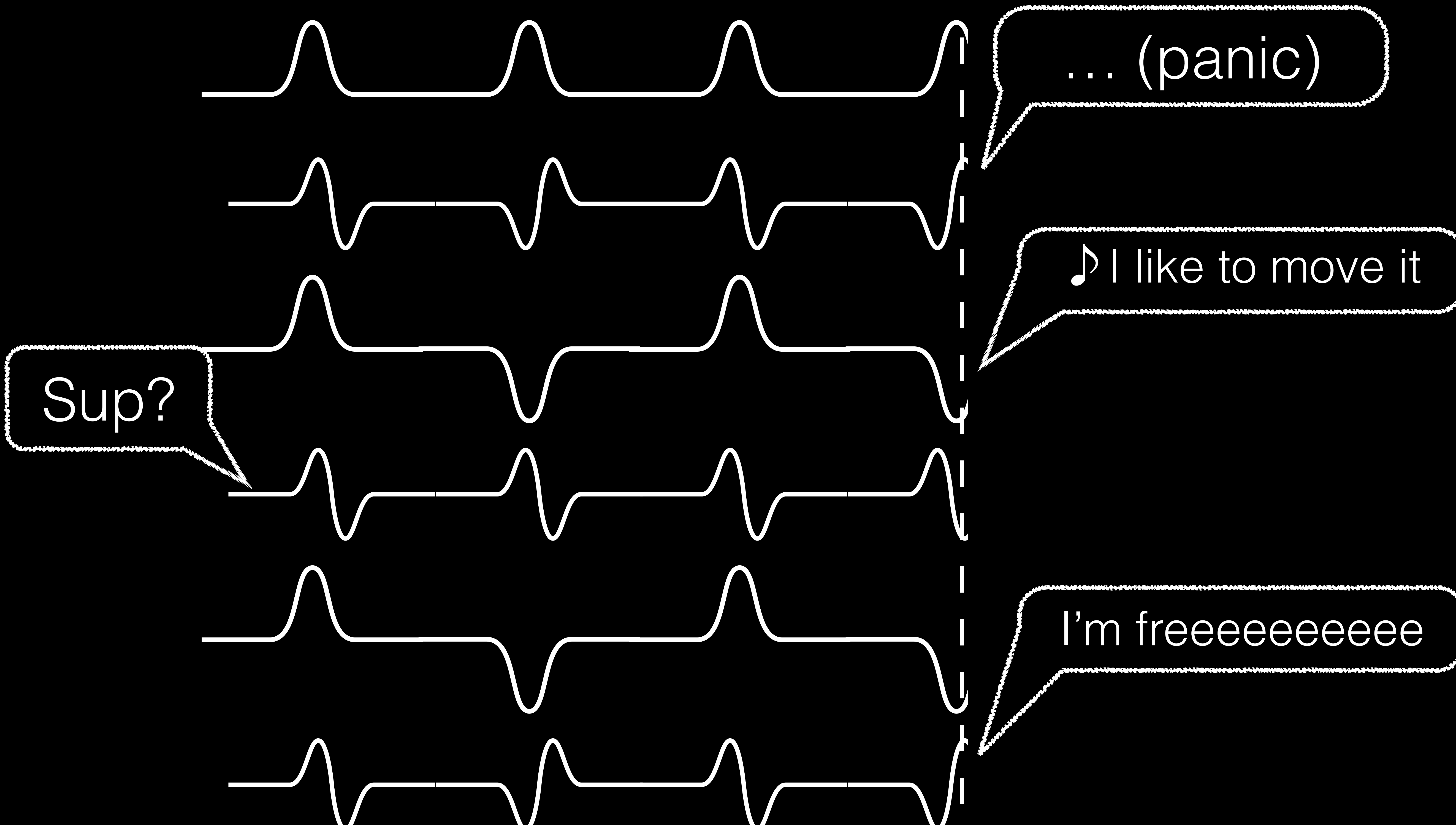
Boundary: Quantum



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

[Brouder et al (2007), Soluyanov-Vanderbilt (2011),…]

Main Goal

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

Efficient way(s) to tell trivial ≃ atomic ≃ classical from topological ≃ quantum

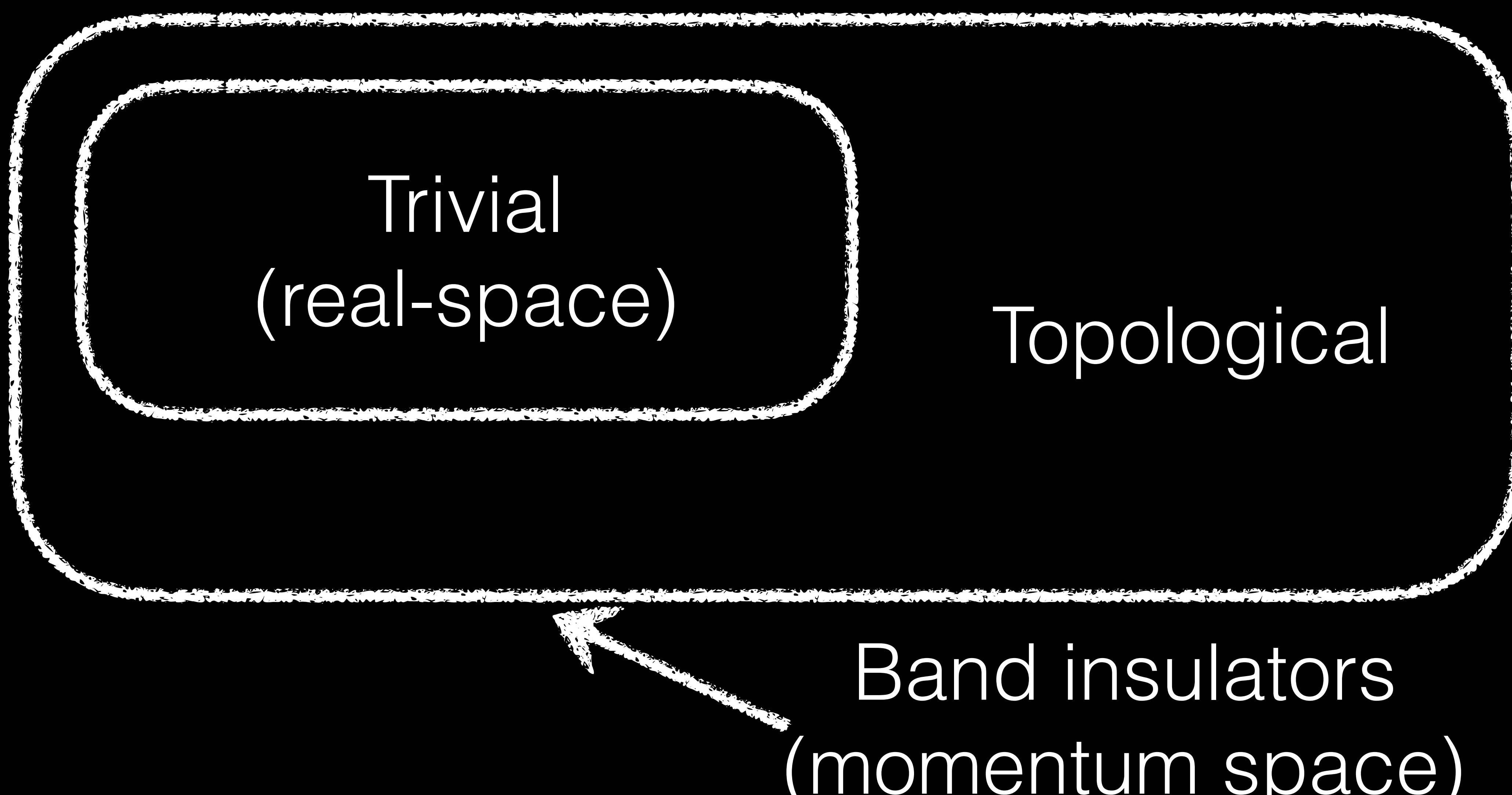
Applications:
large-scale materials discovery

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

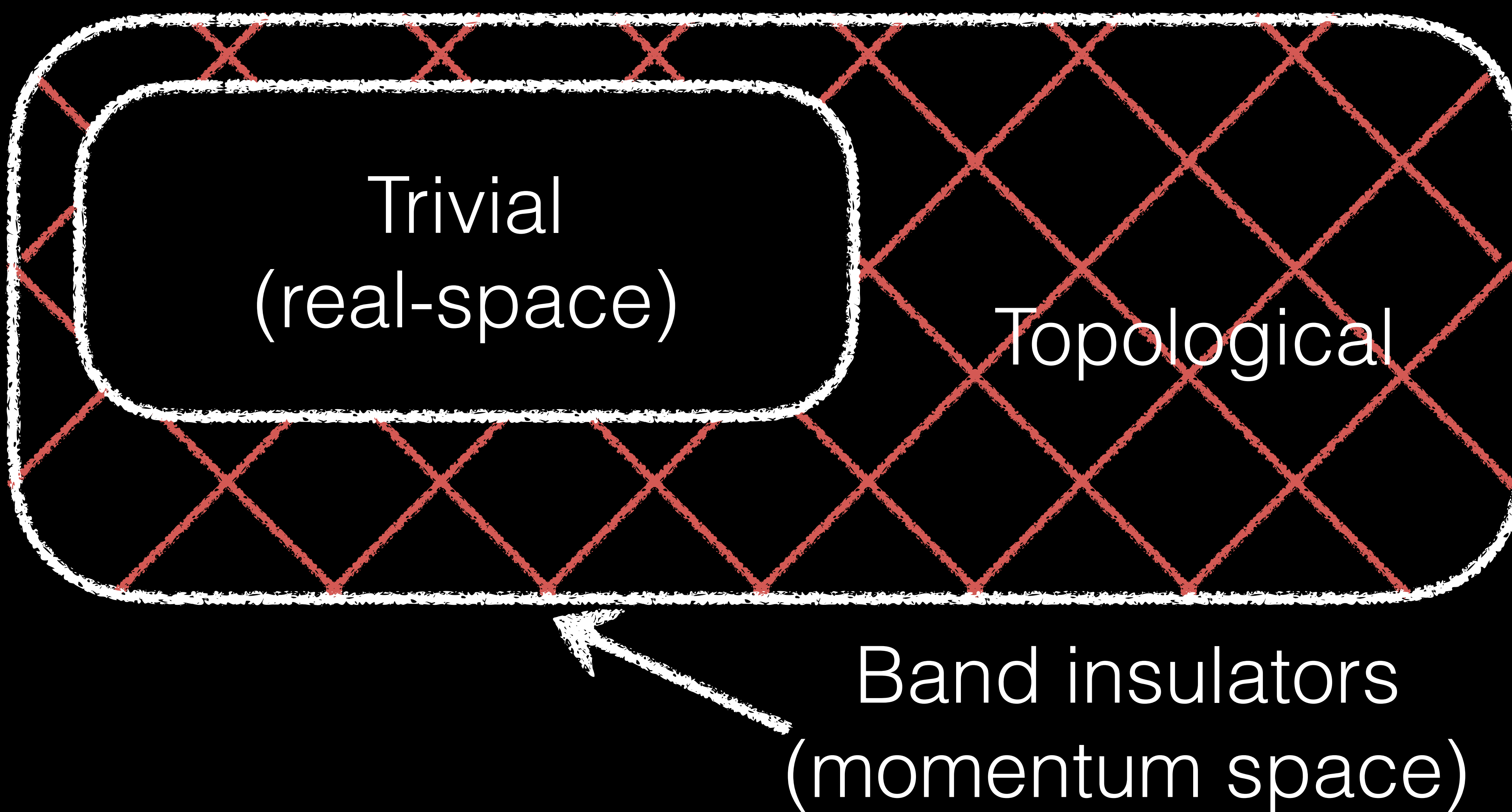
Efficient way(s) to tell trivial ≃ atomic ≃ classical from topological ≃ quantum



Main Goal

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

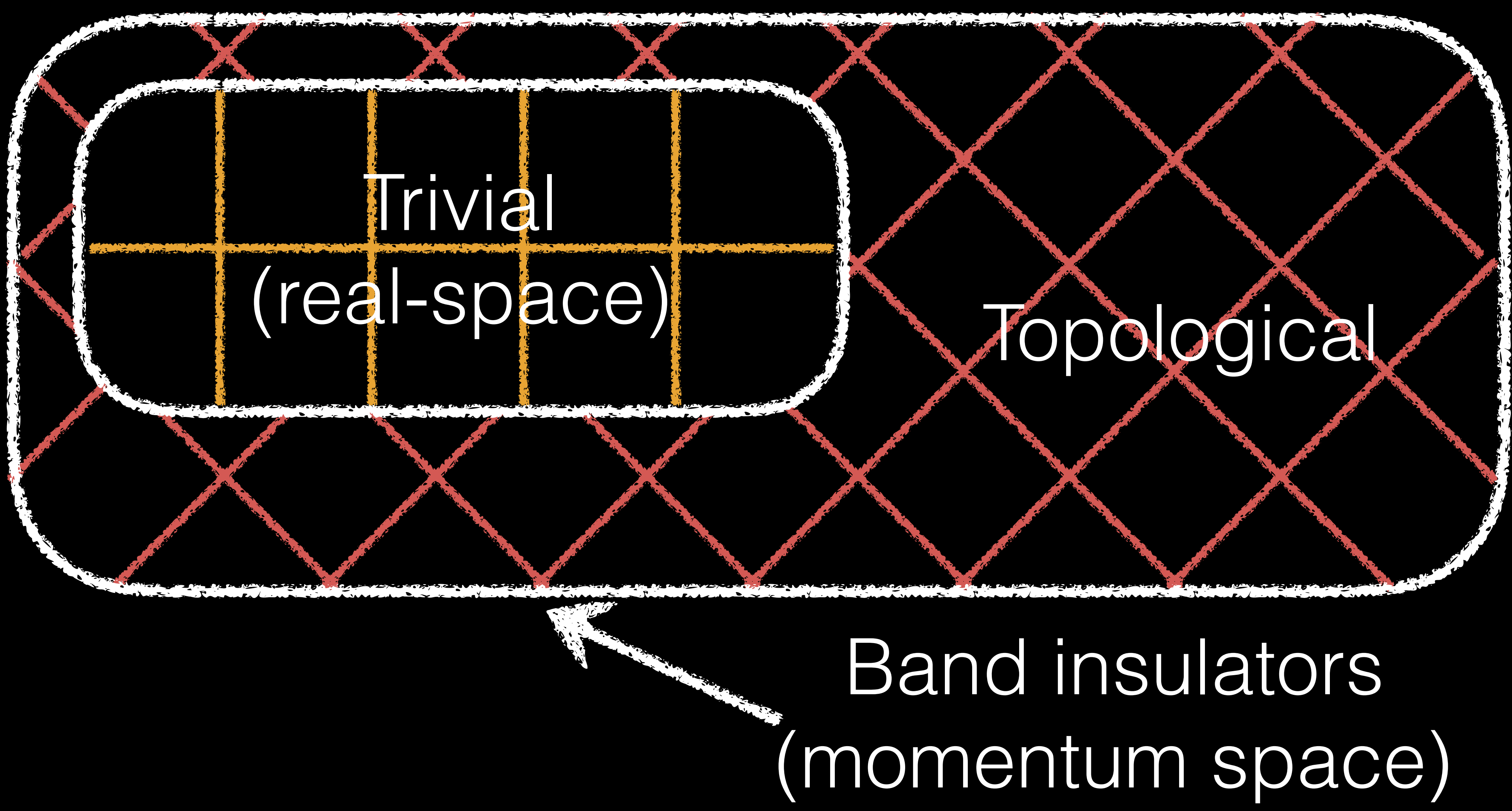
Efficient way(s) to tell trivial ≃ atomic ≃ classical from topological ≃ quantum



Main Goal

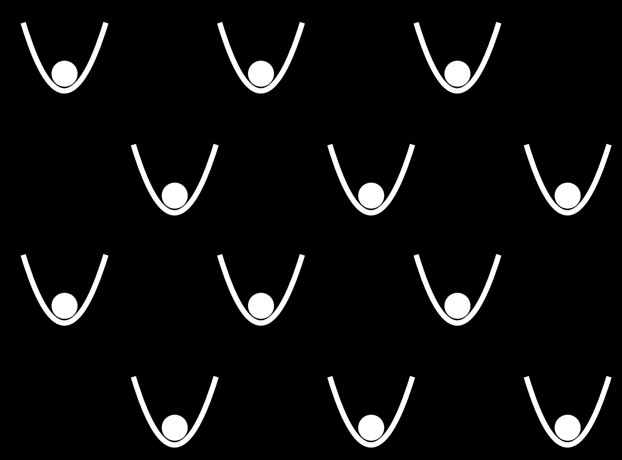
HCP, Vishwanath & Watanabe, 1703.00911
Bradlyn et al, 1703.02050

Efficient way(s) to tell trivial ≃ atomic ≃ classical from topological ≃ quantum



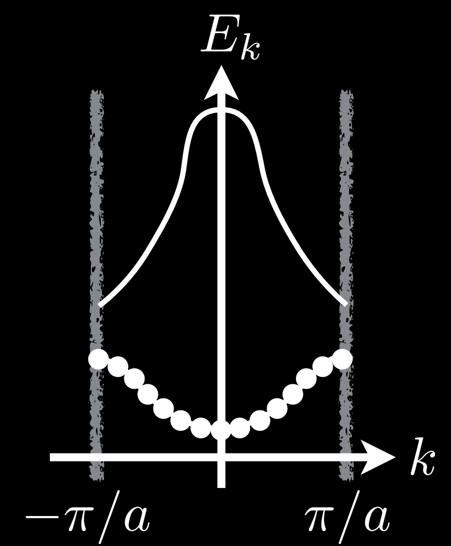
How to compare?

Real space



- Lattice sites
- Reps of site-sym. groups

Momentum space



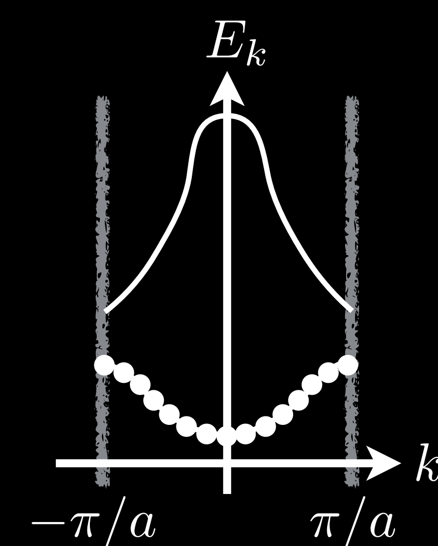
- Energy bands
- Bloch wave functions
  - Reps at high-sym. momenta

How to compare?

Real space

- Lattice sites
- Reps of site-sym. groups

Momentum space

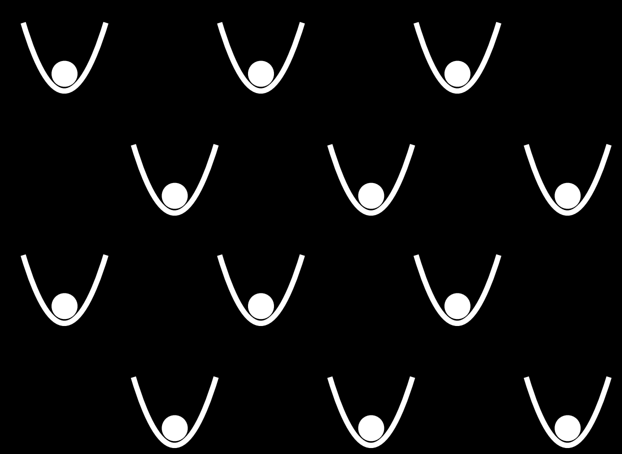


- Energy bands
- Bloch wave functions
  - Reps at high-sym. momenta

Fourier Trans.

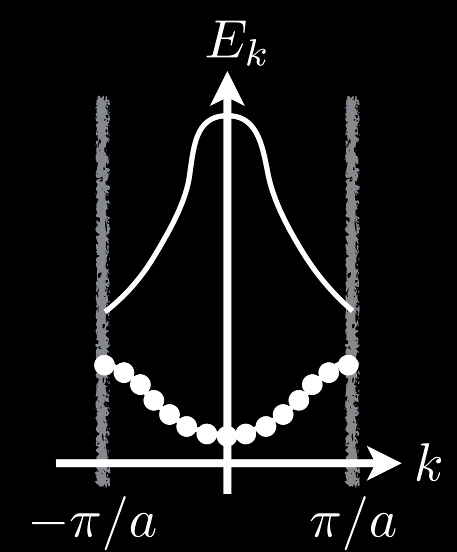
How to compare?

Real space



- Lattice sites
- Reps of site-sym. groups

Momentum space



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

Fourier Trans.

Wannier Fns. (if exist)

How to compare?

Real space

Momentum space

Straight-forward

Fourier Trans.

Wannier Fns.
(if exist)

Hard—requires knowing the Bloch wave functions over the BZ

How to compare?

Real space | Momentum space

Straight-forward

Fourier Trans.

Wannier Fns.
(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

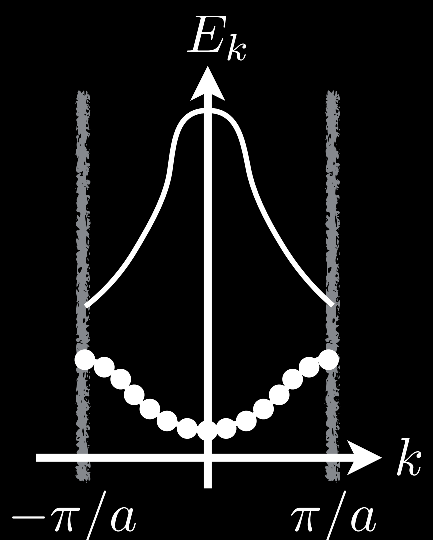
real vs. *momentum* spaces

Specifying sym. reps in…

Real space

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

Momentum space

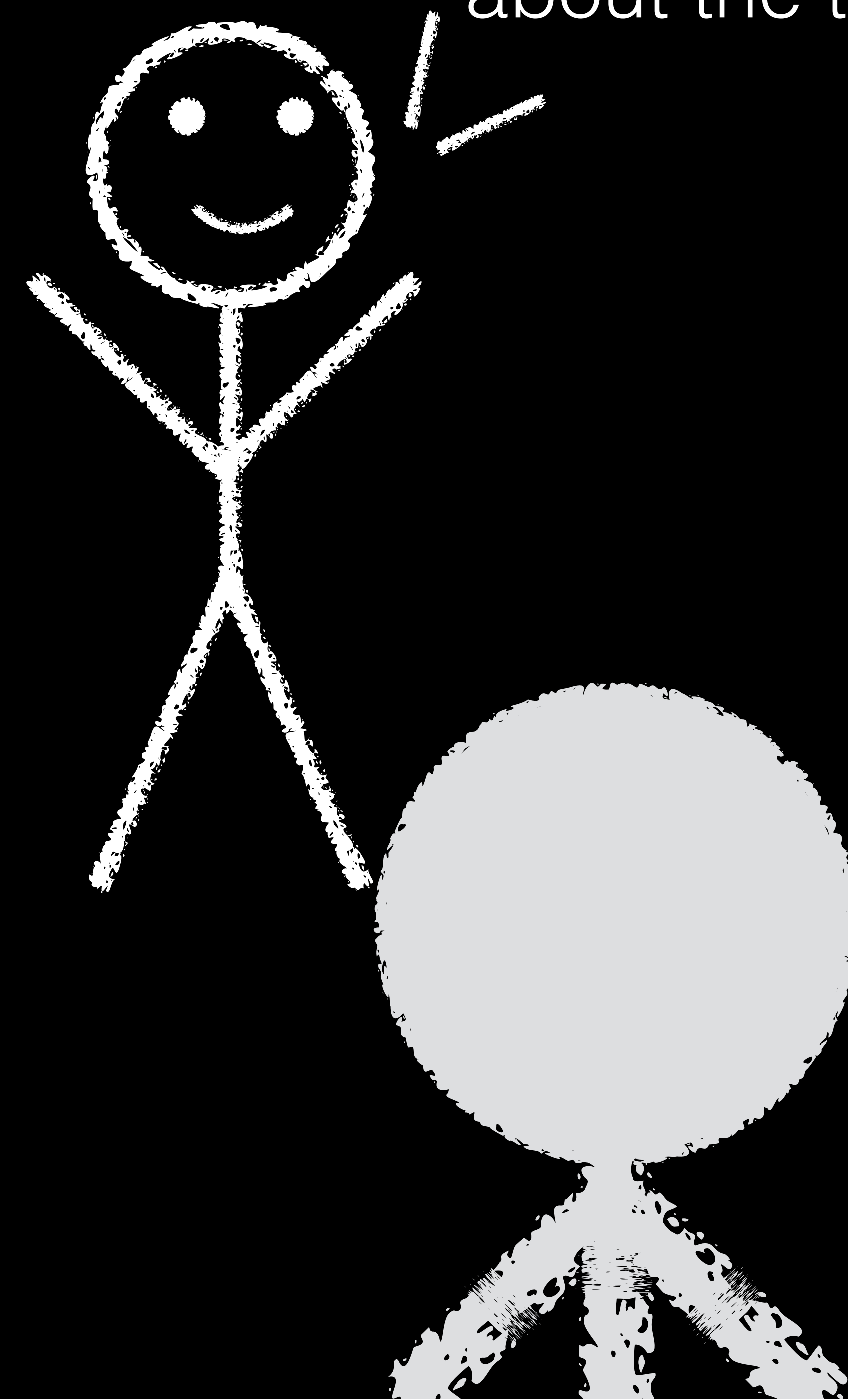


- *Restricted knowledge* on the *full set* of band insulators

“Bootstrapping” from the trivial

Real space

I’ve computed everything
about the trivial states!



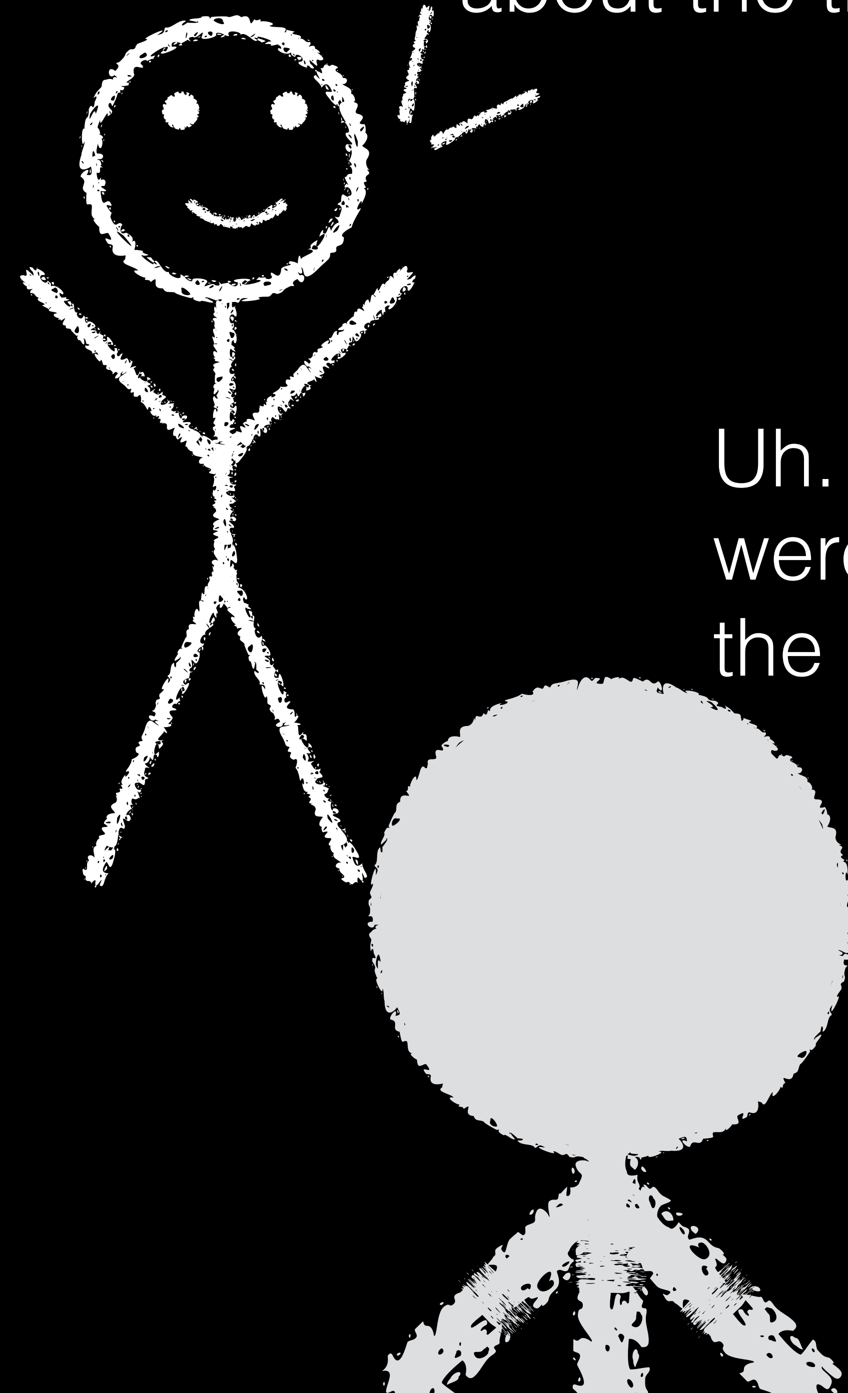
- *Full knowledge* on a *restricted set* of band insulators (i.e., trivial)

“Bootstrapping” from the trivial

Real space

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

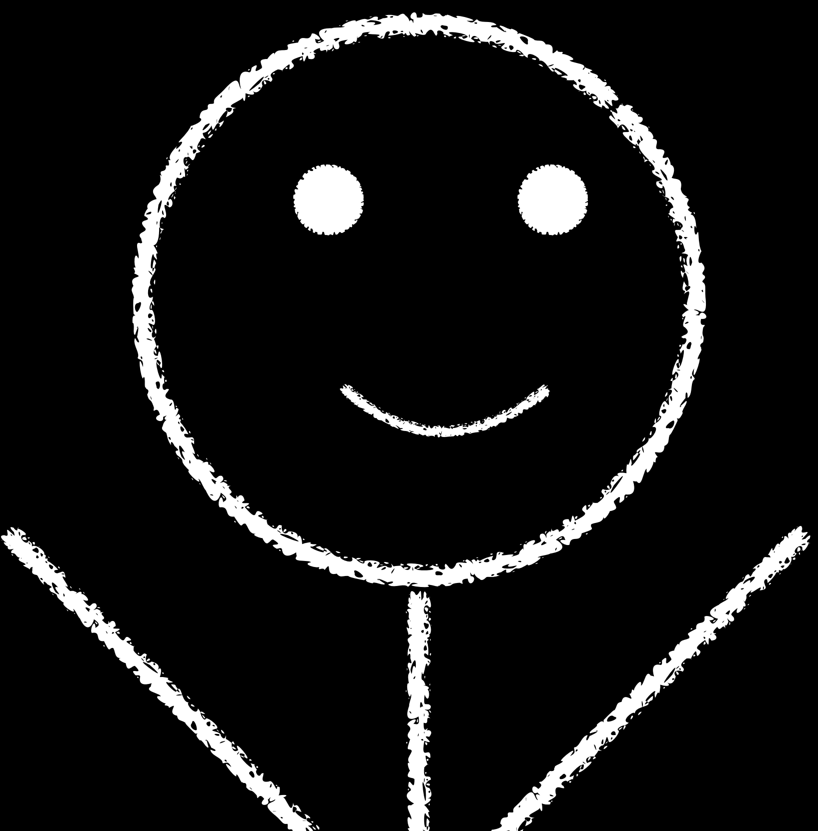
I’ve computed everything about the trivial states!



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

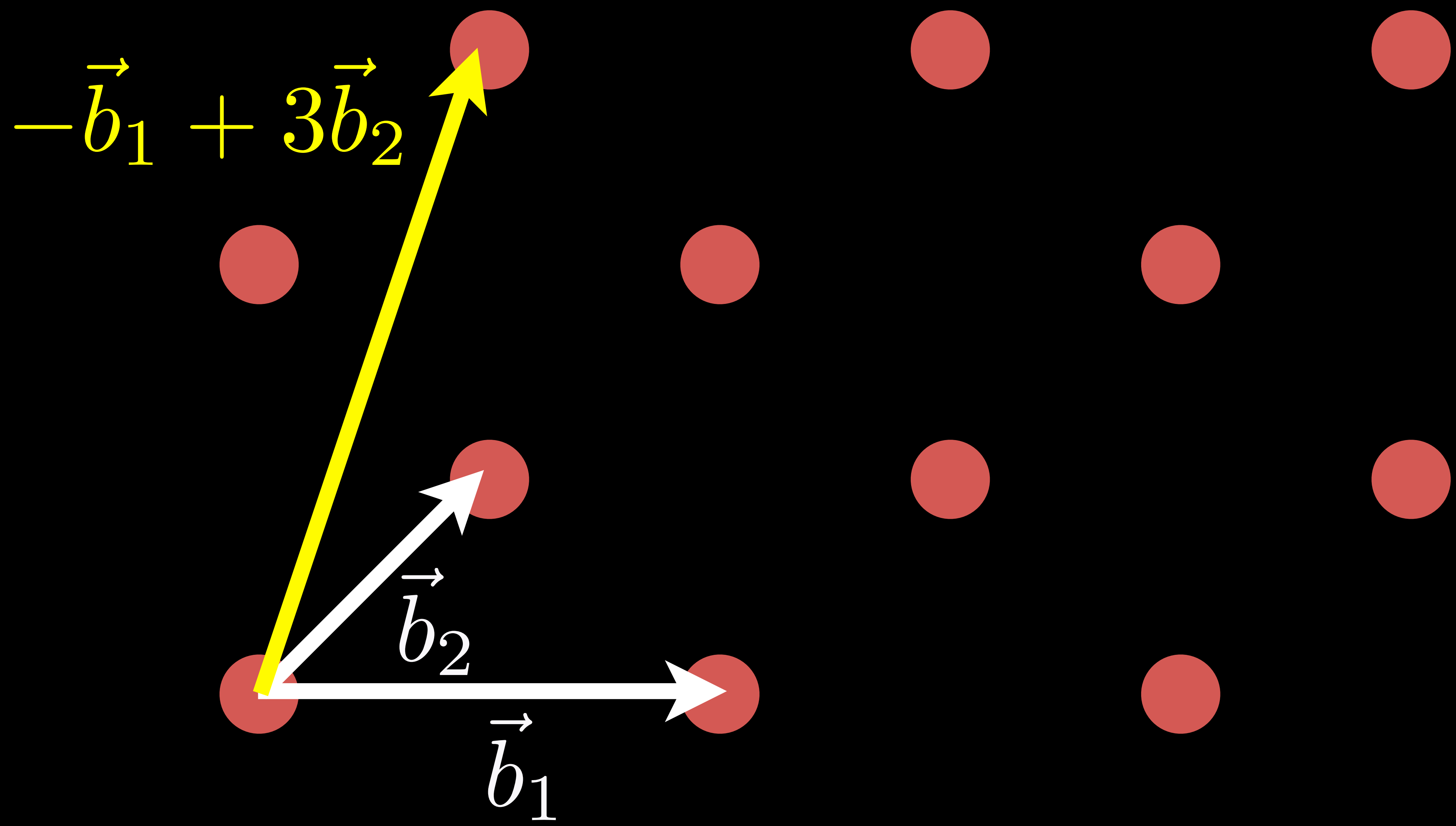
Outline aka Take-homes

- 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
  - ➡ By viewing band structures as a “vector space”
- Comparing momentum vs real space
  - ➡ symmetry-based indicators of band topology
- Applications
  - ➡ High throughput materials prediction

Punchline 1



Band structures form a “vector space”

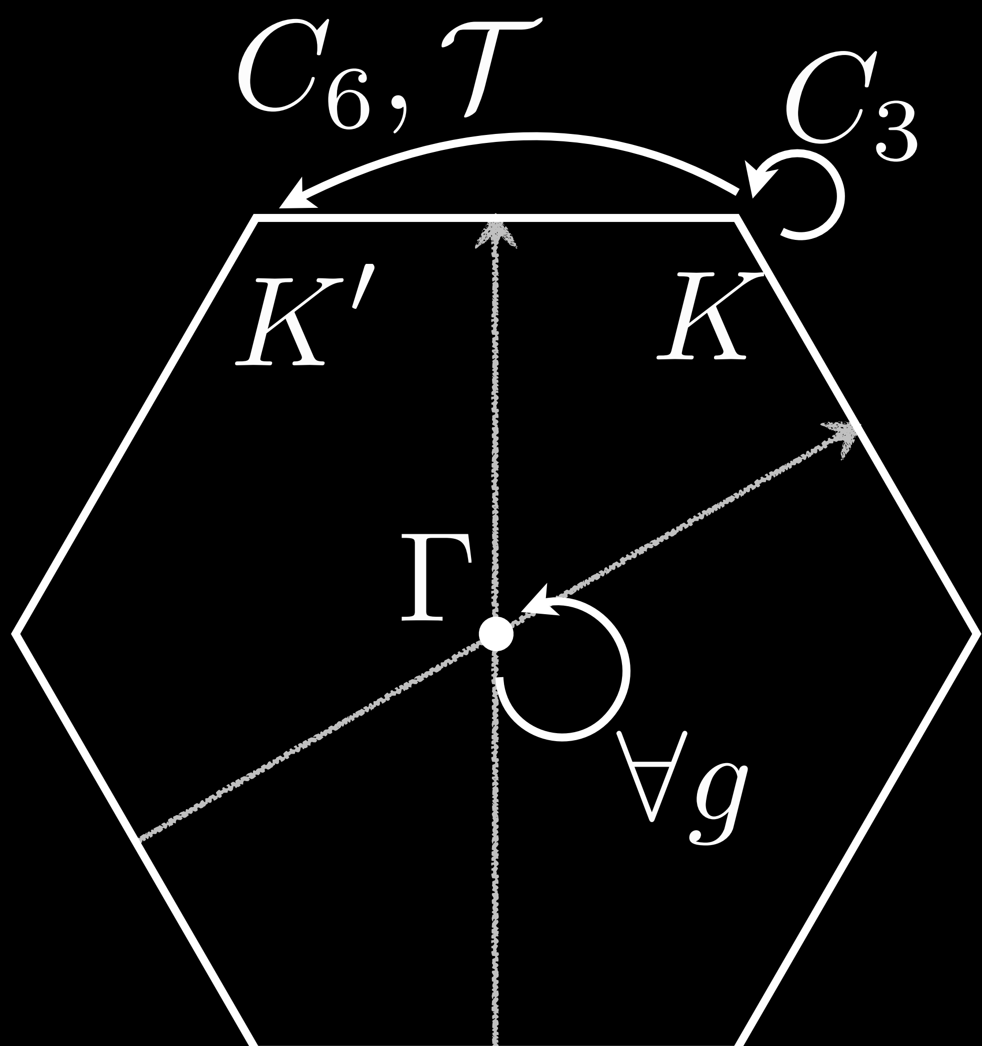
“Vector space”?

(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

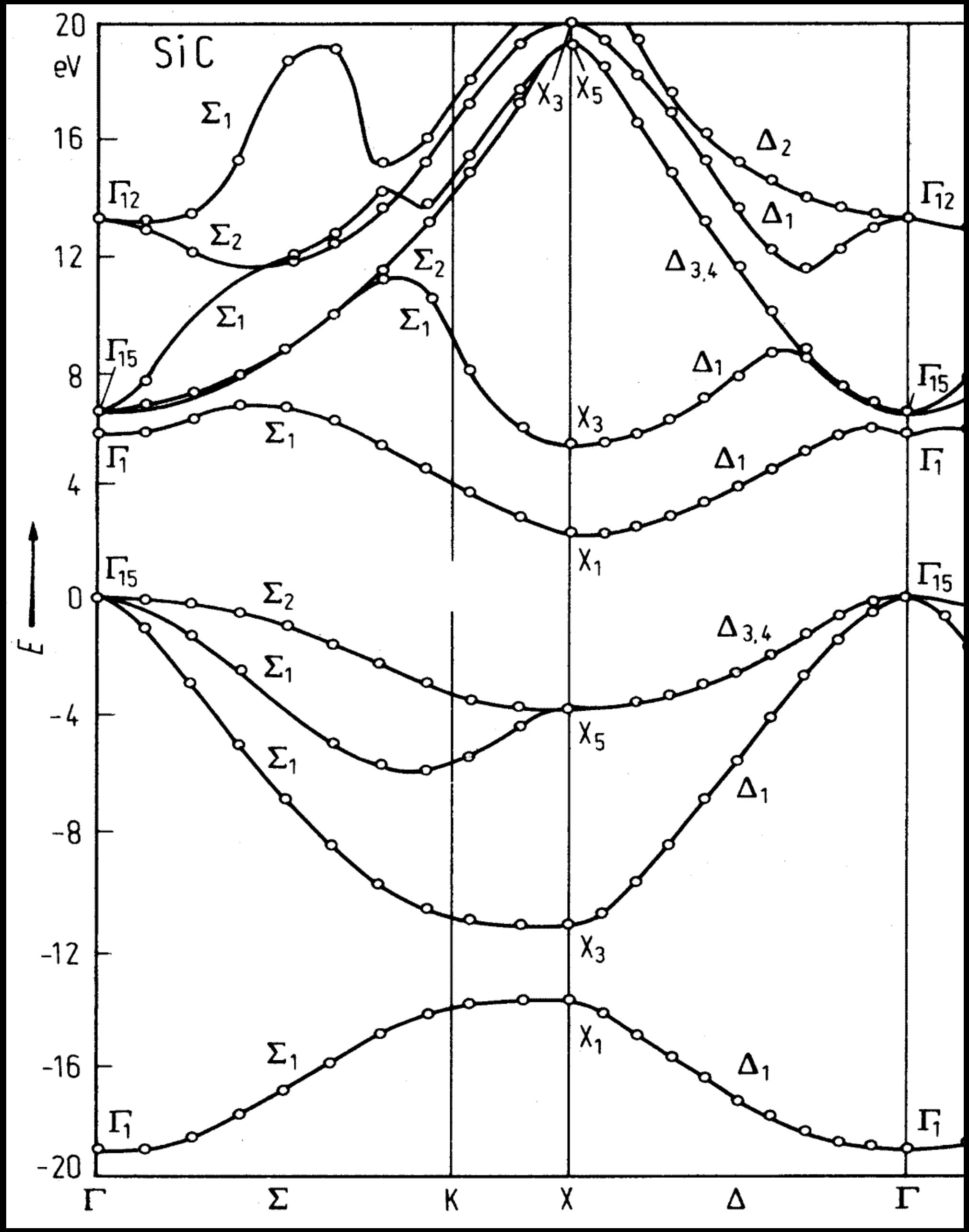
(i) Leaves a momentum invariant

- (Degenerate) Bloch wave functions furnish (irreducible) representations

(ii) Relates two momenta

- Energies identical
- Wave functions symmetry-related

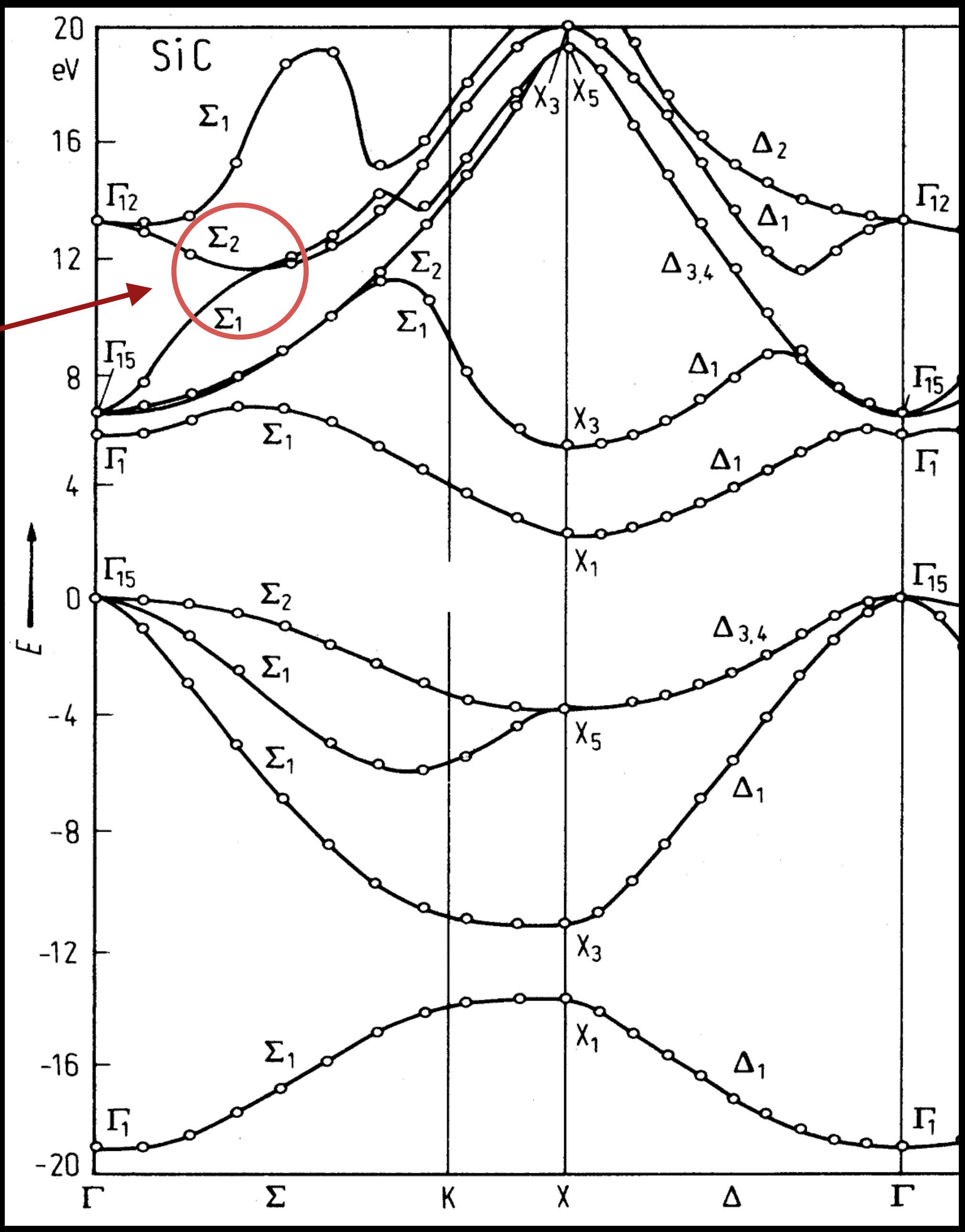
Sym. reps of band structures



[Hemstreet & Fong (1974)]

Sym. reps of band structures

Bands can cross only when they carry different symmetry labels

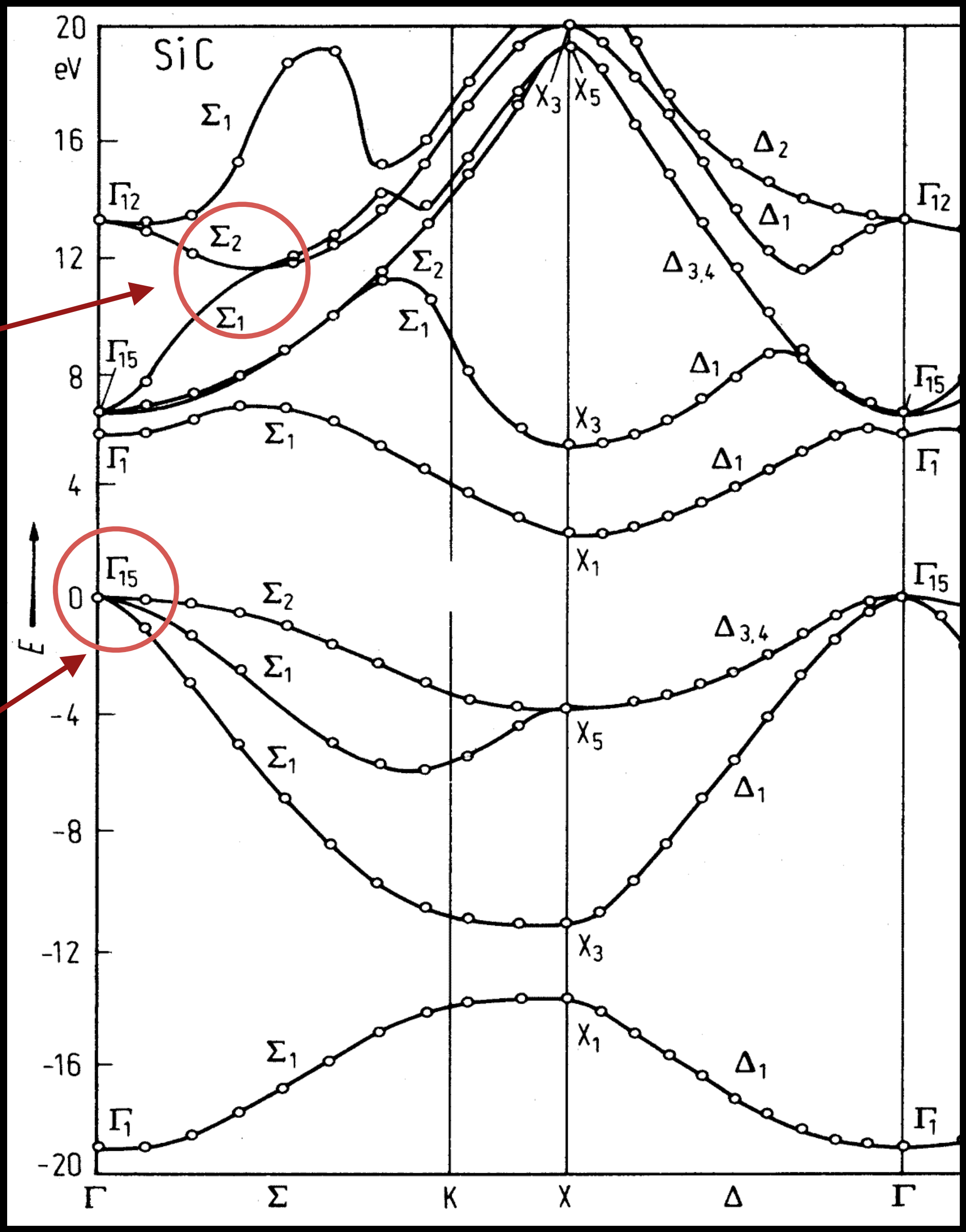


[Hemstreet & Fong (1974)]

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"

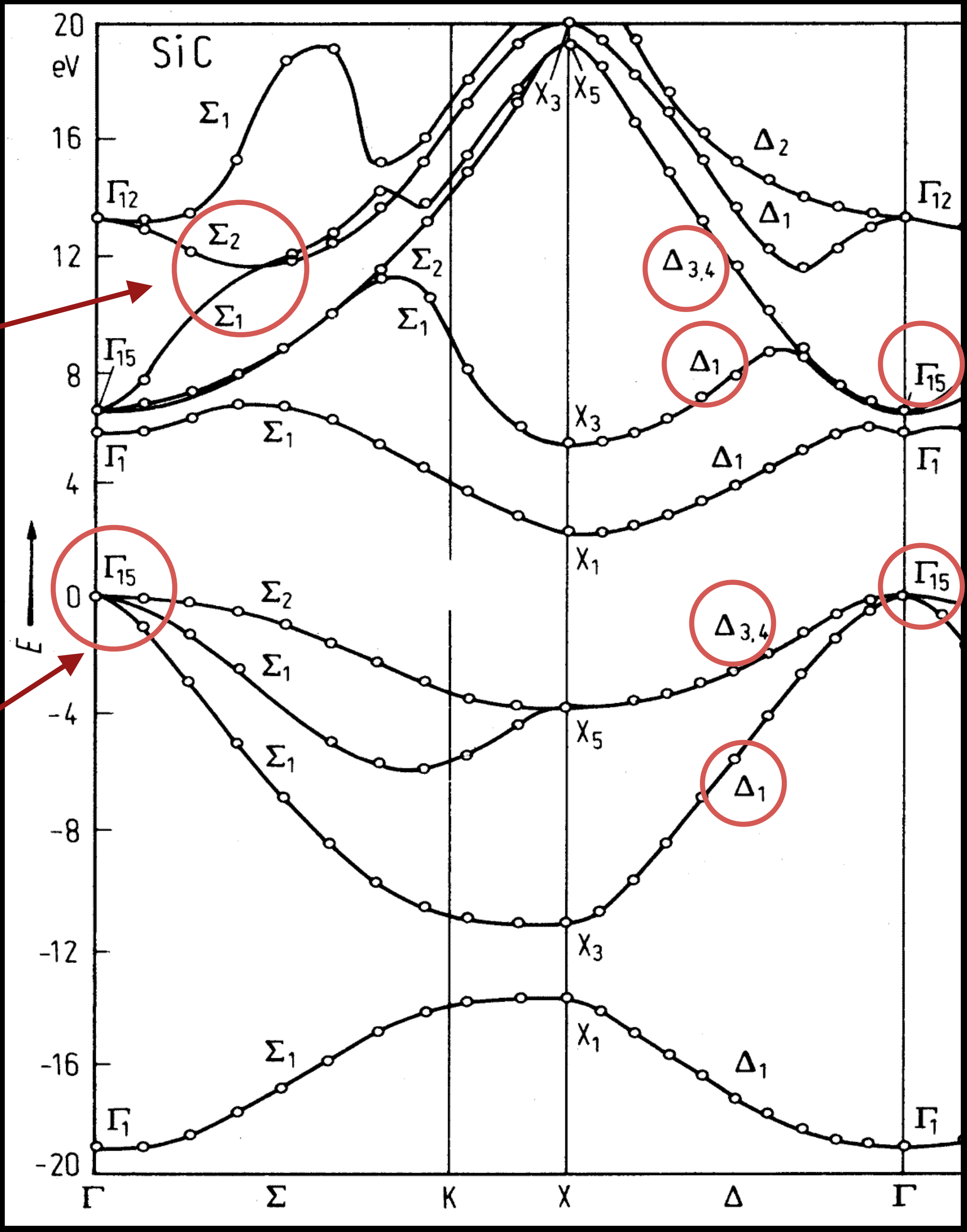


[Hemstreet & Fong (1974)]

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"

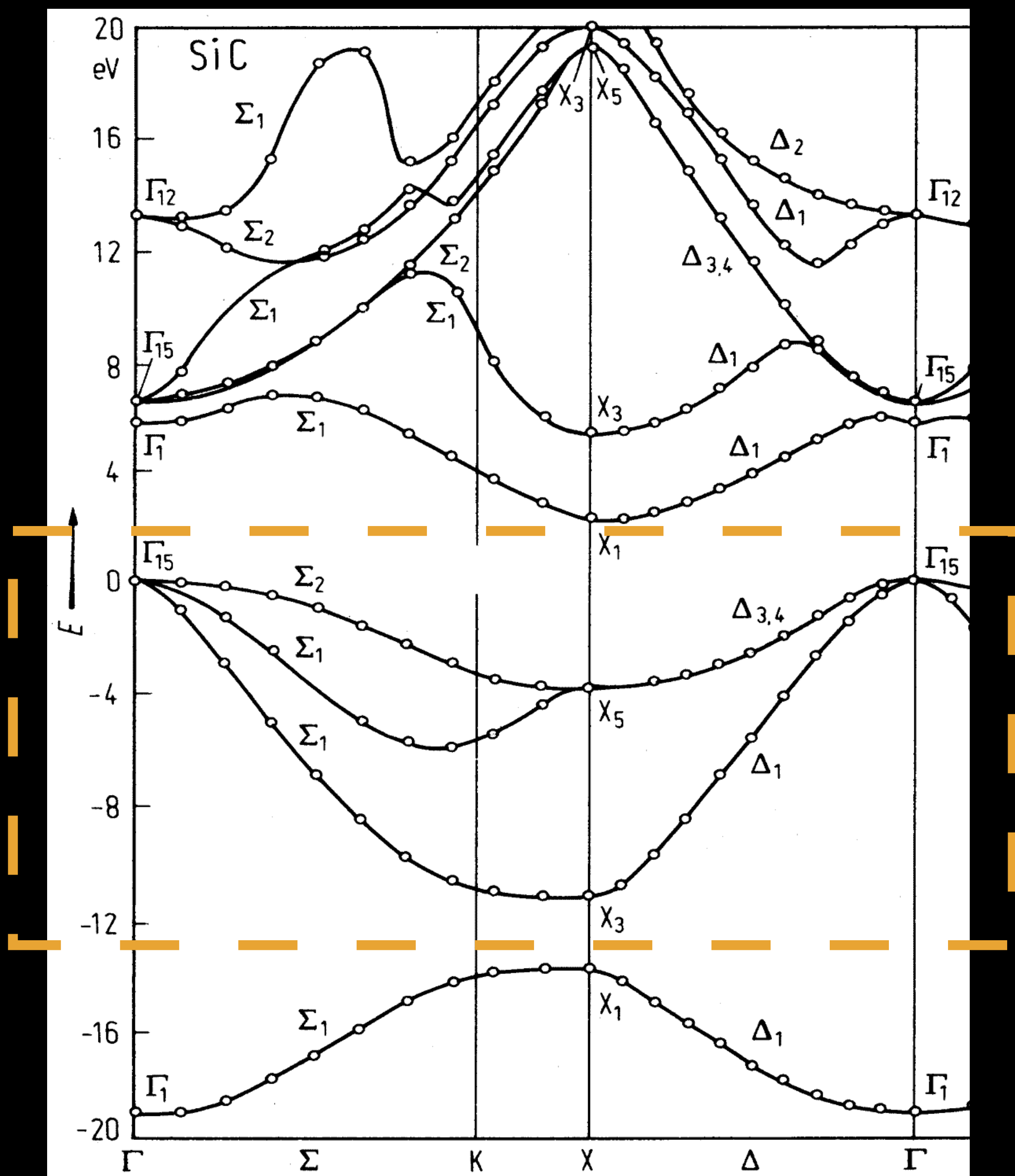


[Hemstreet & Fong (1974)]

Irreps follow rules under symmetry lowering

$$\Gamma_1 \to \Delta_1$$
$$\Gamma_{12} \to \Delta_1 \oplus \Delta_2$$
$$\Gamma_{15} \to \Delta_1 \oplus \Delta_{3,4}$$

Topology meets band symmetries

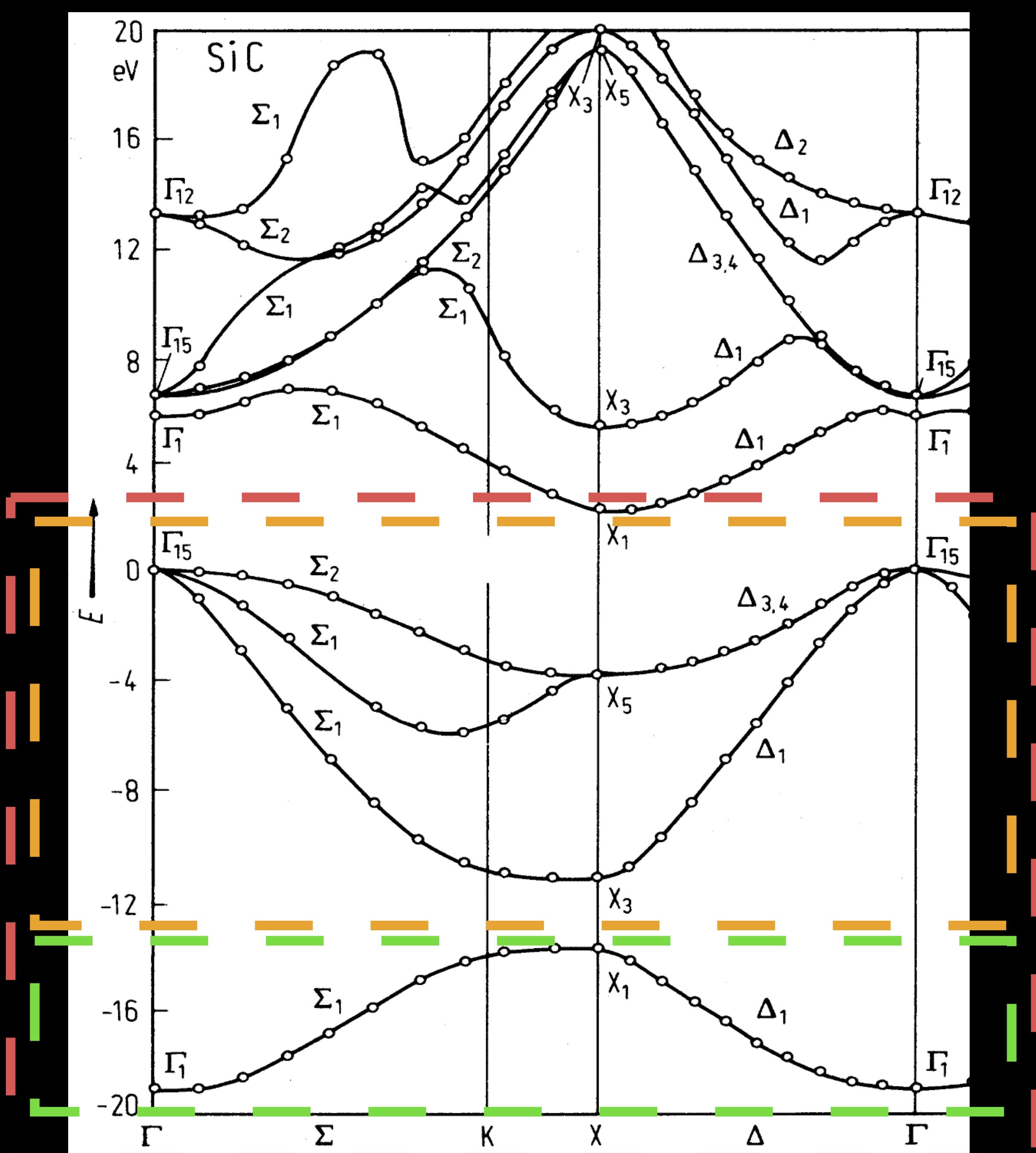


[Hemstreet & Fong (1974)]

- 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

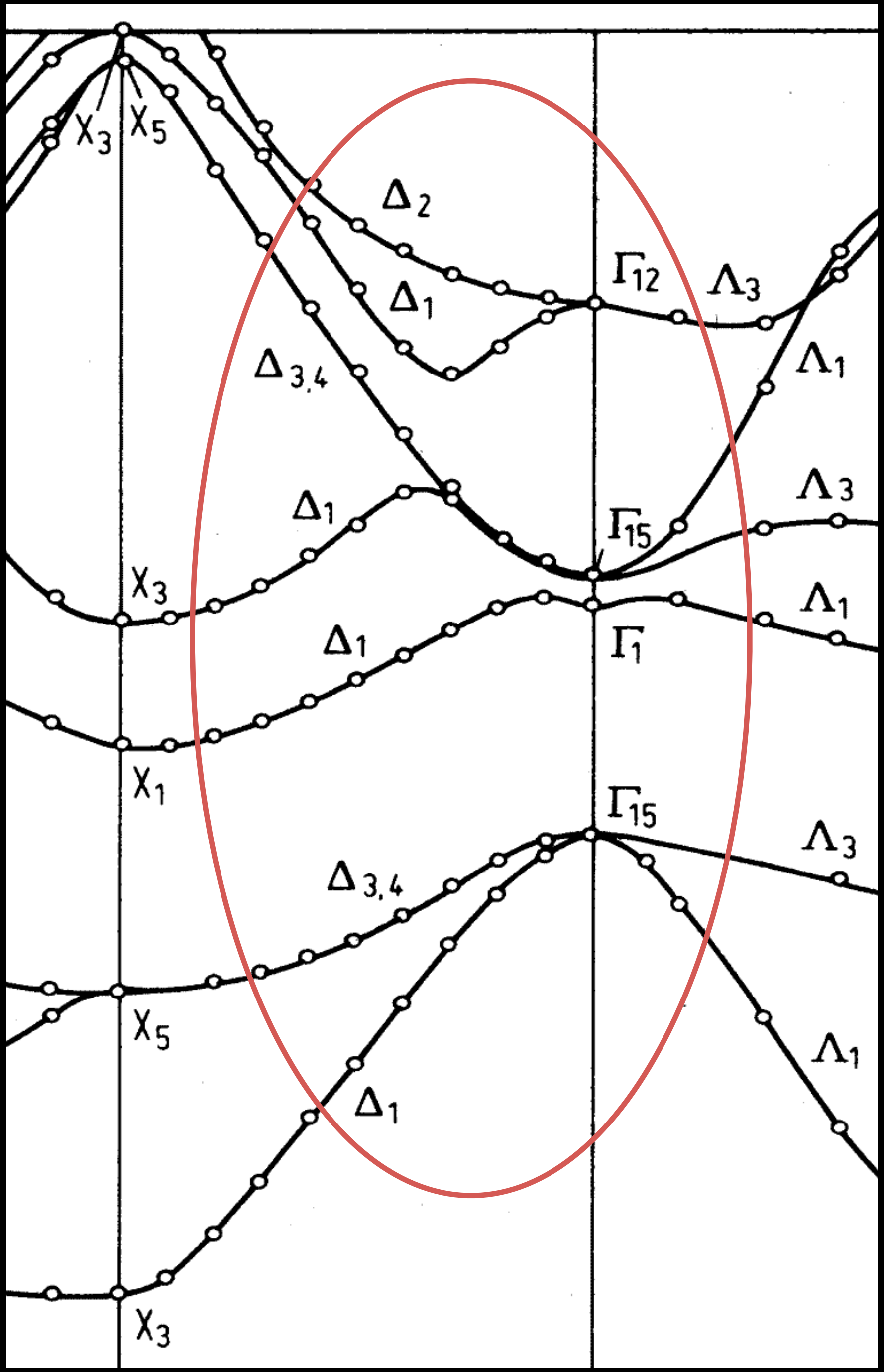


[Hemstreet & Fong (1974)]

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

Imposing Compatibility Relations

- But these counts are not independent: "Compatibility Relations"



$$\begin{cases} \Gamma_1 \to \Delta_1 \\ \Gamma_{12} \to \Delta_1 \oplus \Delta_2 \\ \Gamma_{15} \to \Delta_1 \oplus \Delta_{3,4} \end{cases}$$

$$\Downarrow$$

$$\begin{cases} n_{\Delta_1} = n_{\Gamma_1} + n_{\Gamma_{12}} + n_{\Gamma_{15}} \\ n_{\Delta_2} = n_{\Gamma_{12}} \\ n_{\Delta_{3,4}} = n_{\Gamma_{15}} \end{cases}$$

The group {BS}

- Generally, integer-valued linear equations

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{pmatrix}}_{\mathcal{C}} \begin{pmatrix} n_{\Gamma_1} \\ n_{\Gamma_{12}} \\ n_{\Gamma_{15}} \\ n_{\Delta_1} \\ n_{\Delta_2} \\ n_{\Delta_{3,4}} \end{pmatrix} = 0$$

- Gapped band structure = solutions to $\mathcal{C}\vec{n} = \vec{0}$

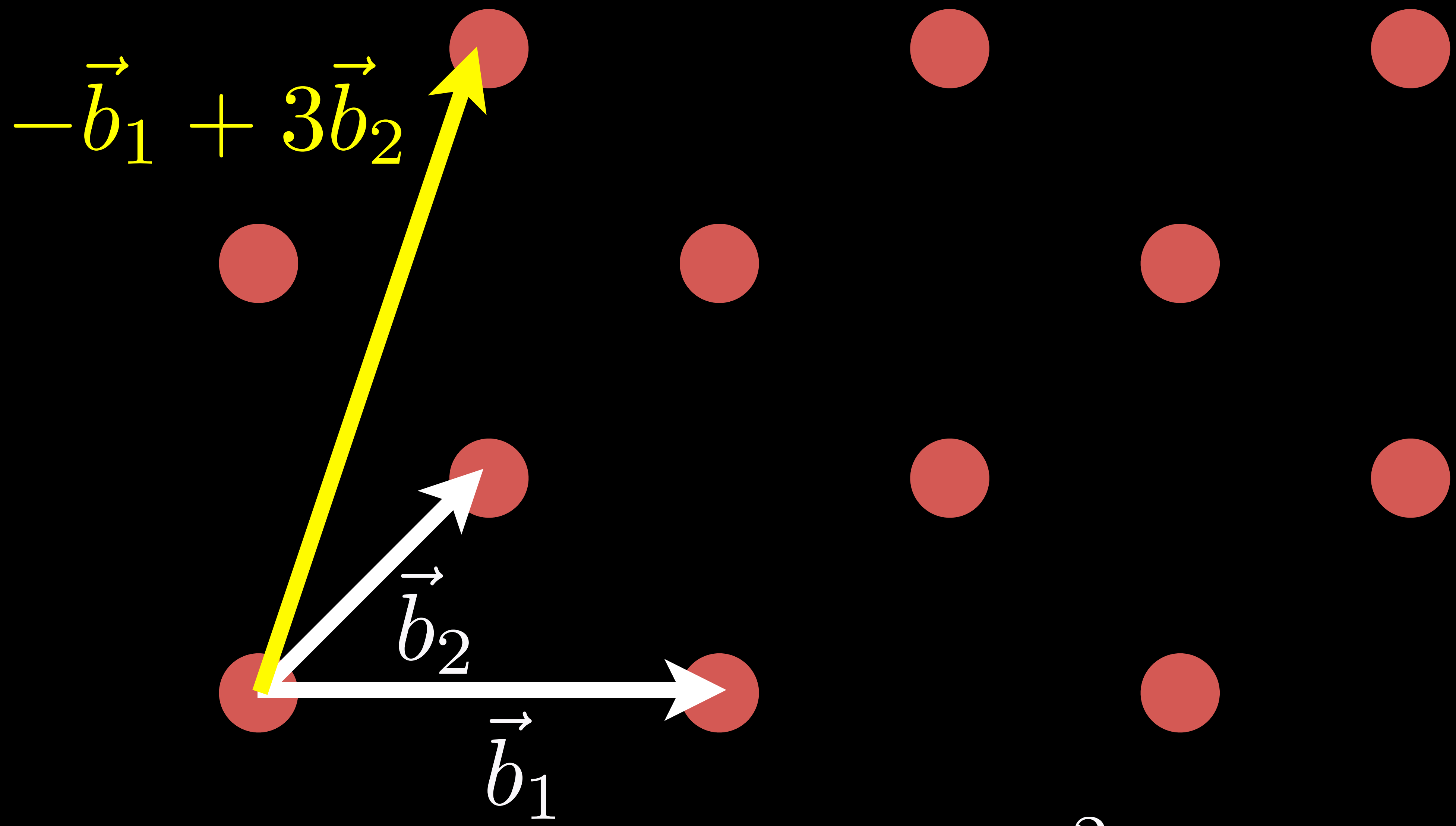
$$\{\mathrm{BS}\} \equiv \ker \mathcal{C} \cap \mathbb{Z}^D \simeq \mathbb{Z}^{d_{\mathrm{BS}}}$$

d_{BS}: dimension of solution space

- $\mathbb{Z}^{d_{\mathrm{BS}}}$ is an abelian group with d_{BS} generators

{Band structures} as a "vector space"

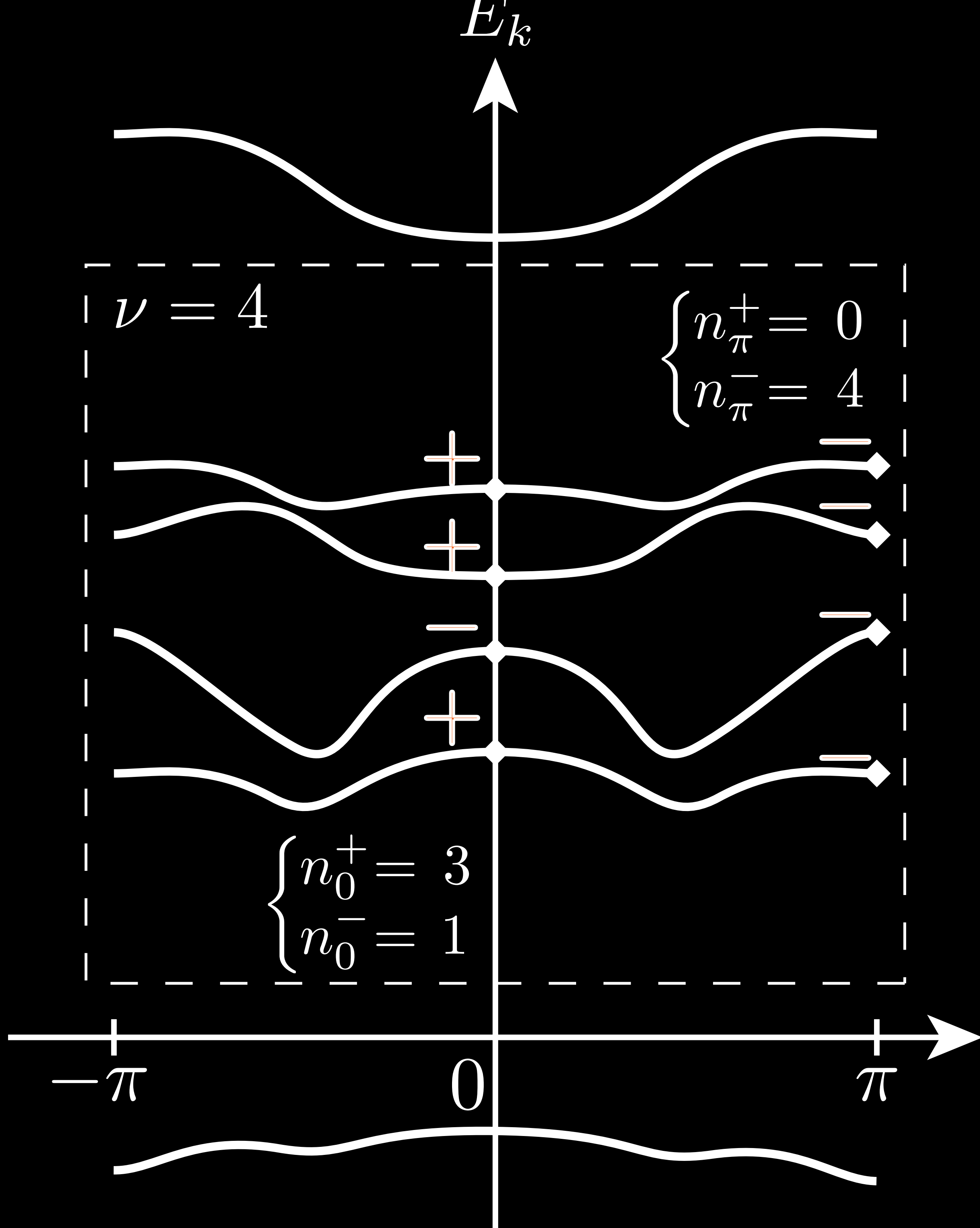
$$\vec{n} \in \{\mathrm{BS}\} \Rightarrow \vec{n} = \sum_{i=1}^{d_{\mathrm{BS}}} m_i \vec{b}_i; \; m_i \in \mathbb{Z}$$



eg. $\{\mathrm{BS}\} = \mathbb{Z}^2$

Example: 1D w/ inversion

[Turner et al (2012), Kruthoff et al (2016)]



- 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

$$\{\mathrm{BS}\} = \mathbb{Z}^3$$

Interlude: What have we done?

[HCP, Vishwanath & Watanabe, 1703.00911]

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)]

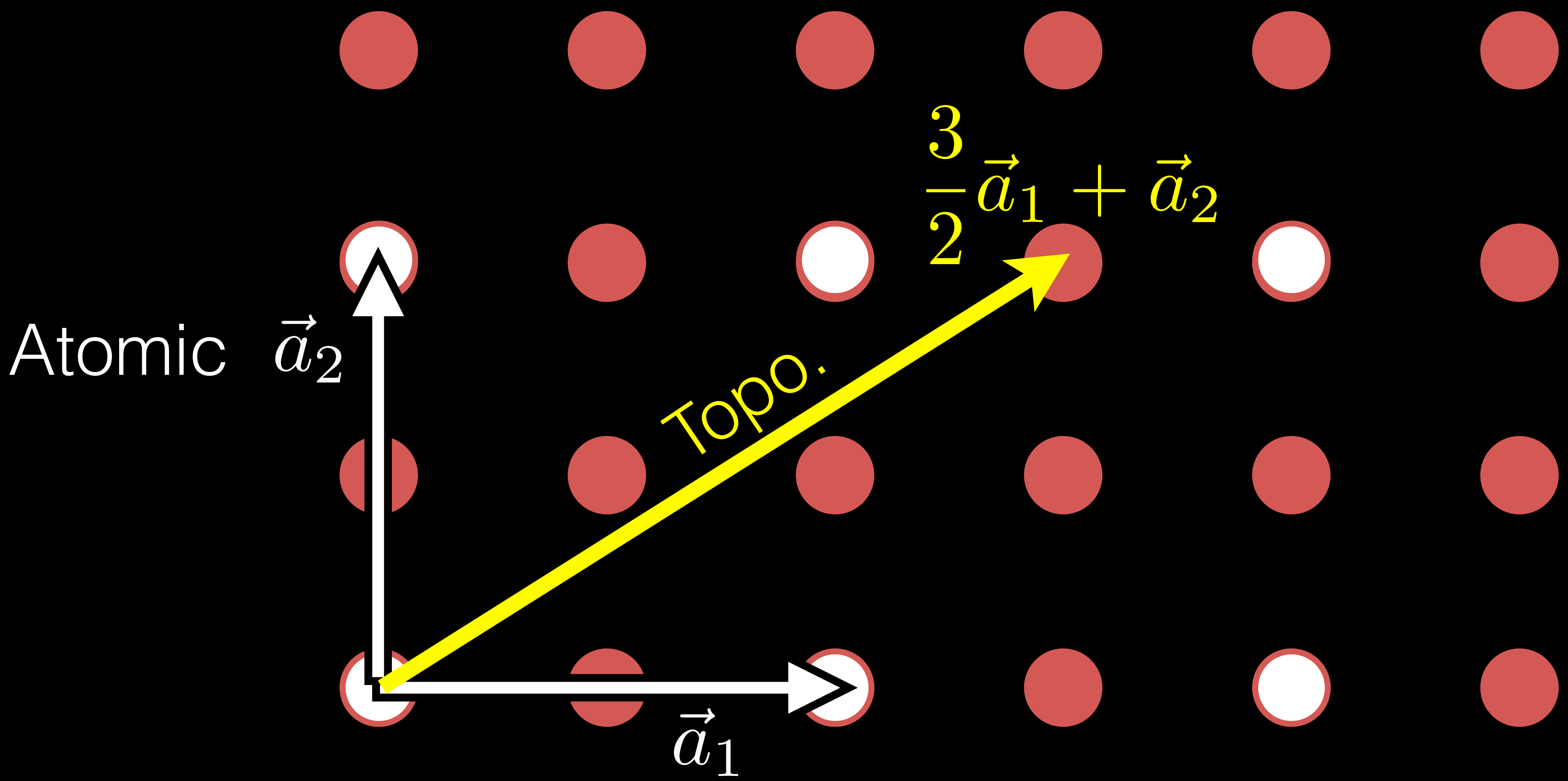
Outline aka Take-homes

- ✓ 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

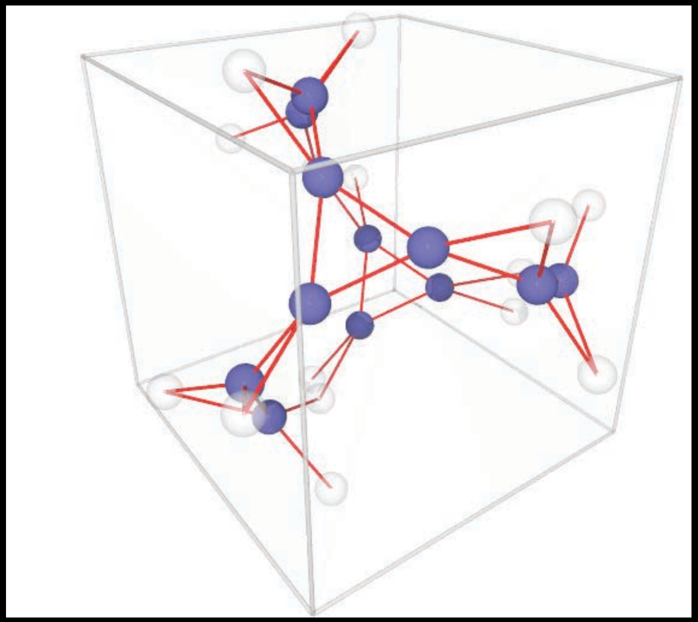
Punchline 2



Real-space (atomic) pictures contain all band-symmetry solutions

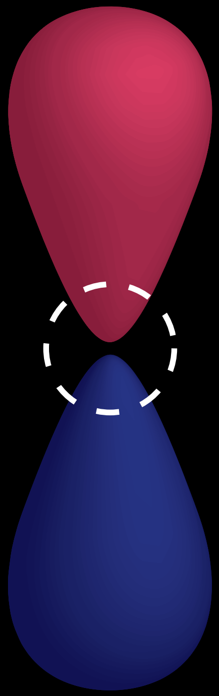
Trivial ≡ Atomic insulators

Trivial band structures: those with a real-space description



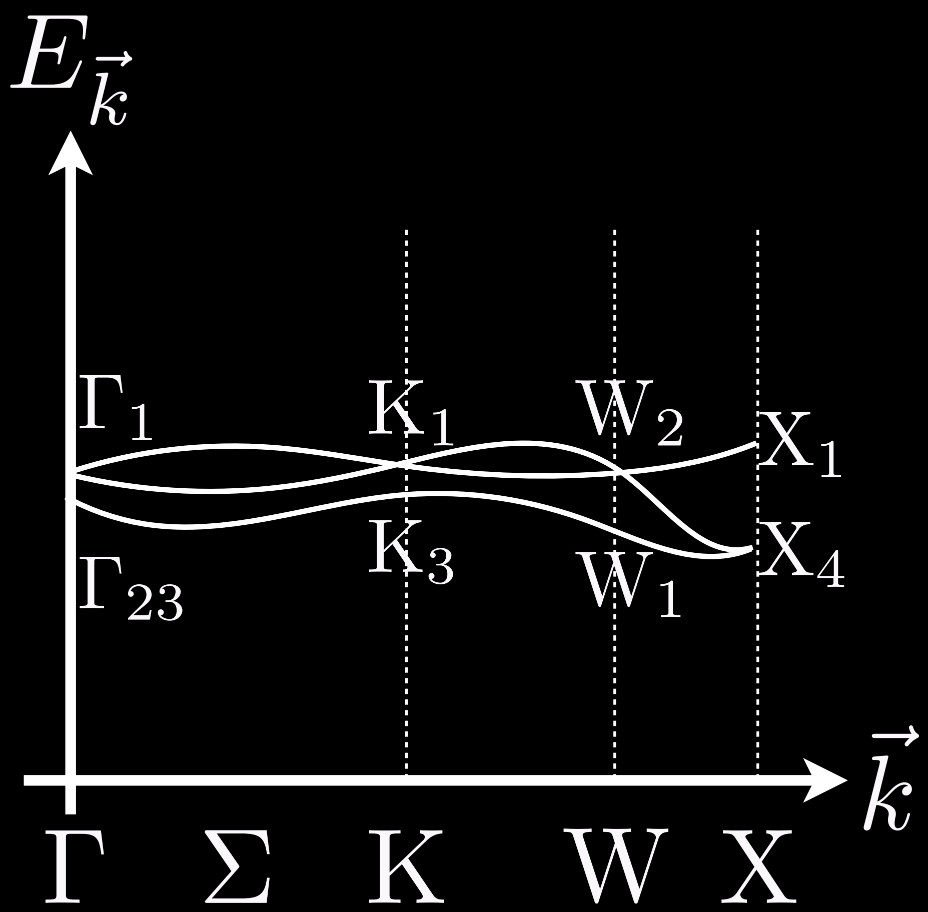
Lattice Points

+



Orbitals

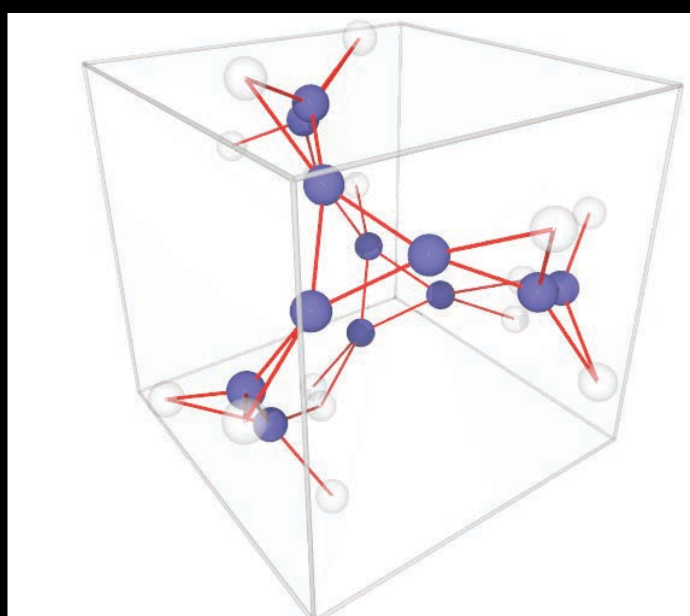
Fourier →



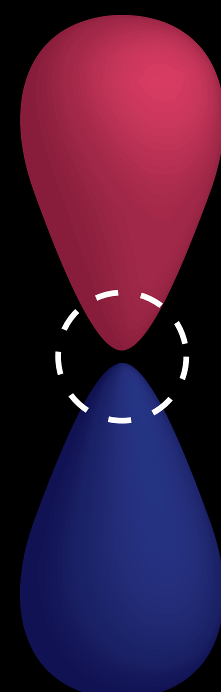
Tight-binding orbitals fix momentum-space sym. reps.

Trivial = Atomic insulators

Trivial band structures: those with a real-space description



+



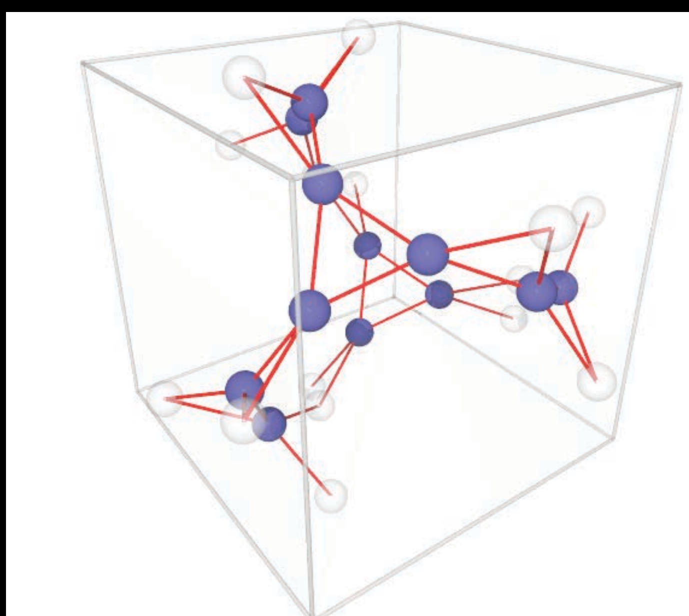
$$\xrightarrow{\text{Fourier}} \quad \vec{a} \in \{\mathrm{BS}\}$$

Lattice Points

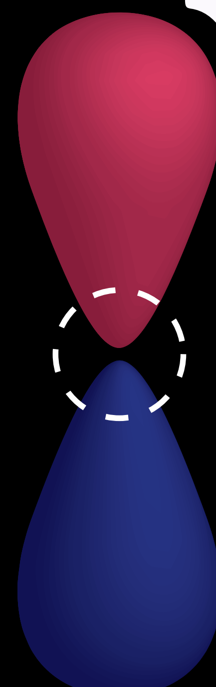
Orbitals

Trivial = Atomic insulators

Trivial band structures: those with a real-space description



+



$\xrightarrow{\text{Fourier}}$ $\vec{a} \in \{\mathrm{BS}\}$

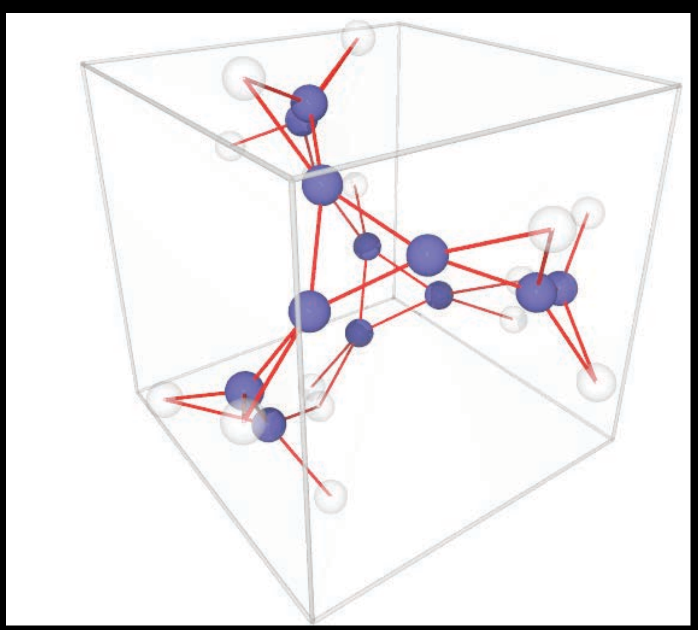
Lattice Points

Orbitals

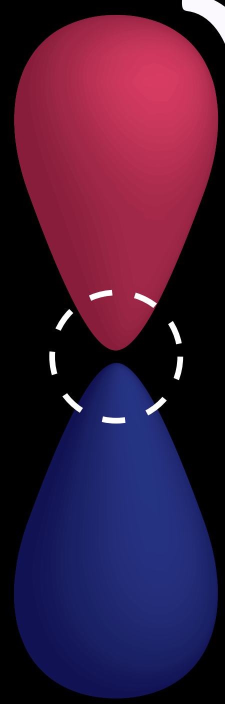
Trivial = Atomic insulators

Trivial band structures: those with a real-space description

$$\left\{ \quad \text{Lattice Points} \quad + \quad \text{Orbitals} \quad \right\} \xrightarrow{\text{Fourier}} \{\vec{a}\} \leq \{\mathrm{BS}\}$$



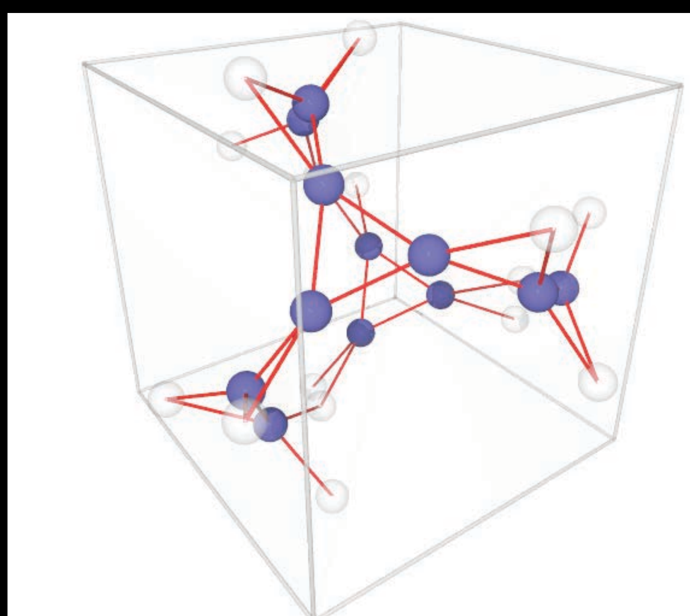
Lattice Points



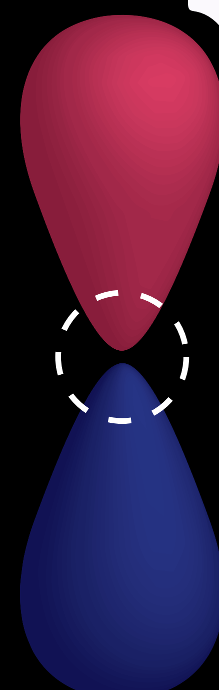
Orbitals

Trivial = Atomic insulators

Trivial band structures: those with a real-space description



+



$$\xrightarrow{\text{Fourier}} \{\vec{a}\} \leq \{\mathrm{BS}\}$$

$$\|$$

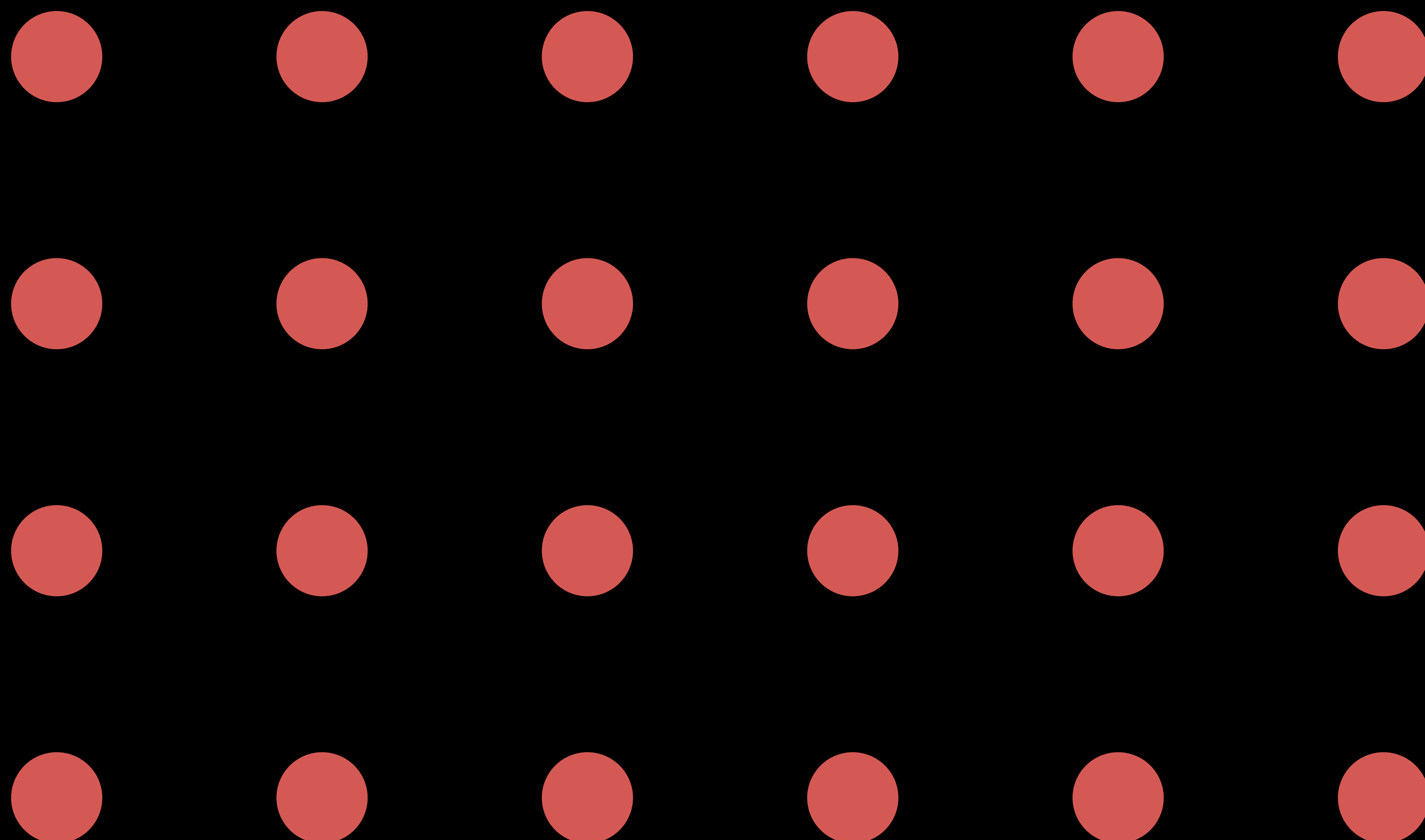
$$\{\mathrm{AI}\} \leq \{\mathrm{BS}\}$$

Lattice Points

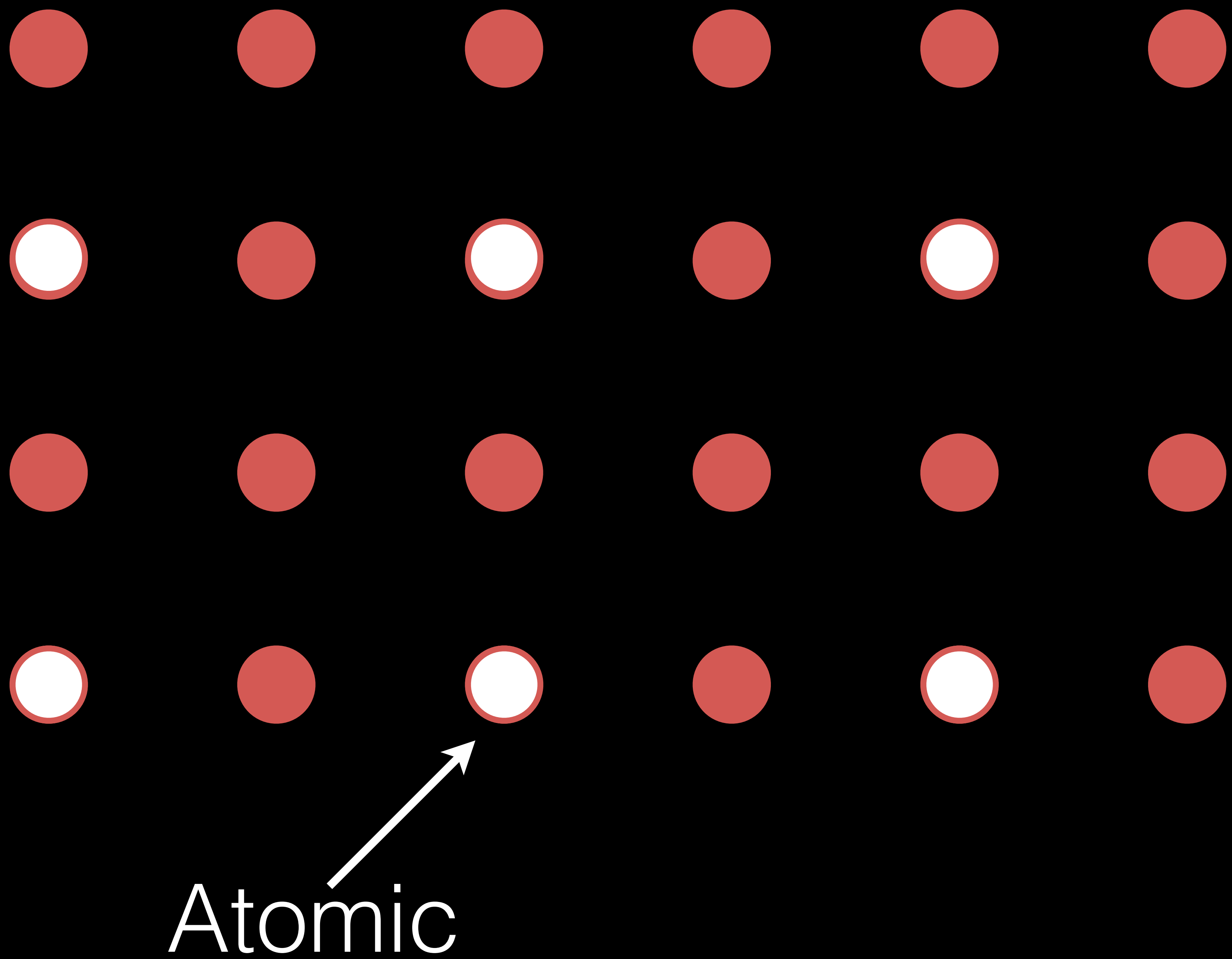
Orbitals

Subgroup from trivial BSs

{BS} vs {AI}

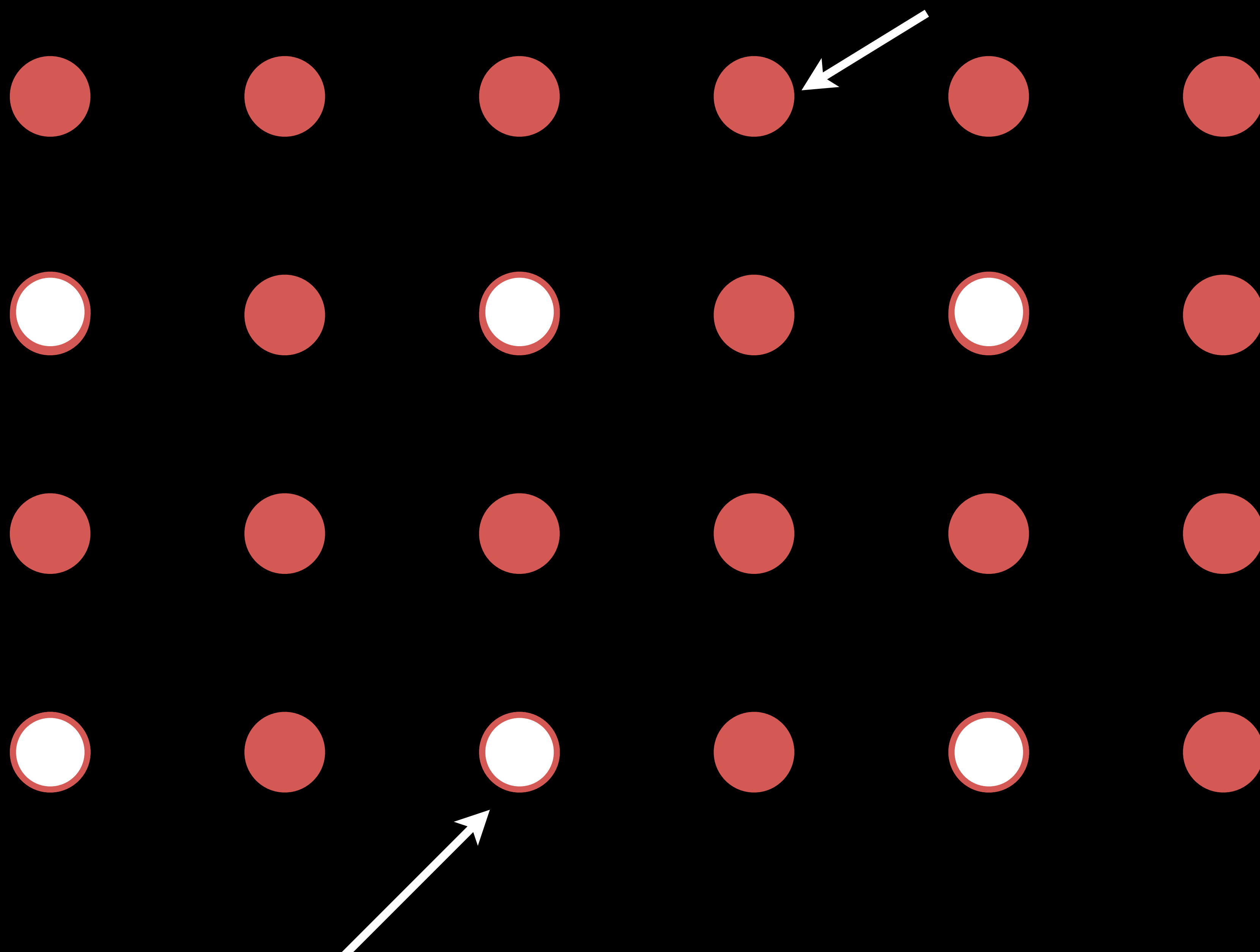


{BS} vs {AI}



{BS} vs {AI}

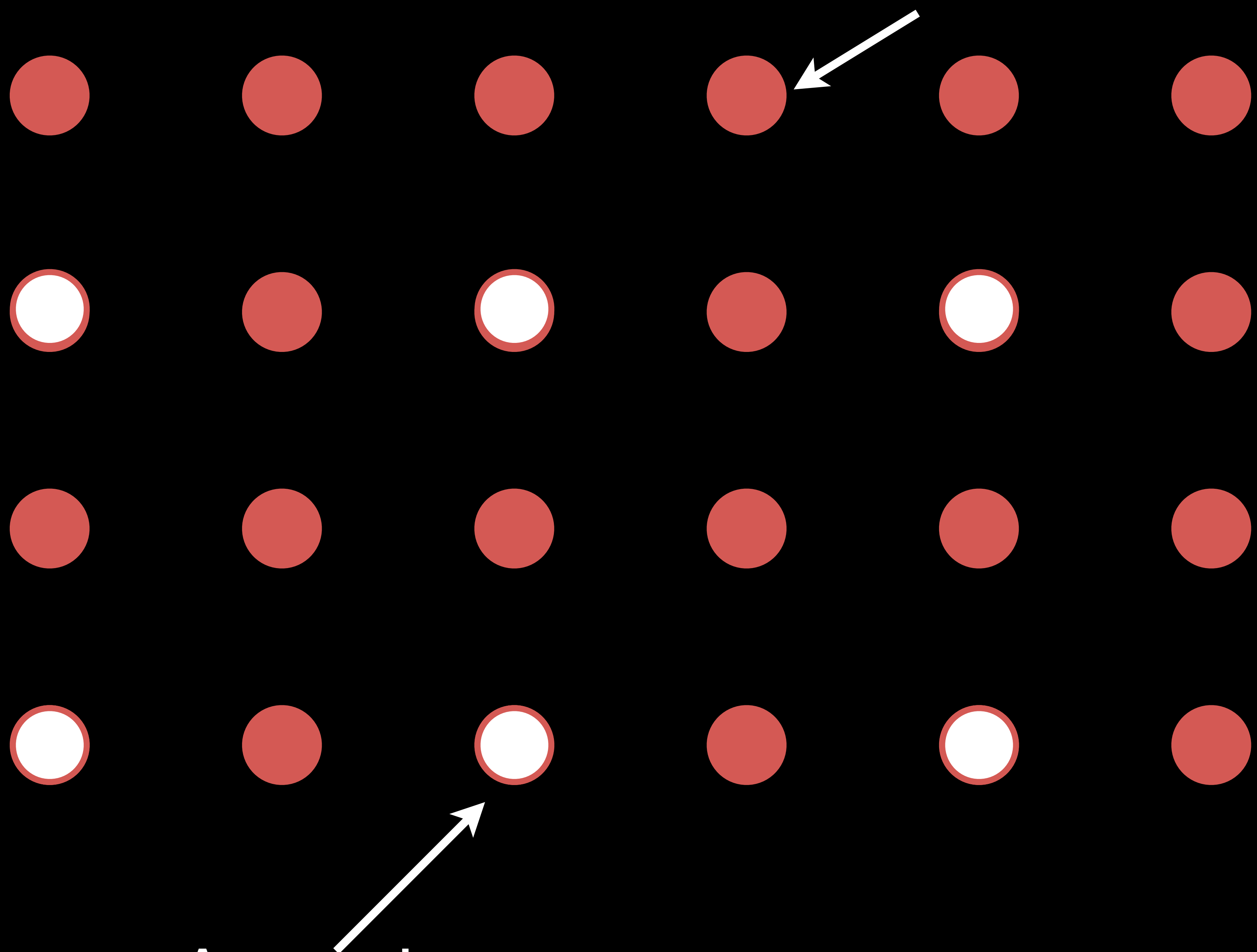
Non-atomic = topological



Atomic

{BS} vs {AI}

Non-atomic = topological



Atomic

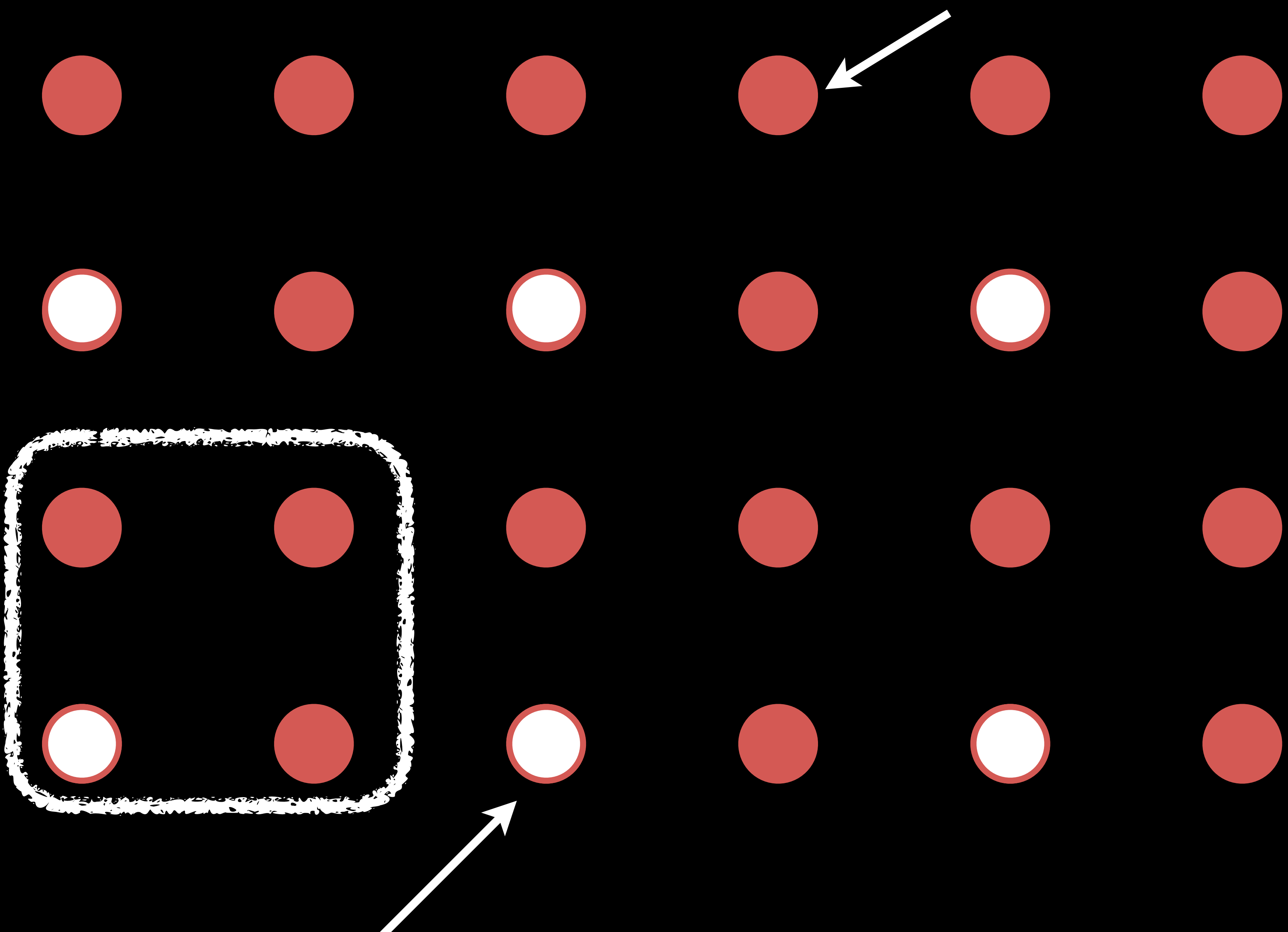
Band topology indicated by

$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}$$

(e.g., $\mathbb{Z}_2 \times \mathbb{Z}_2$)

{BS} vs {AI}

Non-atomic = topological



Atomic

Band topology indicated by

$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}$$

(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,

$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}$$

is a finite abelian group.

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

⇒ Basis for {BS} constructible from that of {AI}

Computing the indicator

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

Let $\{\mathbf{a}_i \mid i = 1,\ldots,d_{\mathrm{AI}}\}$ be a complete basis for {AI}.

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

$$\mathbf{b} = \sum_{i=1}^{d_{\mathrm{AI}}} q_i \mathbf{a}_i$$

for some rational coefficients q_i ; in addition

- *Any* q_i is fractional ⇒ $\mathbf{b}$ is topological
- All q_i are integers ⇒ $\mathbf{b}$ *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, $X_{\mathrm{BS}} = \mathbb{Z}_2$
  - simply the quantum spin Hall index
- For 3D,

$$X_{\mathrm{BS}} = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

TR & inversion symmetric systems

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

$$X_{\mathrm{BS}} = \underbrace{\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2}_{\text{Weak TIs}} \times \mathbb{Z}_4$$

TR & inversion symmetric systems

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

$$X_{\mathrm{BS}} = \underbrace{\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2}_{\text{Weak TIs}} \times \underbrace{\mathbb{Z}_4}_{\text{Strong TI \& something more, protected by TR \& inversion}}$$

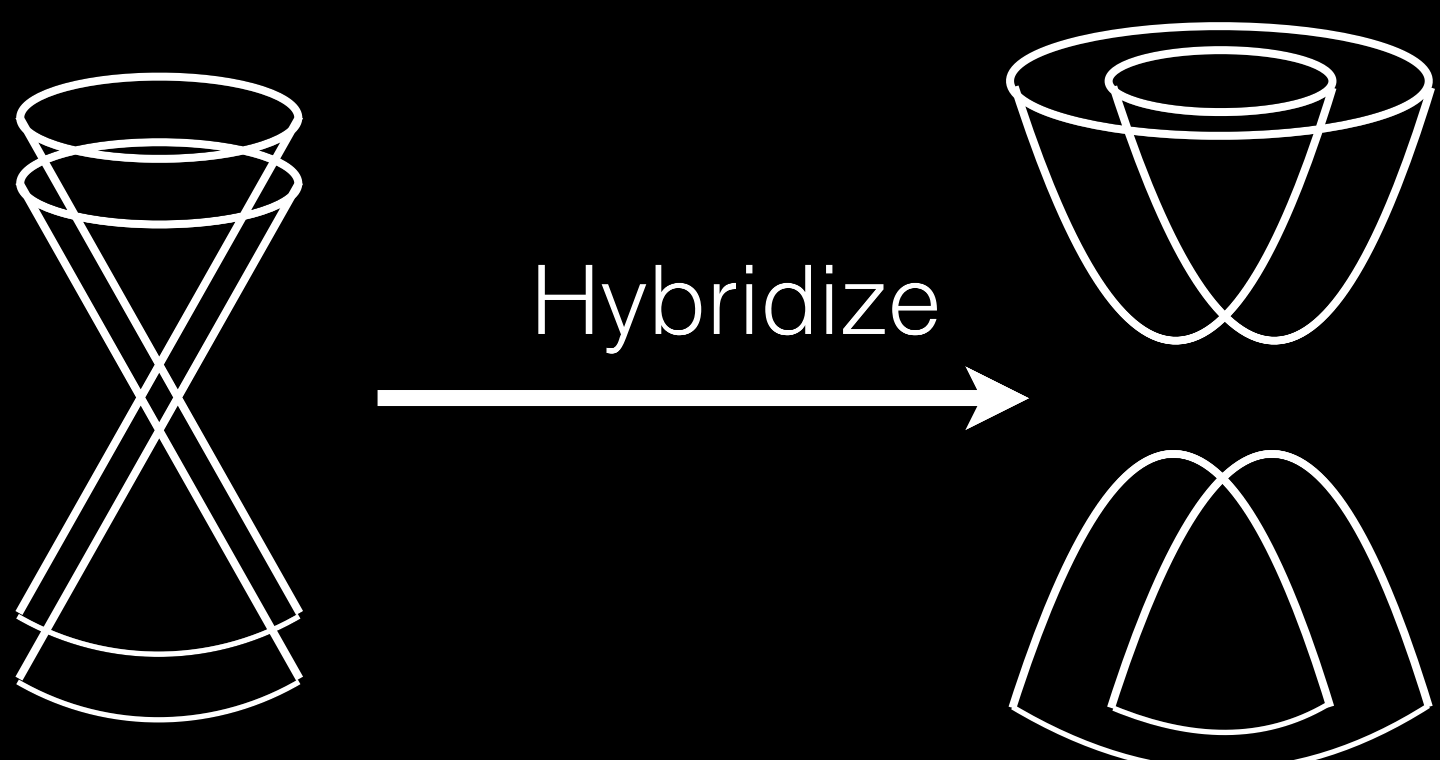
Weak TIs

Strong TI
&
something more,
protected by TR & inversion

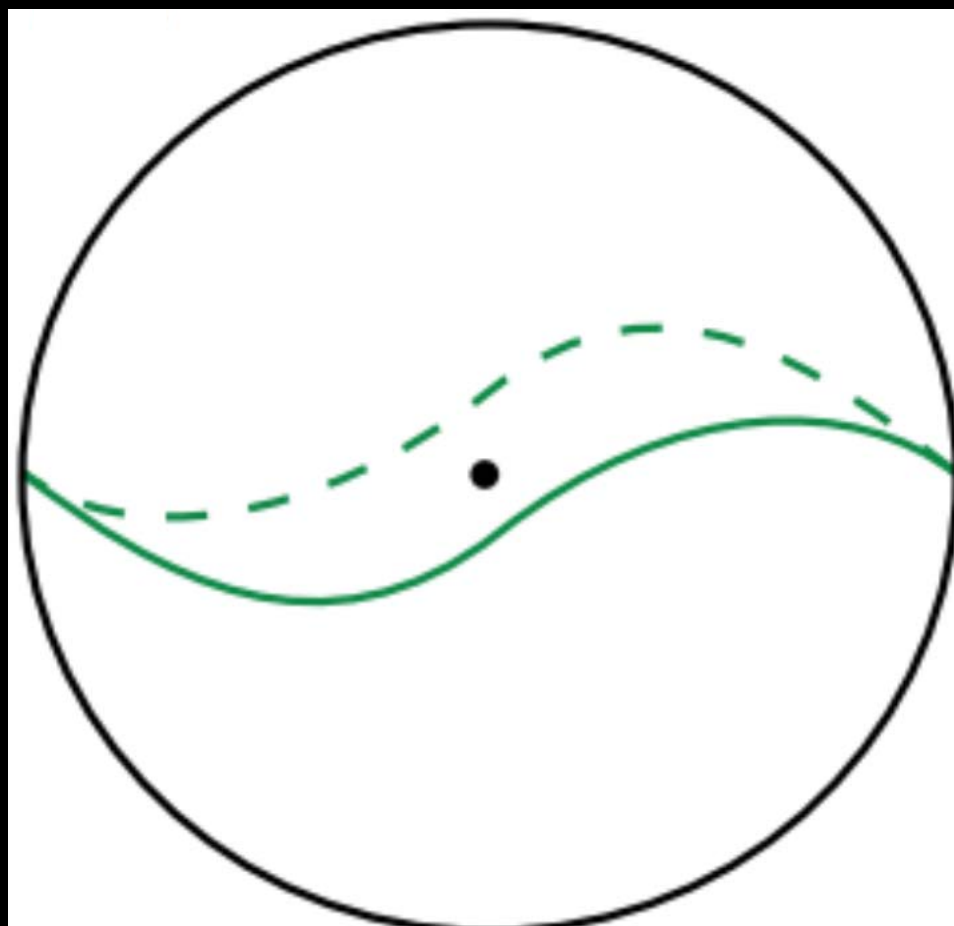
[HCP, Vishwanath & Watanabe, 1703.00911]

“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?



[Fang & Fu, 1709.01929]

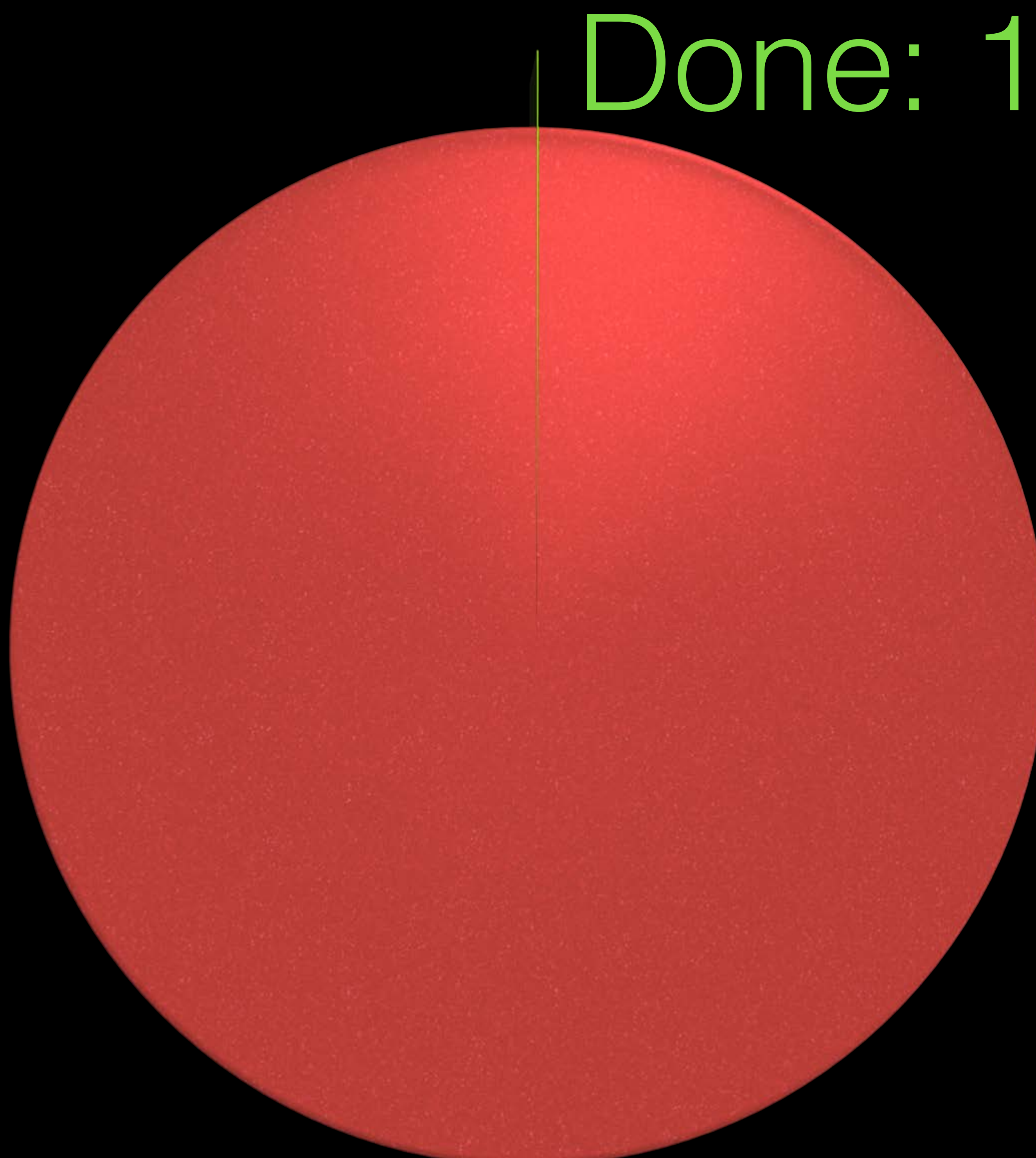
Inversion-symmetric
open-boundary conditions

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!



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.

MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}
1.1 I	1	(1)	1	1.3 IV	1	(1)	2	2.5 II	9	(2,2,2,4)	2	2.7 IV	5	(2)	2
1.2 II	1	(1)	2	2.4 I	9	(2,2,2,4)	1	2.6 III	1	(1)	2				

d: Rank of the band structure group {BS}
X_{BS}: Symmetry-based indicators of band topology
ν_{BS}: Set of ν bands are symmetry-forbidden from being isolated by band gaps if $\nu \notin \nu_{\mathrm{BS}}\mathbb{Z}$

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

MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}
3.1 I	5	(2)	1	7.24 I	1	(1)	2	10.47 IV	7	(2,2)	2	13.70 IV	4	(2)	4
3.2 II	1	(1)	2	7.25 II	1	(1)	4	10.48 IV	6	(2)	2	13.71 IV	3	(2)	4
3.3 III	1	(1)	1	7.26 III	1	(1)	2	10.49 IV	8	(2)	2	13.72 IV	5	(2)	2
3.4 IV	3	(2)	2	7.27 IV	1	(1)	4	11.50 I	6	(2)	2	13.73 IV	3	(2)	4
3.5 IV	1	(1)	2	7.28 IV	1	(1)	2	11.51 II	5	(2,2,4)	4	13.74 IV	4	(2)	4
3.6 IV	3	(1)	2	7.29 IV	1	(1)	4	11.52 III	2	(1)	2	14.75 I	5	(2)	2
4.7 I	1	(1)	2	7.30 IV	1	(1)	4	11.53 III	1	(1)	2	14.76 II	5	(2,4)	4
4.8 II	1	(1)	4	7.31 IV	1	(1)	2	11.54 III	5	(2,2,4)	2	14.77 III	1	(1)	4
4.9 III	1	(1)	2	8.32 I	2	(1)	1	11.55 IV	3	(2)	4	14.78 III	1	(1)	4
4.10 IV	1	(1)	4	8.33 II	1	(1)	2	11.56 IV	5	(2)	2	14.79 III	5	(2,4)	2
4.11 IV	1	(1)	2	8.34 III	1	(1)	1	11.57 IV	3	(2)	4	14.80 IV	3	(2)	4
4.12 IV	1	(1)	2	8.35 IV	1	(1)	2	12.58 I	10	(2,2)	1	14.81 IV	3	(2)	4
5.13 I	3	(1)	1	8.36 IV	1	(1)	2	12.59 II	7	(2,2,4)	2	14.82 IV	3	(2)	4
5.14 II	1	(1)	2	9.37 I	1	(1)	2	12.60 III	1	(1)	2	14.83 IV	5	(2)	2
5.15 III	1	(1)	1	9.38 II	1	(1)	4	12.61 III	1	(1)	2	14.84 IV	3	(2)	4
5.16 IV	2	(1)	2	9.39 III	1	(1)	2	12.62 III	7	(2,2,4)	1	15.85 I	6	(2,2)	2
5.17 IV	1	(1)	2	9.40 IV	1	(1)	2	12.63 IV	5	(2)	2	15.86 II	5	(2,4)	4
6.18 I	3	(1)	1	9.41 IV	1	(1)	4	12.64 IV	5	(2)	2	15.87 III	1	(1)	2
6.19 II	1	(1)	2	10.42 I	15	(2,2,2)	1	13.65 I	7	(2,2)	2	15.88 III	2	(1)	2
6.20 III	1	(1)	1	10.43 II	9	(2,2,2,4)	2	13.66 II	5	(2,2,4)	4	15.89 III	5	(2,4)	2
6.21 IV	1	(1)	2	10.44 III	1	(1)	2	13.67 III	1	(1)	2	15.90 IV	4	(2)	2
6.22 IV	2	(1)	2	10.45 III	1	(1)	2	13.68 III	3	(1)	2	15.91 IV	3	(2)	4
6.23 IV	2	(1)	2	10.46 III	9	(2,2,2,4)	1	13.69 III	5	(2,2,4)	2				

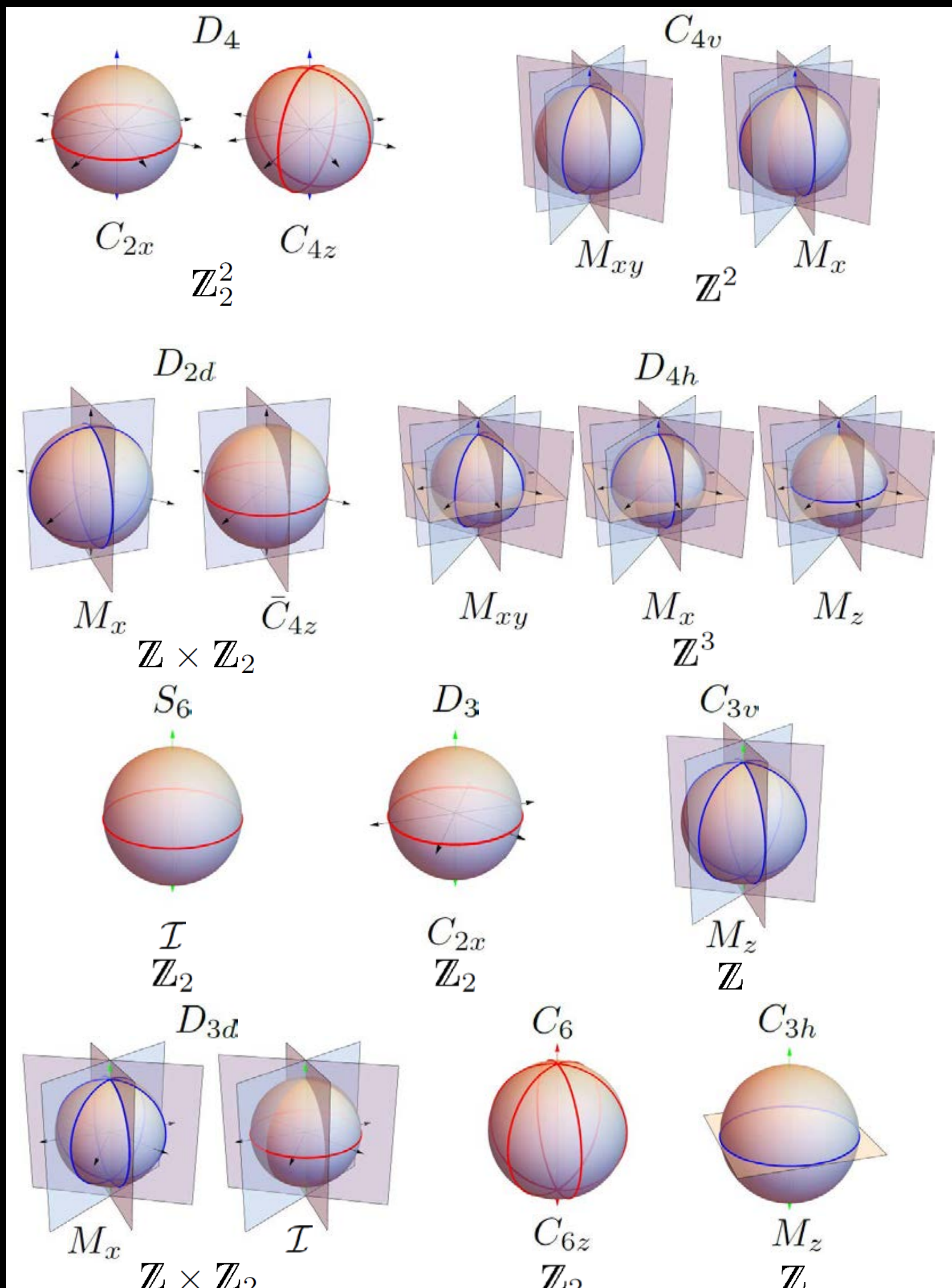
d: Rank of the band structure group {BS}
X_{BS}: Symmetry-based indicators of band topology
ν_{BS}: Set of ν bands are symmetry-forbidden from being isolated by band gaps if $\nu \notin \nu_{\mathrm{BS}}\mathbb{Z}$

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

MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}	MSG	d	X_{BS}	ν_{BS}
16.1 I	1	(1)	2	23.51 III	3	(1)	1	29.101 III	1	(1)	4	33.151 IV	1	(1)	4
16.2 II	1	(1)	2	23.52 IV	1	(1)	2	29.102 III	1	(1)	4	33.152 IV	1	(1)	4
16.3 III	5	(2)	1	24.53 I	4	(1)	2	29.103 III	1	(1)	4	33.153 IV	1	(1)	4
16.4 IV	1	(1)	2	24.54 II	1	(1)	4	29.104 IV	1	(1)	4	33.154 IV	1	(1)	4
16.5 IV	1	(1)	4	24.55 III	2	(1)	2	29.105 IV	1	(1)	8	33.155 IV	1	(1)	4
16.6 IV	1	(1)	4	24.56 IV	3	(1)	2	29.106 IV	1	(1)	4	34.156 I	3	(1)	2
17.7 I	5	(1)	2	25.57 I	1	(1)	2	29.107 IV	1	(1)	4	34.157 II	1	(1)	4
17.8 II	1	(1)	4	25.58 II	1	(1)	2	29.108 IV	1	(1)	4	34.158 III	1	(1)	2
17.9 III	1	(1)	2	25.59 III	3	(1)	1	29.109 IV	1	(1)	4	34.159 III	3	(1)	2
17.10 III	3	(2)	2	25.60 III	5	(2)	1	29.110 IV	1	(1)	4	34.160 IV	2	(1)	4
17.11 IV	2	(1)	4	25.61 IV	1	(1)	4	30.111 I	3	(1)	2	34.161 IV	1	(1)	4
17.12 IV	5	(1)	2	25.62 IV	1	(1)	2	30.112 II	1	(1)	4	34.162 IV	2	(1)	4
17.13 IV	4	(1)	2	25.63 IV	1	(1)	4	30.113 III	1	(1)	2	34.163 IV	3	(2)	4
17.14 IV	3	(1)	4	25.64 IV	1	(1)	4	30.114 III	1	(1)	2	34.164 IV	3	(1)	2
17.15 IV	3	(1)	4	25.65 IV	1	(1)	4	30.115 III	3	(1)	2	35.165 I	2	(1)	2
18.16 I	3	(1)	2	26.66 I	1	(1)	2	30.116 IV	2	(1)	4	35.166 II	1	(1)	2
18.17 II	1	(1)	4	26.67 II	1	(1)	4	30.117 IV	3	(2)	4	35.167 III	2	(1)	1
18.18 III	3	(2)	2	26.68 III	1	(1)	2	30.118 IV	1	(1)	4	35.168 III	4	(2)	1
18.19 III	1	(1)	2	26.69 III	3	(1)	2	30.119 IV	3	(1)	2	35.169 IV	1	(1)	4
18.20 IV	2	(1)	4	26.70 III	1	(1)	2	30.120 IV	2	(1)	4	35.170 IV	2	(1)	2
18.21 IV	1	(1)	4	26.71 IV	1	(1)	4	30.121 IV	2	(1)	4	35.171 IV	2	(1)	4
18.22 IV	2	(1)	4	26.72 IV	1	(1)	4	30.122 IV	2	(1)	4	36.172 I	1	(1)	2
18.23 IV	3	(1)	2	26.73 IV	1	(1)	2	31.123 I	2	(1)	2	36.173 II	1	(1)	4
18.24 IV	3	(1)	2	26.74 IV	1	(1)	2	31.124 II	1	(1)	4	36.174 III	1	(1)	2
19.25 I	1	(1)	4	26.75 IV	1	(1)	4	31.125 III	1	(1)	2	36.175 III	2	(1)	2
19.26 II	1	(1)	8	26.76 IV	1	(1)	4	31.126 III	2	(1)	2	36.176 III	1	(1)	2
19.27 III	1	(1)	4	26.77 IV	1	(1)	4	31.127 III	1	(1)	2	36.177 IV	1	(1)	2
19.28 IV	1	(1)	4	27.78 I	1	(1)	2	31.128 IV	2	(1)	4	36.178 IV	1	(1)	4
19.29 IV	1	(1)	4	27.79 II	1	(1)	4	31.129 IV	1	(1)	4	36.179 IV	1	(1)	2
19.30 IV	1	(1)	4	27.80 III	1	(1)	2	31.130 IV	1	(1)	4	37.180 I	2	(1)	2
20.31 I	3	(1)	2	27.81 III	5	(2)	2	31.131 IV	1	(1)	4	37.181 II	1	(1)	4
20.32 II	1	(1)	4	27.82 IV	1	(1)	2	31.132 IV	2	(1)	2	37.182 III	1	(1)	2
20.33 III	1	(1)	2	27.83 IV	1	(1)	4	31.133 IV	2	(1)	4	37.183 III	4	(2)	2
20.34 III	2	(1)	2	27.84 IV	1	(1)	4	31.134 IV	2	(1)	2	37.184 IV	1	(1)	2
20.35 IV	3	(1)	2	27.85 IV	1	(1)	4	32.135 I	3	(1)	2	37.185 IV	2	(2)	4
20.36 IV	1	(1)	4	27.86 IV	1	(1)	4	32.136 II	1	(1)	4	37.186 IV	2	(1)	2
20.37 IV	3	(1)	2	28.87 I	4	(1)	2	32.137 III	1	(1)	2	38.187 I	1	(1)	2
21.38 I	2	(1)	2	28.88 II	1	(1)	4	32.138 III	3	(2)	2	38.188 II	1	(1)	2
21.39 II	1	(1)	2	28.89 III	1	(1)	2	32.139 IV	1	(1)	4	38.189 III	2	(1)	1
21.40 III	4	(2)	1	28.90 III	2	(1)	2	32.140 IV	2	(1)	4	38.190 III	3	(1)	1
21.41 III	3	(1)	1	28.91 III	3	(2)	2	32.141 IV	3	(1)	2	38.191 III	3	(1)	1
21.42 IV	1	(1)	2	28.92 IV	4	(1)	2	32.142 IV	2	(1)	4	38.192 IV	1	(1)	2
21.43 IV	2	(1)	2	28.93 IV	2	(1)	4	32.143 IV	3	(1)	4	38.193 IV	1	(1)	2
21.44 IV	2	(1)	2	28.94 IV	1	(1)	4	33.144 I	1	(1)	4	38.194 IV	1	(1)	4
22.45 I	1	(1)	2	28.95 IV	2	(1)	4	33.145 II	1	(1)	8	39.195 I	1	(1)	2
22.46 II	1	(1)	2	28.96 IV	4	(1)	4	33.146 III	1	(1)	4	39.196 II	1	(1)	4
22.47 III	3	(1)	1	28.97 IV	3	(1)	2	33.147 III	1	(1)	4	39.197 III	2	(1)	2
22.48 IV	1	(1)	2	28.98 IV	3	(1)	4	33.148 III	1	(1)	4	39.198 III	1	(1)	2
23.49 I	1	(1)	2	29.99 I	1	(1)	4	33.149 IV	1	(1)	4	39.199 III	3	(2)	2
23.50 II	1	(1)	2	29.100 II	1	(1)	8	33.150 IV	1	(1)	8	39.200 IV	1	(1)	4

& ~20 more pages

Physical consequence



etc.

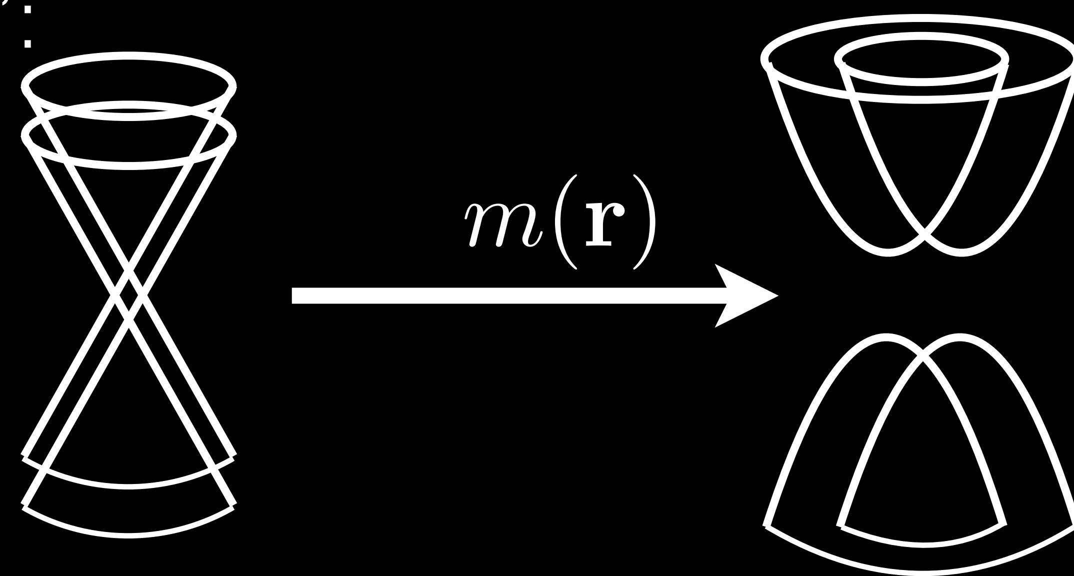
In class AII (spin-orbit coupled with time-reversal $\mathcal{T}^2$=-1), nontrivial X_{BS} implies (up to energetics):

- 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 AII 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

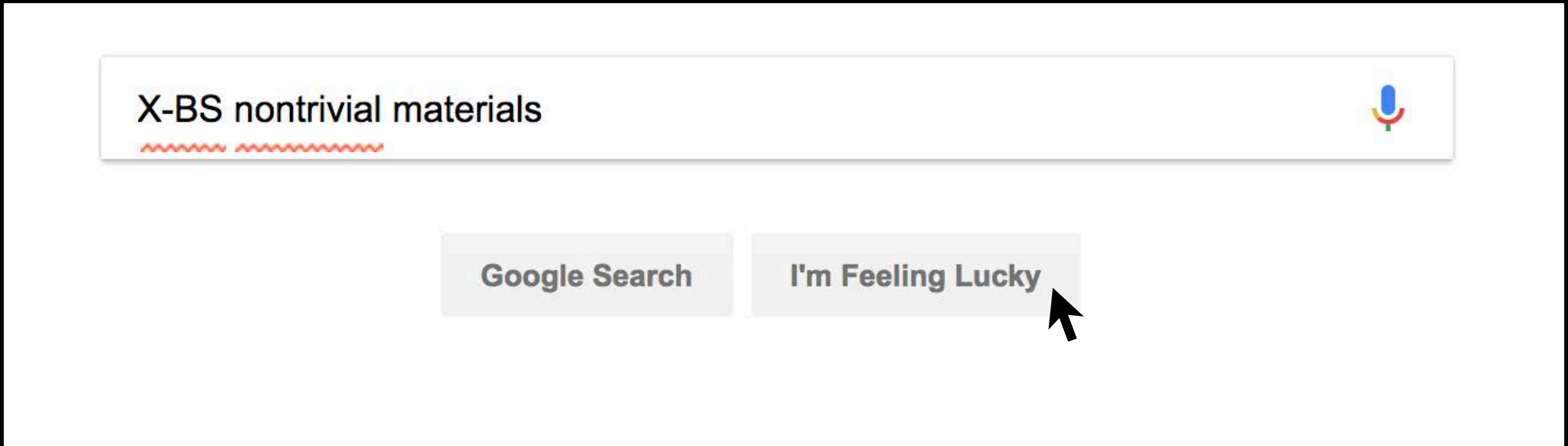
1. Why “band structures” instead of “band insulators”?
   - Gap condition *only* imposed at high-symmetry momenta; could have *irremovable* gapless points at generic momenta

     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

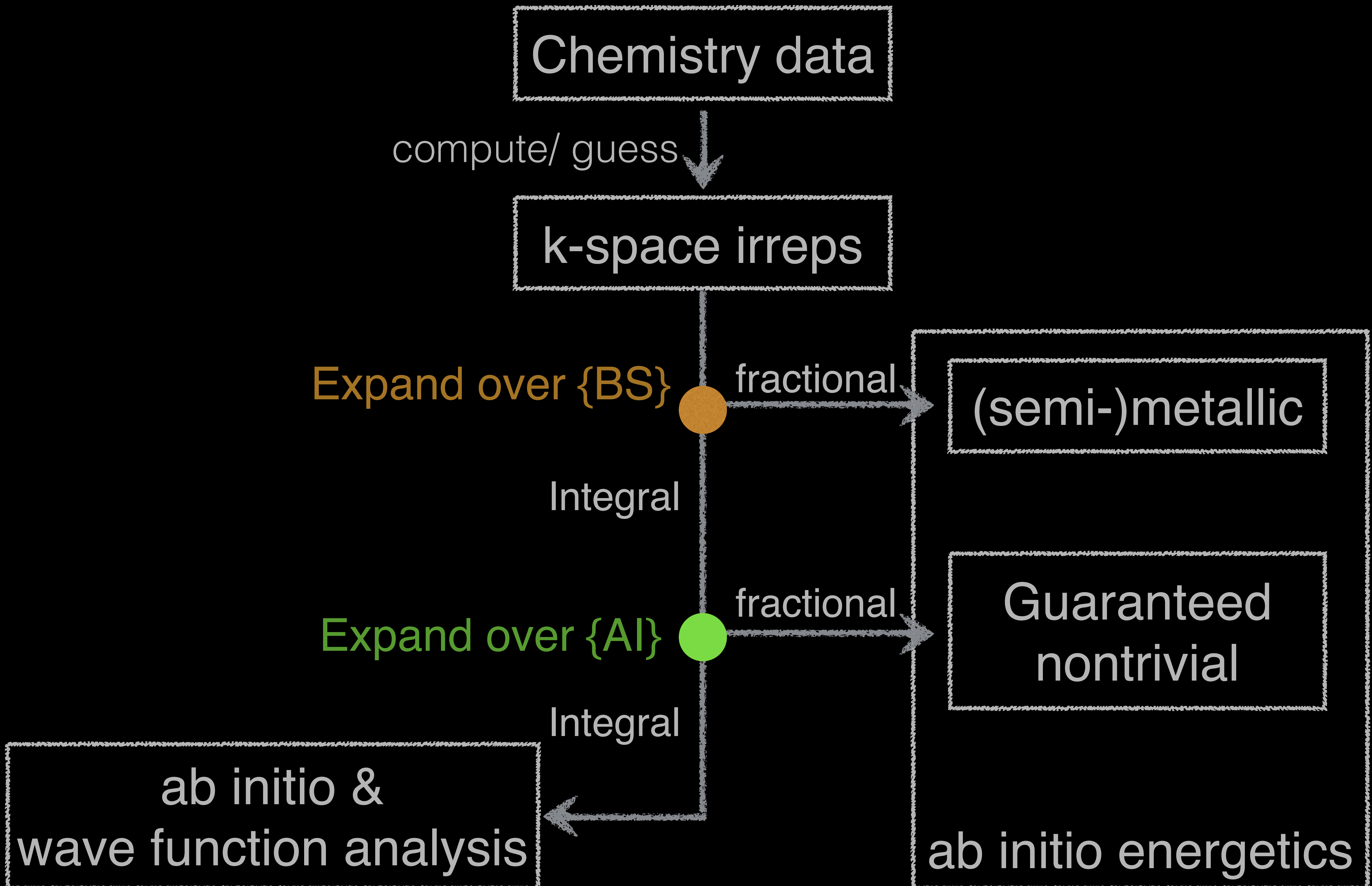
Outline aka Take-homes

- ✓ 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…



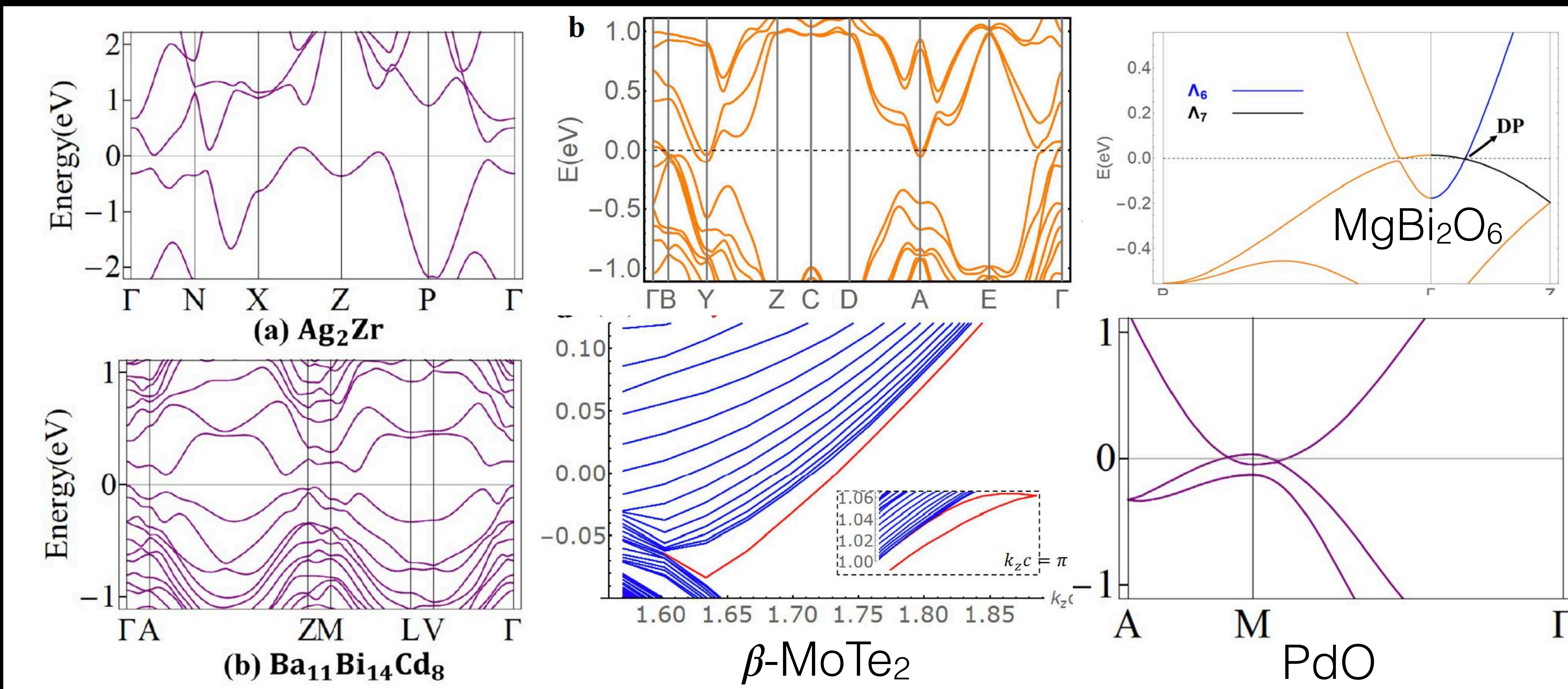
Materials analysis flow



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 Dirac SM

Non-magnetic materials search

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

1807.10271]

$\mathcal{SG}$	X_{BS}	Topological insulators
2	$\mathbb{Z}_3^2 \times \mathbb{Z}_4$	Ag_2F_5
11	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	BBeLi
12	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ag_4K_2 Ba_2Cd Bi_4Pb ,$PdSe_6$
14	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag_2Te
15	$\mathbb{Z}_2 \times \mathbb{Z}_4$	MoP_4[
51	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$AlPt_2$[
55	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Bi_6In_2
58	$\mathbb{Z}_4$	Bi_2Hf[
59	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag_3Sb
60	$\mathbb{Z}_4$	Au_2Pt
62	$\mathbb{Z}_4$	AsCdN 68],FS GeHfP Ge_2W P_2Zr[8 94],SiS AlLaP
63	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AgS_3T Ga[10 AlLa[1
64	$\mathbb{Z}_2 \times \mathbb{Z}_4$	As[115
65	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ag_3Te
69	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Be_2Zn
71	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AsTeT
72	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Br_2Hg
87	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Hf_5Te_4
121	$\mathbb{Z}_2$	Ag_2S_4
122	$\mathbb{Z}_2$	As_2Cd
123	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	$BaGe_3$
127	$\mathbb{Z}_4 \times \mathbb{Z}_8$	B_4Y[1
129	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$HfSb_2$[
136	$\mathbb{Z}_4$	Ag_5Cs
139	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Ag_2Zr $CaGe_2$

$\mathcal{SG}$	X_{BS}	Topological crystalline insulators
2	$\mathbb{Z}_3^2 \times \mathbb{Z}_4$	CsHg[256]
11	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$BaSb_2$[257],$MoTe_2$[258],
12	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$Al_4Cl_{51}Zr_{12}$[262],Al_4Na_4 $As_4Ba_3Zn_2$[269],Ba_3Cd_2 Cl_8NSc_5[277],NbP_2[278]
14	$\mathbb{Z}_2 \times \mathbb{Z}_4$	LaSbSe[285],AsSY[286],
51	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$GaPt_2$[287]
55	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ca_5Ga_2Sb_6$[288]
58	$\mathbb{Z}_4$	Bi_3RbS_5[289]
59	$\mathbb{Z}_2 \times \mathbb{Z}_4$	BrNTi[290]
62	$\mathbb{Z}_4$	$HgSr_3$[291],LaSbTe[292]
63	$\mathbb{Z}_2 \times \mathbb{Z}_4$	BaGe[293],BaSi[294], B [301] $Cd_2FSb_5Sr_5$[302],PbSr[3
64	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ca_5Ga_2N_4$[308],Li[309]
69	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$Ge_6Li_2Sr_4$[310]
71	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ba_3Bi_4Li_4$[311],Ba_3Li_4S
87	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Au_4Ti[312]
88	$\mathbb{Z}_4$	O_4PbPd_2[313]
123	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	As_3CsZn_4[314],As_3RbZn
129	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AsGeNb[316],GeHfS[317 GeSeZr[317],HfSSi[317,
137	$\mathbb{Z}_4$	Ba_2LiN[322]
139	$\mathbb{Z}_2 \times \mathbb{Z}_8$	$AsBa_2$[323],$AsCa_2$[324] Ba_2Bi[325],Ba_2Sb[326],
140	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Bi[330],$GePt_3$[331]
148	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Mo_3S_4[332]
164	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$BaSi_2$[333],BiTe[334],Bi_2
166	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$AsNaTe_2Zr_2$[340],As_3Cd As_3Cd_4Na[341],As_3Cd_4 ClZr[348],Hg[349],P[350] BrLa[351]
187	$\mathbb{Z}_3 \times \mathbb{Z}_3$	CHf[352],$InNbSe_2$[353,
189	$\mathbb{Z}_3 \times \mathbb{Z}_3$	AgAsCa[4, 356],AgCaP[GeLiY[358],AsLuPd[359
191	$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	B_2Zr[360]
193	$\mathbb{Z}_{12}$	Pb_3SZr_5[361]
194	$\mathbb{Z}_{12}$	AsHgK[362, 363],C[364]
221	$\mathbb{Z}_4 \times \mathbb{Z}_8$	Ba_3OPb[368, 369],CaPd NY[373],$OPbSr_3$[368, 3

$\mathcal{SG}$	Topological (semi-)metals
11	Br_9TeW[396],CBrHgNS[397],Li_7Sn_3[398],Mo_2S_2Sb[399]
15	BaI_4La[400]
51	AuCd[401],AuTi[402]
52	Ag_2BiO_3[403],Bi_3Sr_2[404]
55	Al_3Pd_5[405],Al_3Pt_5[406],BCl_6Sc_4[407], $Bi_9Ca_9Cd_4$[408], $Bi_9Ca_9Zn_4$[409],$Bi_9Cd_4Sr_9$[408],$In_5S_{13}Y_4$[410]
57	AlCaPd[411], BiK_2Sn[412]
58	$C_{60}K$[413]
59	Ag_3Sn[414]
60	F_4NaTi[415],O_2Re[416]
61	AgF_2[417]
62	$AgAuF_7$[418],AgF_3K[419],$AlPt_2$[420] Bi_3Ca_5[421],Bi_3Sr_5[422],Ca_5Sb_3[423] $GeNb_3Te_6$[424],$GePd_2Y$[425],N_3Nb_2[426],Nb_3Si[427] PdSbZr[428],$SiTa_3Te_6$[428],$AuLu_2$[429],GeLa[430],$GeLaPd_2$[430],$GeLuPd_2$[431],$LuPd_2Si$[432],LuPt[433], $LuPt_2Si$[434]
63	AgCa[435], AuCa[436], BiZr[437], Ga_3PdSr[438], Ga_5Zr_3[439], GeSc[440], GeY[441], HfSb[442],$K_3O_4Pd_2$[443],$K_3O_4Pt_2$[444],K_4P_3[445, 446], N_5NaTa_3[447],PdY[448],SiY[449], Sr_3Tl_5[450],LuSi[451],Al_6Re[452]
64	$AgCs_2F_4$[453],$Au_{10}Ca_4In_3$[454],Bi[455, 456],$LaSb_2$[457]
65	$C_7Re_2Sc_5$[458],$Ge_{10}La_7Li_8$[459]
71	$ReSi_2$[460]
74	Ag_2La[461],Au_2La[461],In_2La[462]
87	Ba_9In_4[463],$In_4Pd_{17}Se_4$[464],$Pt_{11}Zr_9$[465], $Pt_{12}Si_5$[466]
88	$Al_{21}Pt_8$[467],$CsFO_3S$[468],Ge_8Pd_{21}[469],LaO_4Pd_2[470]
123	$AgPPt_5$[471],$AlPPt_5$[471],$AsInPd_5$[472],$AsPd_5Tl$[473] $AsPt_5Tl$[473],As_2BaPd_2[474],BaP_2Pd_2[475],CaPb[476] CdPd[477],$CdPd_5Se$[478],CdPt[479],Cd_3Zr[480] $FKNb_4O_5$[481],HgPd[482],$HgPd_5Se$[483],HgPt[484],Hg_2Pt[484] $InPPd_5$[485],$InPPt_5$[485],PPd_5Tl[485],PPt_5Tl[485] PdTi[486],Pd_5SeZn[487],SiSr[488],Sr[489],C_2Re[490],AsLa[491],LaSb[492]
127	$AlSc_2Si_2$[493],Au_2Ca_2Pb[494],Au_2InY_2[495],B_2Ta_3[496] B_4W[497],C_2B_2Y[498],Ga_2MgSc_2[499],Ca_3Hg_2[500] Ga_2Nb_3[501],Ga_2Ta_3[502],Ge_2Hf_3[503],Hg_2Sr_3[504, 505] $InPd_2Y_2$[506],In_5Ti_2[507],$LiSi_2Y_2$[508],$PbPd_2Y_2$[509],N_2Re[510]
129	AgMgSb[511],AsNbSi[512],AsSiTa[513], BaMgSi[514],BiKMg[515],GeTeZr[516],MoNTa[517]
130	$AlMg_4Si_3$[518],Se_3Tl_5[519]
131	OPd[520]
136	$AlNb_2$[521],$AlTa_2$[522],Bi_2MgO_6[523], O_2Pb[524, 525],O_2Pd[526],O_2Pt[527],O_2Re[528]

Stron

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

Thanks!