

Title: Lattice homotopy: the physics of moving things around and calling them the same

Speakers: Hoi Chun Po

Series: Condensed Matter

Date: February 25, 2020 - 3:30 PM

URL: <http://pirsa.org/20020018>

Abstract: While the concept of topology is often introduced by contrasting oranges with bagels, the idea of topologically distinct quantum phases of matter is far more abstract. In this talk, we will focus on a more tangible form of topology that also arises in quantum condensed matter system: when the sites in a lattice are dragged around in a symmetric manner, what attributes of the lattice would remain unchanged? Such deformation can be viewed as the lattice analog of the familiar (mental) exercise of transforming a bagel into a coffee mug. We will first introduce the mathematical framework for identifying the topological classes of lattices, and then discuss how these invariants can constrain and inform the more abstract notion of topological phases of matter that emerge.

Lattice Homotopy:

moving things around &
calling them the same

Adrian (Hoi Chun) Po
MIT

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Perimeter Institute @Perimeter · Feb 14

On [#ValentinesDay](#), how about some love for the fascinating fields of physics? We created dating profiles for a bunch of them.
hubs.ly/H0n0QQn0 [#Physics](#) [#STEM](#) [#Love](#)



CONDENSED MATTER

I am complex, but don't let that scare you off. Sometimes that means I'm scattered, but under great pressure, I can do amazing things. Exotic and unusual, I'm looking for someone who can help harness my untapped potential.

Hobbies: Packing lots of stuff into teeny, tiny spaces, just to see what happens.

Likes: Liquids right now, but it's just a phase.



5



12



Confession: this slide inspired by Liujun's talk last week :)

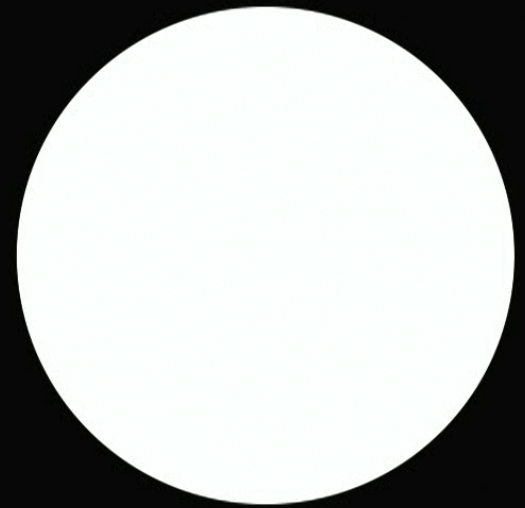
Packing in teeny, tiny spaces

Atoms in a crystal



20 nm

A strand of human hair



20 μm

vs

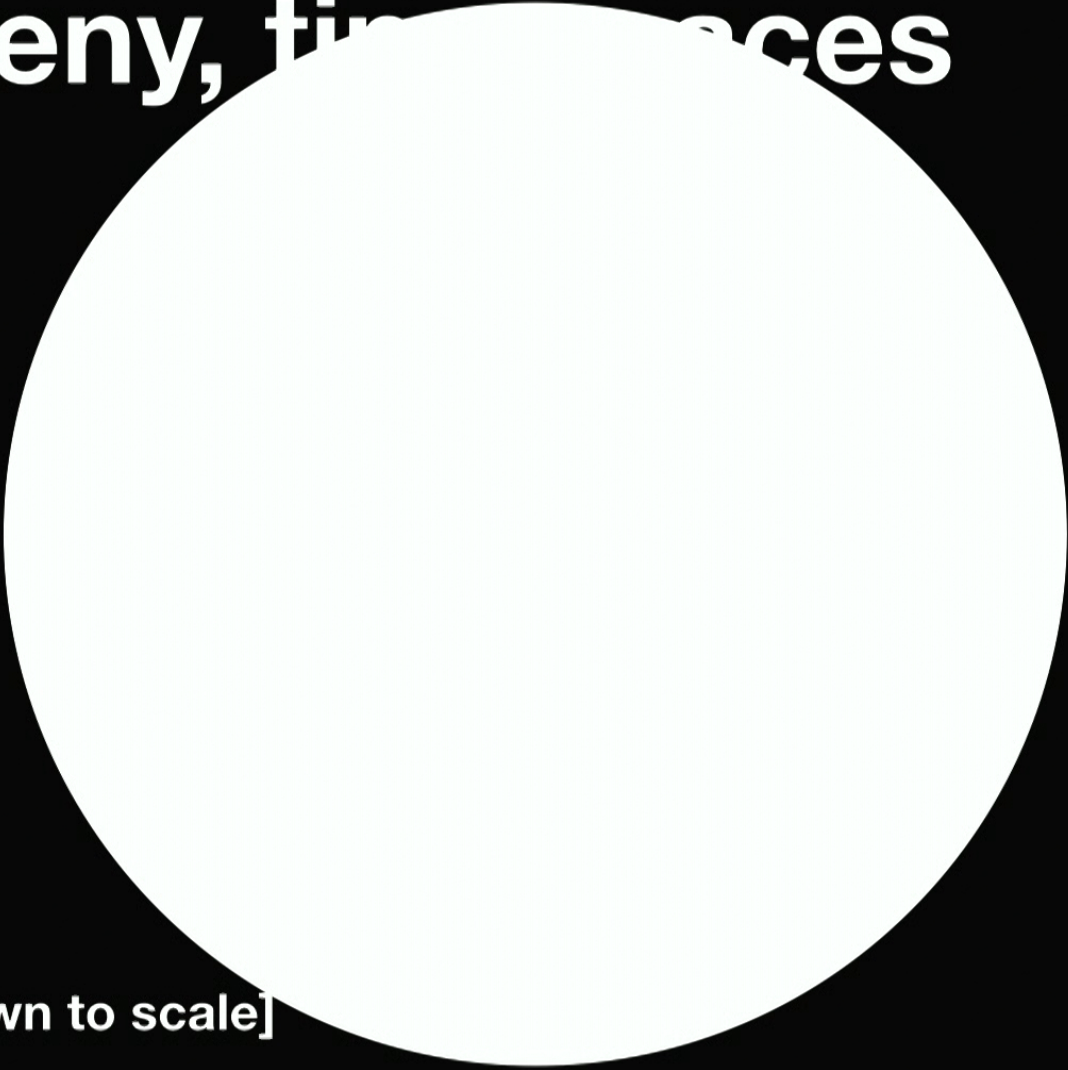
[Not drawn to scale]

Packing in teeny, tiny spaces


1 pixel

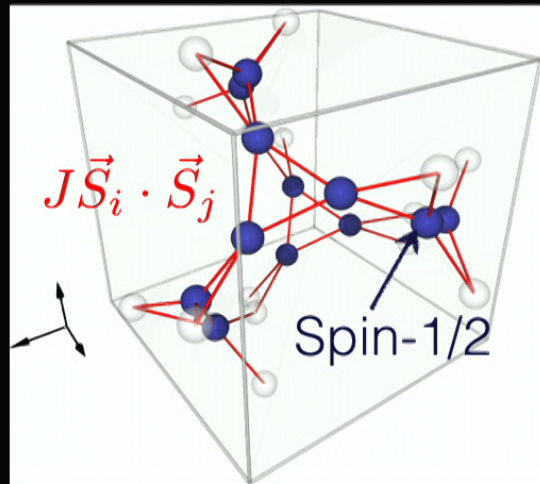
VS

[Drawn to scale]



microscopic
Packing lots of stuff into teeny, tiny spaces,
just to see what happens.
Macroscopic

THE problem of quantum many-body problems

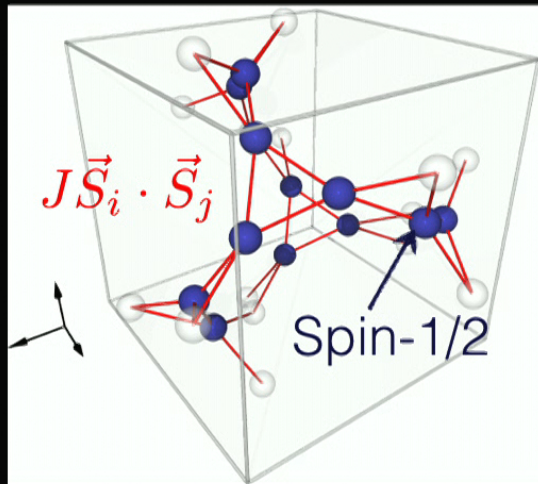


Consider the anti-ferromagnetic Heisenberg model on the hyperkagome lattice.

Find its ground state(s). [5 pts]

Simple to state, (almost) impossible to answer

Why simple?



- O(1) number of parameters
 - What degrees of freedom
 - How they are arranged
 - How they are coupled

Why impossible?

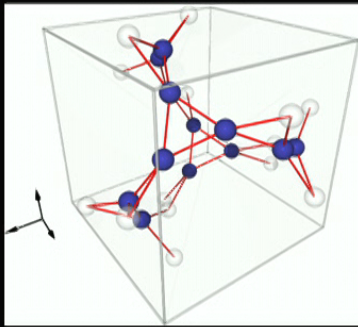
- V spin-1/2 $\Rightarrow$ dimension = 2^V
- $1\mu\text{m}$ sample in 2D $\Rightarrow 2^{10^8} \simeq 2^{10^8}$ GB
- Total data “stored” in our world $\lesssim 2^{40}$ GB



Parameters

“The Convenient
illusion of Hilbert space”
[Poulin et al PRL 2011]

**Packing in
teeny, tiny spaces**

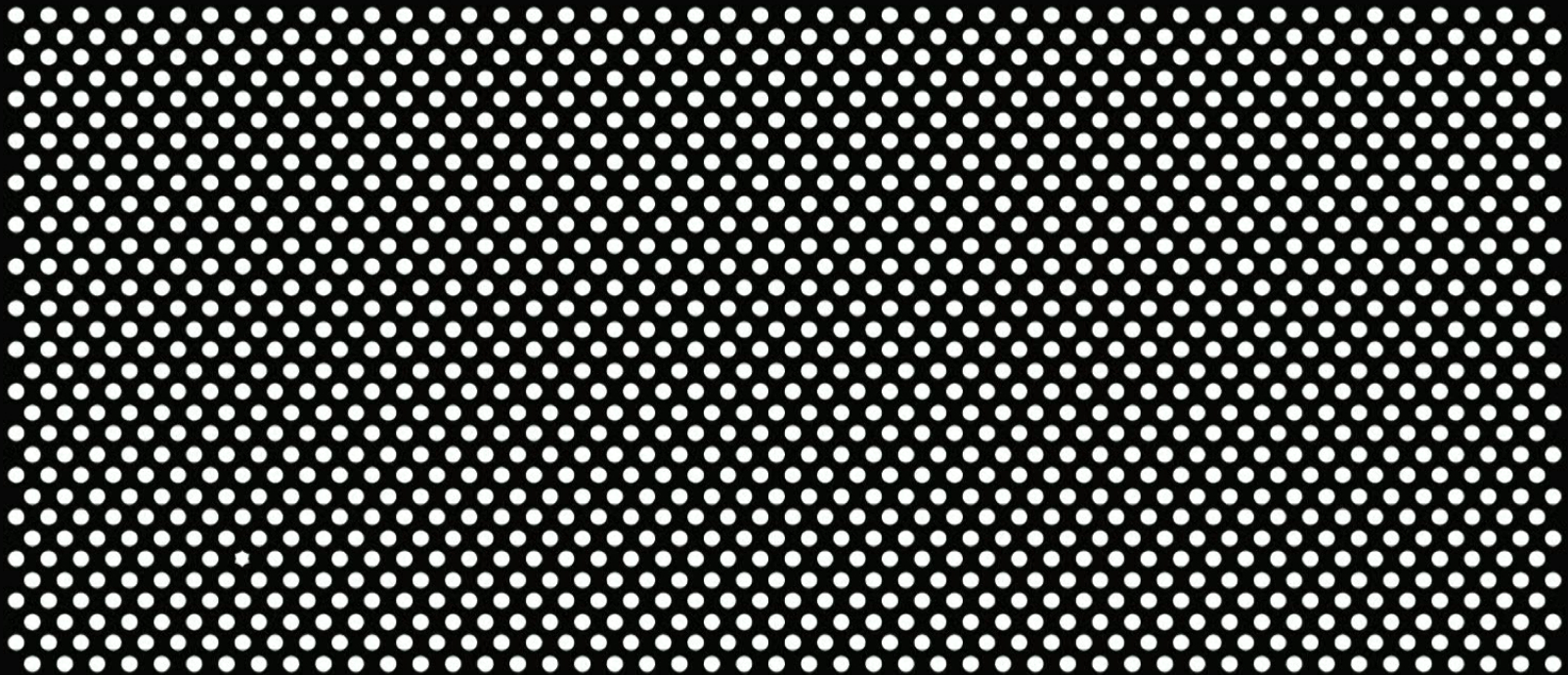


What happens?



The
Grand Problem

Packing in teeny, tiny spaces: What information is important?





CONDENSED MATTER

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maybe Psychology!

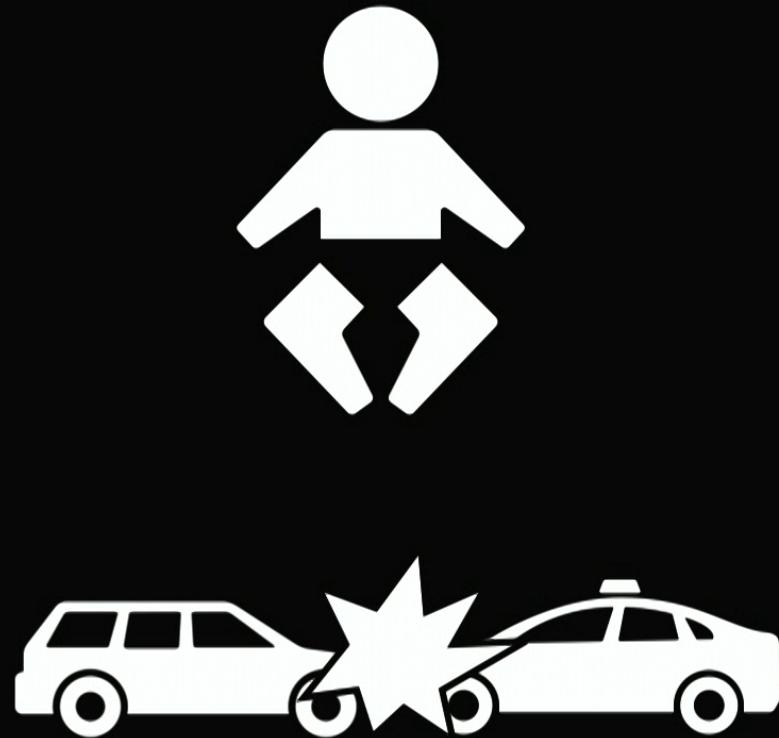
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Sensorimotor play (Piaget)

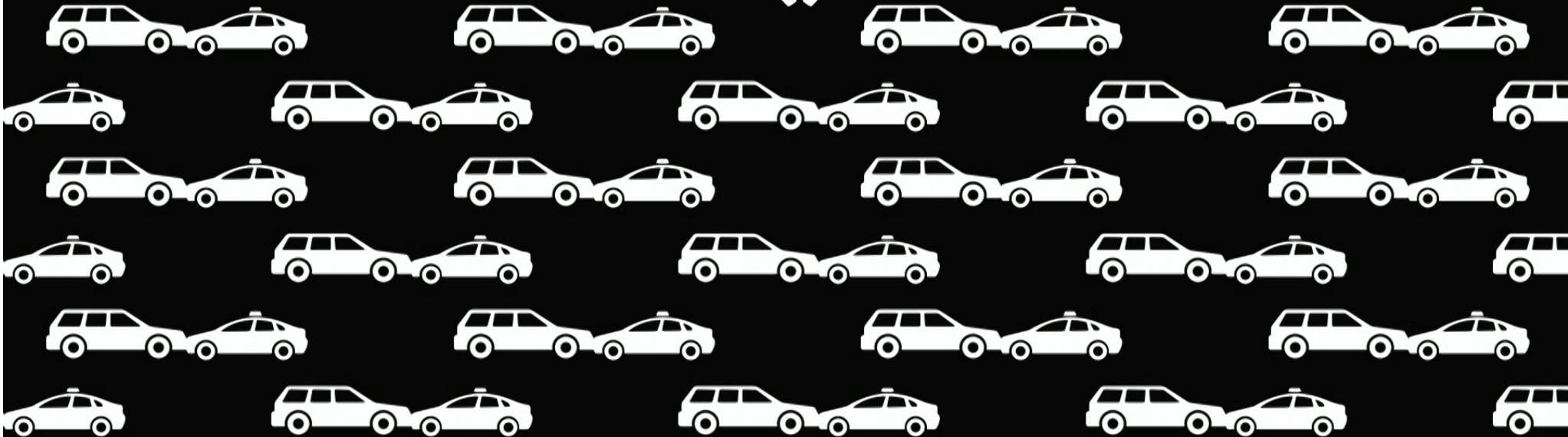


Sensorimotor play (Piaget)



Back to condensed matter...

What are the invariants?

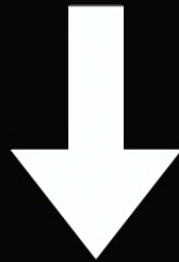


Overarching theme

How does the conventional notion of topology interact with our understanding on quantum ground states?

Lattice homotopy

What are the robust (topological) data in a lattice under smooth, symmetric deformation?



What are their implications on quantum phases of matter?

Outline aka take-homes

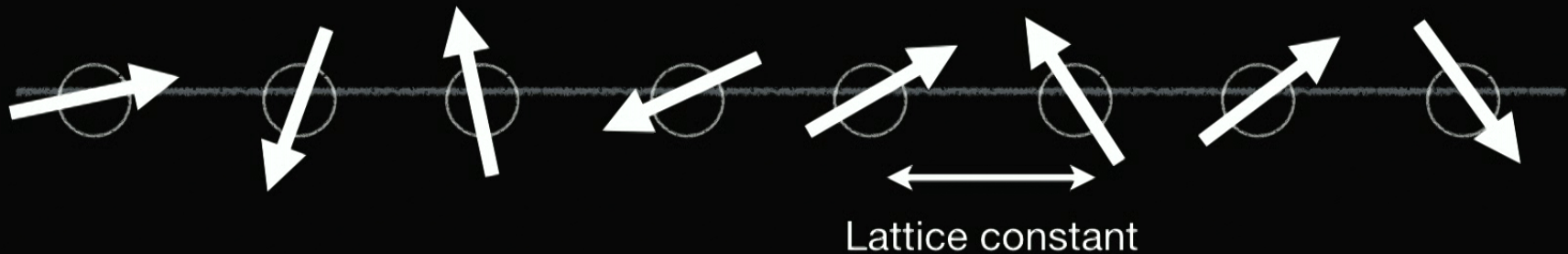
- Lieb-Schultz-Mattis theorem: no-go for “boring” phases
 - A motivating example of lattice constraints
- Lattice homotopy: general framework & quantum magnets
 - Generalization of Lieb-Schultz-Mattis to utilize the full space group
- Application to atomic insulators
 - Uncovering topologically nontrivial quantum materials

Lieb-Schultz-Mattis (LSM)

[1D result: Ann. Phys. 1961]

[Higher dimensions: Affleck PRB 1988; Oshikawa PRL 2000; Hastings, PRB 2004]

- Setup: 1D spin chain w/ translation & spin-rotation sym.



- Microscopic: a spin-1/2 per unit cell
- Macroscopic: ground state must be
 - (i) Symmetry breaking; or
 - (ii) Gapless

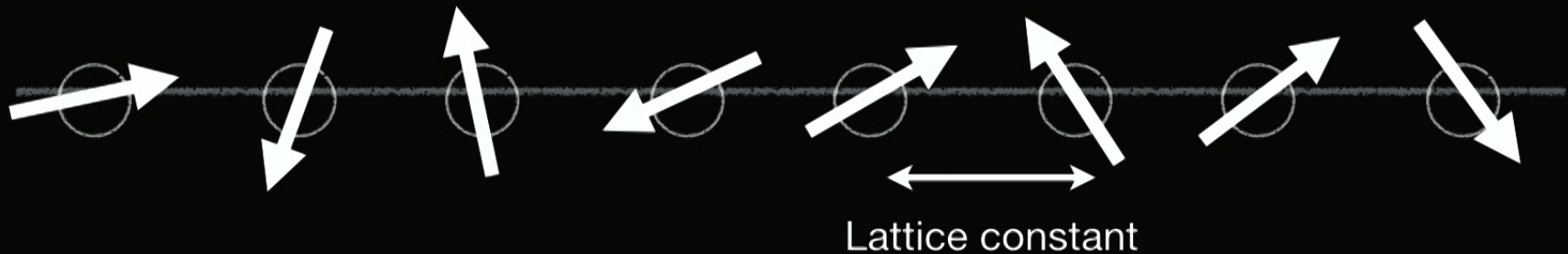
Gapped, unique ground state

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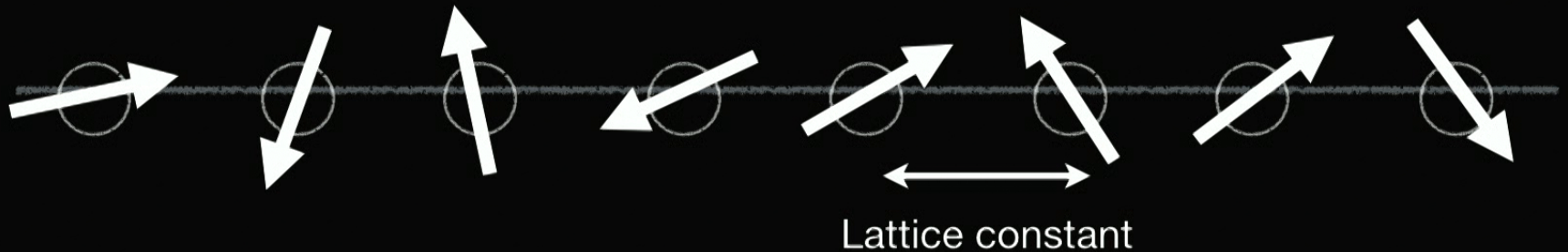


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~~Gapped, unique ground state~~

NON Lieb-Schultz-Mattis

- Setup: 1D spin chain w/ translation & spin-rotation sym.

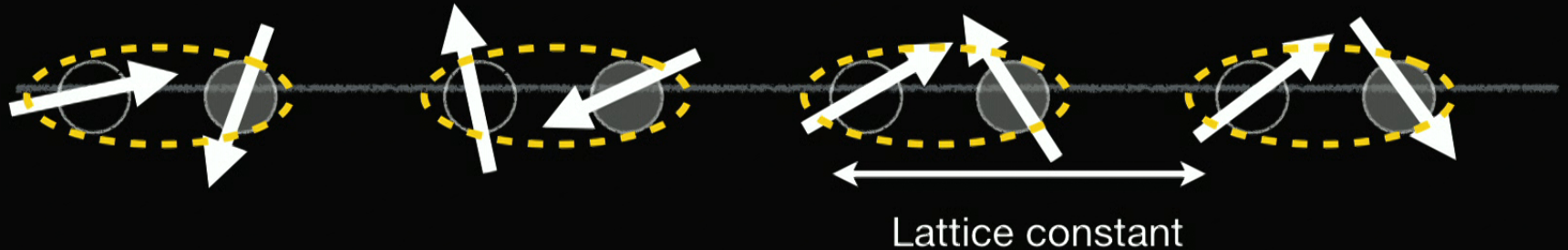


- Microscopic: a **spin-1** per unit cell
- Macroscopic: **ground state can be gapped and symmetric**
 - Haldane/ AKLT chain, an early example of a symmetry-protected topological order

[Haldane PRL 1983, Affleck et al PRL 1987]

NON Lieb-Schultz-Mattis II

- Setup: 1D spin chain w/ translation & spin-rotation sym.



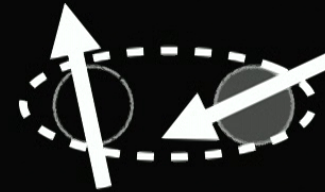
- Microscopic: **two spin-1/2's** per unit cell
- Macroscopic: **ground state can be gapped and symmetric**
 - **Independent singlets**

Heuristic explanation

- Consider a single unit cell



VS



Spin-1/2
two degenerate states

Two spin-1/2's

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

Non-degenerate w/ singlet

Heuristic explanation

- Translation sym.: extend to a ring of odd length L



vs



$$\frac{1}{2} \otimes \frac{1}{2} \otimes \dots \otimes \frac{1}{2} = \dots \oplus \frac{L-2}{2} \oplus \frac{L}{2}$$

$$0 \otimes 0 \otimes \dots \otimes 0 = 0$$

Always half-integer:
any state is degenerate

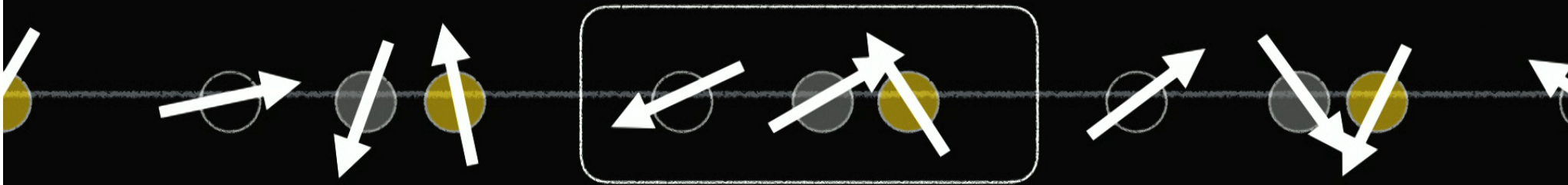
Non-degenerate
ground state is possible

Lattice homotopy: a primer

Micro. data:

- (i) Lattice translation and spin-rotation symmetries
- (ii) Half-integer vs integer spin per unit cell

E.g. Three spin-1/2's in a unit cell

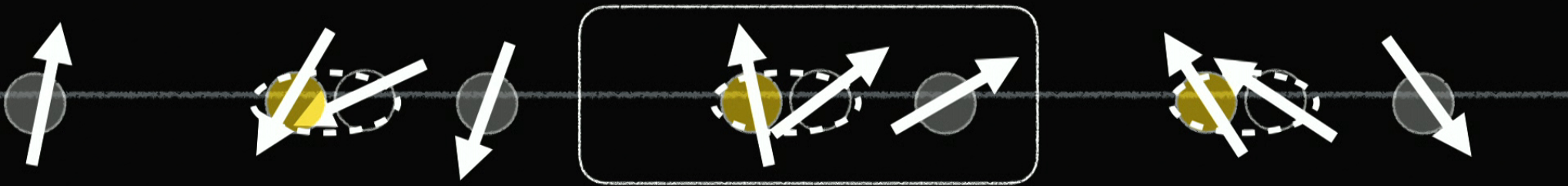


Lattice homotopy: a primer

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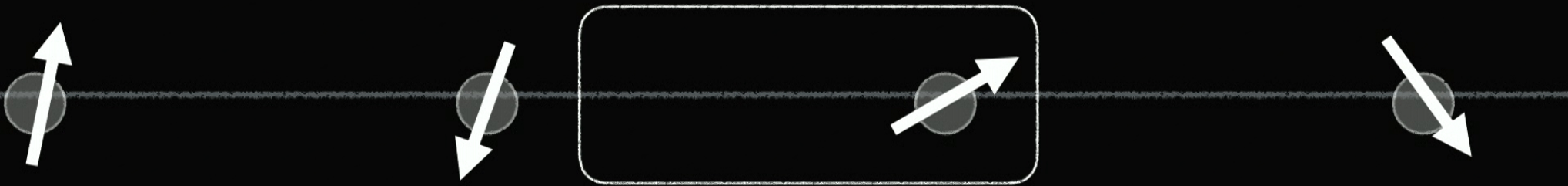


Lattice homotopy: a primer

Topological micro. data:

- (i) Lattice translation and spin-rotation symmetries
- (ii) Half-integer vs integer spin per unit cell

E.g. Half-integer spin in a unit cell



Is this the only invariant?



CONDENSED MATTER

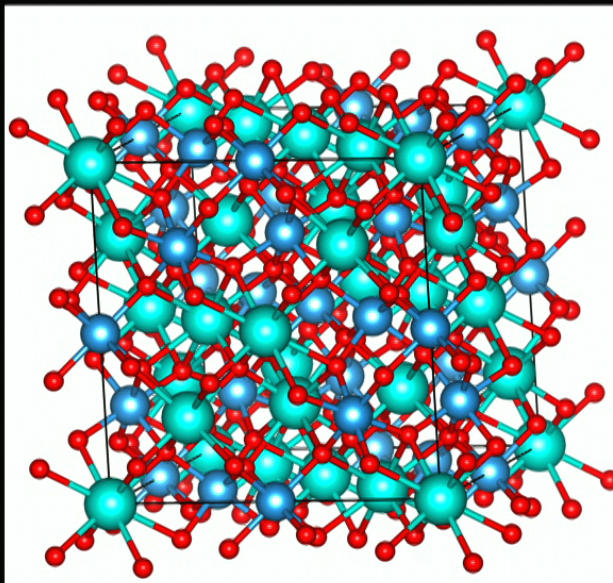
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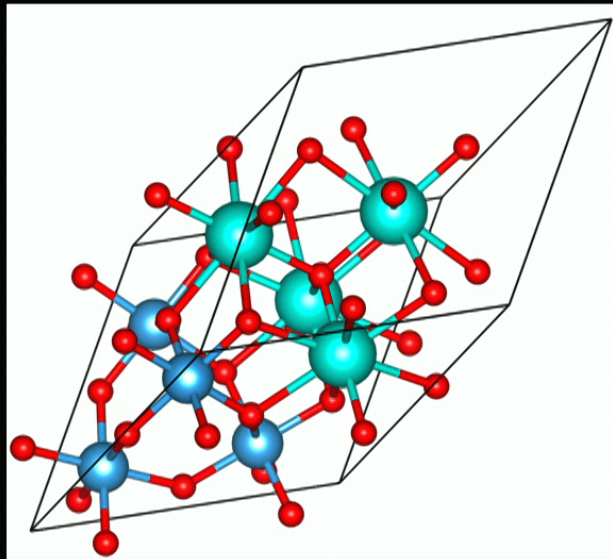
Materials can be complex...



Yb₂Ti₂O₇: spin liquid candidate
[Ross et al PRX 2011]

[crystal data from Springer Materials & Materials Project; visualization w/ VESTA]

Materials can be complex...



4 Kramers doublet
per unit cell

Yb₂Ti₂O₇: spin liquid candidate
[Ross et al PRX 2011]

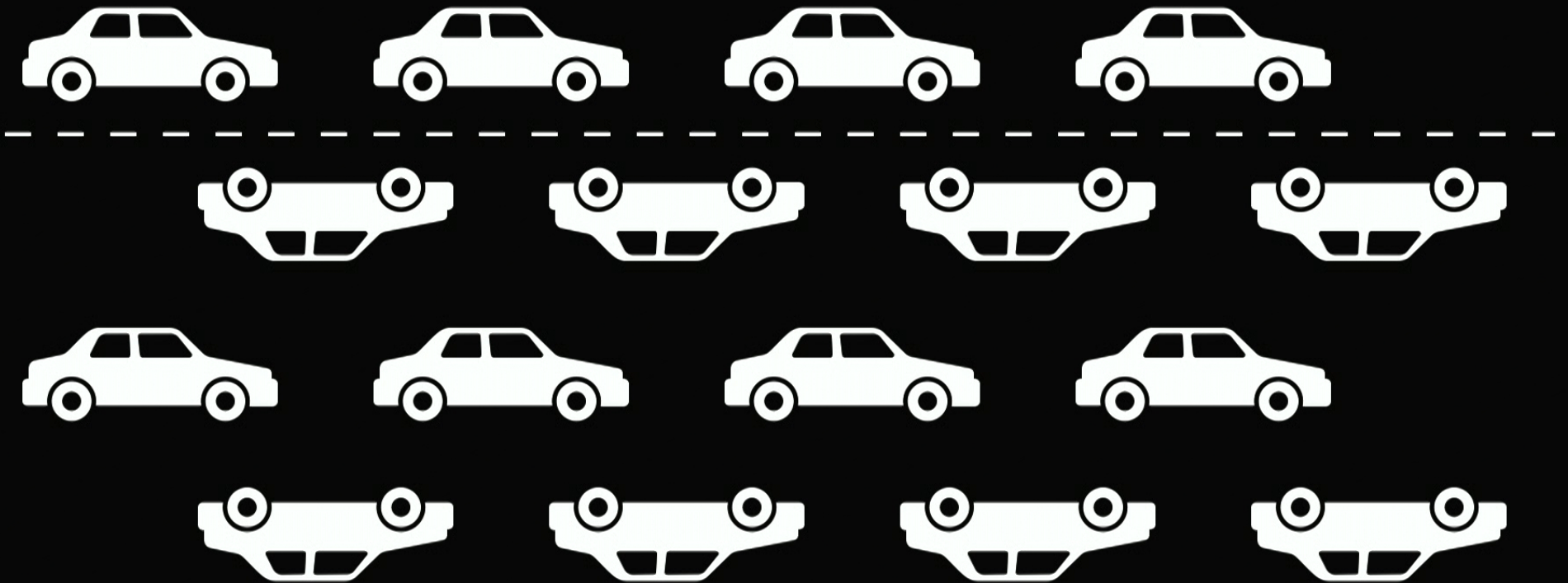
[crystal data from Springer Materials & Materials Project; visualization w/ VESTA]

Complex, but orderly:

make better use of spatial symmetries

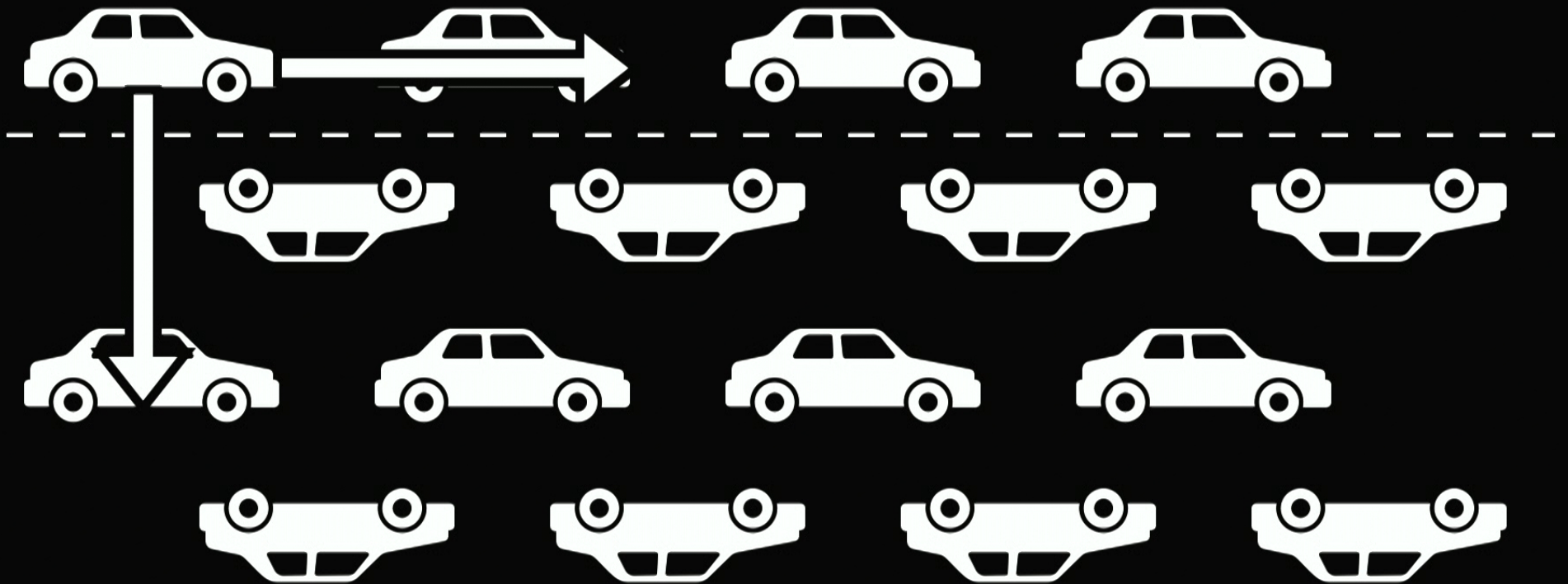
Nonsymmorphic symmetry

E.g.: Glide = reflect & half-translation



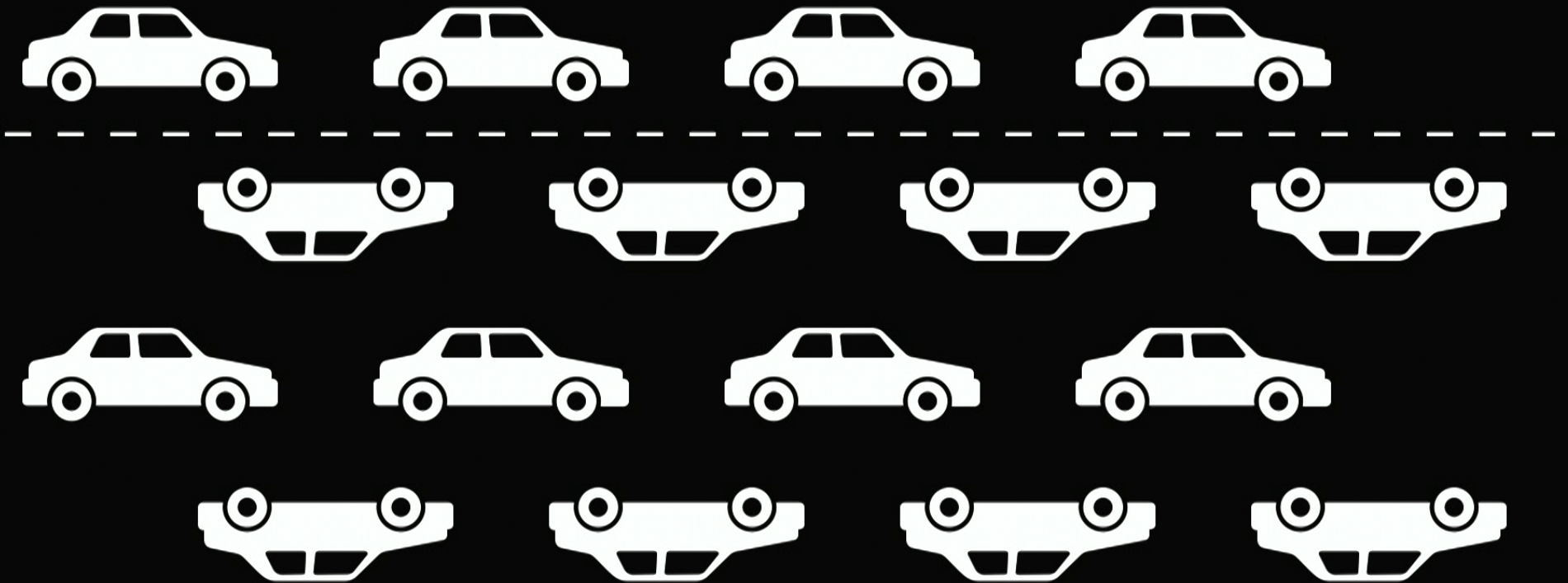
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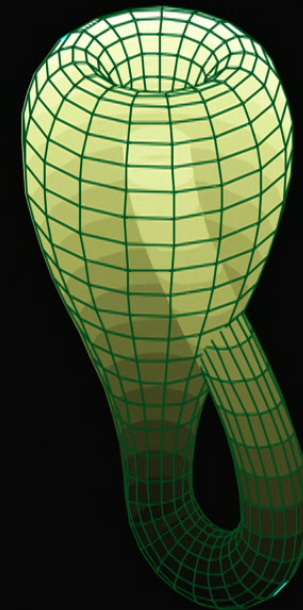
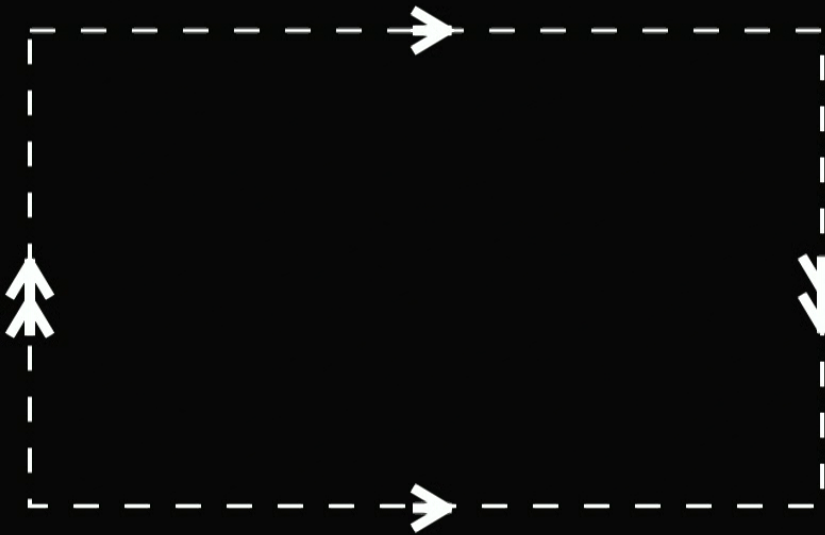
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Nonsymmorphic LSMs

E.g.: Glide = reflect & half-translation

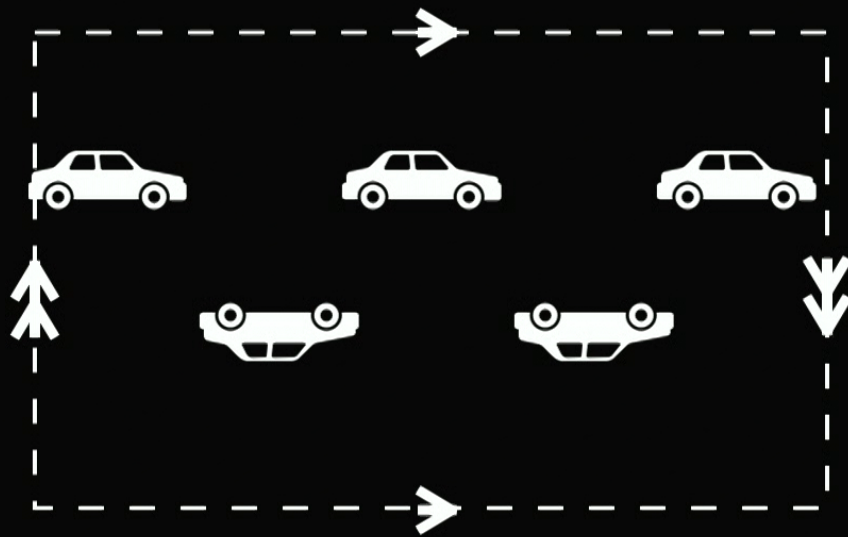


Klein bottle

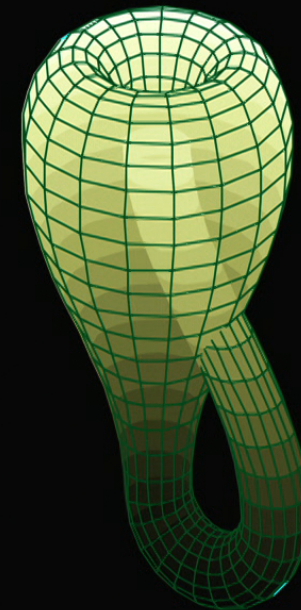
[fig. from wiki]

Nonsymmorphic LSMs

E.g.: Glide = reflect & half-translation



5 cars = $2\frac{1}{2}$ unit cells!

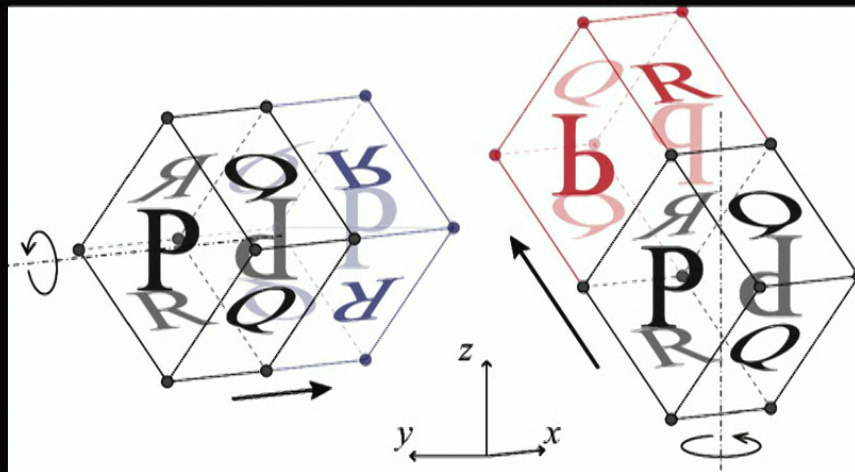


Klein bottle

[fig. from wiki]

Nonsymmorphic LSMs

- Tightened constraints by putting any 3D crystal onto one of the 10 “Bieberbach manifolds”



[Watanabe, HCP, Vishwanath, Zaletel PNAS 2015]

[Also earlier: Parameswaran Nat Phys 2013, Roy 1212.2944]

Table 1. Summary of $\nu_{\min}$ for elementary space groups

ITC no.	Key elements	Minimal filling			Manifold name
		AI*	Ent [†]	Bbb [‡]	
1	(Translation)	2	2	2	Torus
4	2_1	4	4	4	Dicosm
144/145	$3_1/3_2$	6	6	6	Tricosm
76/78	$4_1/4_3$	8	8	8	Tetracosm
77	4_2	4	4	4	
80	4_1	4	4	4	
169/170	$6_1/6_5$	12	12	12	Hexacosm
171/172	$6_2/6_4$	6	6	6	
173	6_3	4	4	4	
19	$2_1, 2_1$	8	4	8	Didicosm
24	$2_1, 2_1$	4	2	4	
7	Glide	4	4	4	First amphicosm
9	Glide	4	4	4	Second amphicosm
29	Glide, 2_1	8	4	8	First amphidicosm
33	Glide, 2_1	8	4	8	Second amphidicosm

*The minimal filling required to form a symmetric atomic insulator.

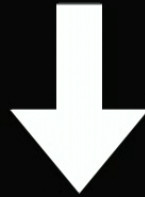
[†] $\nu_{\min}$ obtained in *Extension to 3D Symmorphic and Nonsymmorphic Crystals*. Bounds are not tight for nos. 19, 24, 29, and 33.

[‡] $\nu_{\min}$ obtained in *Alternative Method: Putting Sym-SRE Insulators on Bieberbach Manifolds*. All bounds are tight.

LSM summary

Micro. topological data:

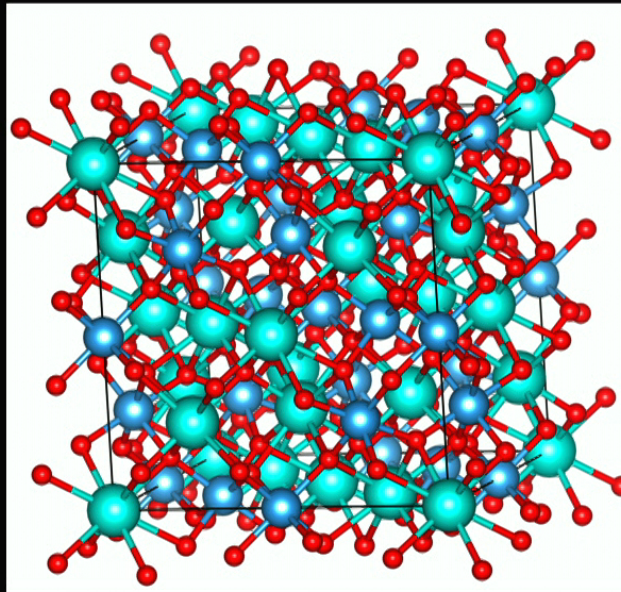
- (i) Half-integer spin per “fundamental domain”



Macro. manifestation: quantum ground state must be

- (i) Symmetry-breaking; or
- (ii) Topologically ordered (e.g. gapped spin liquids); or
- (iii) Gapless

Downside...

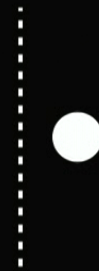


Not covered by this generalization

Outline aka take-homes

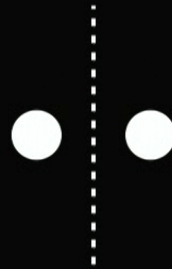
- ✓ Lieb-Schultz-Mattis theorem: no-go for “boring” phases
 - A motivating example of lattice constraints
- Lattice homotopy: general framework & quantum magnets
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Some more crystalline sym.



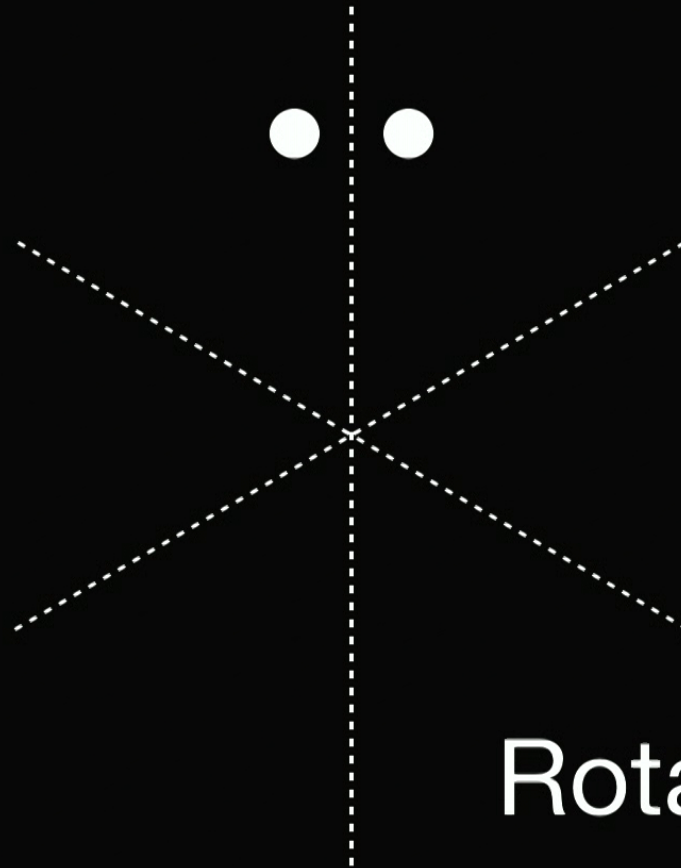
Mirror

Some more crystalline sym.



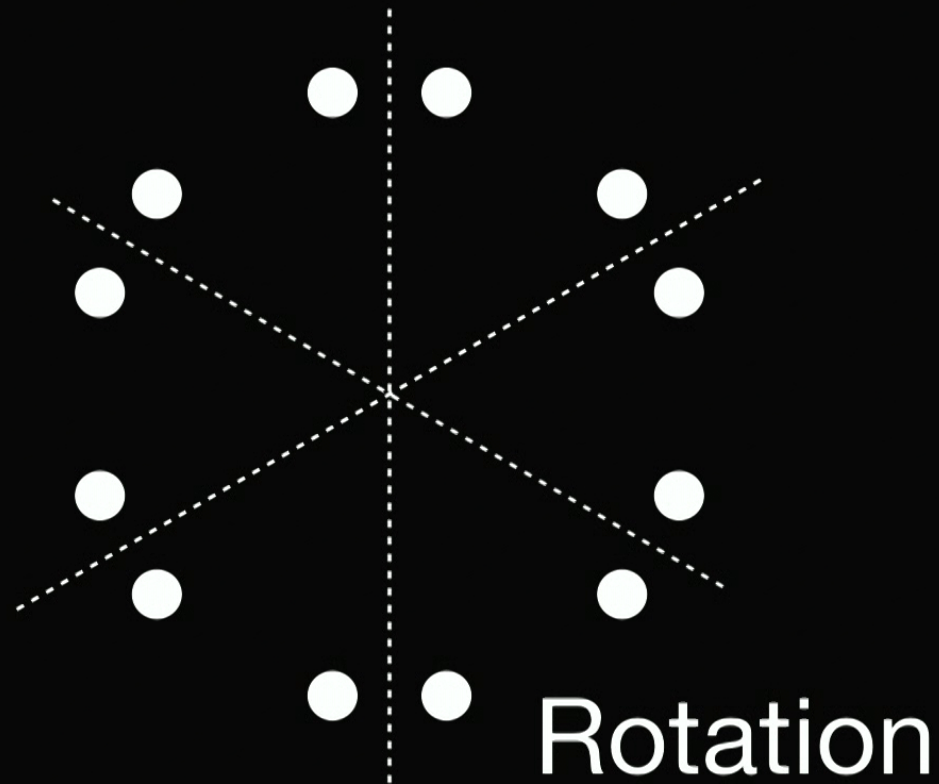
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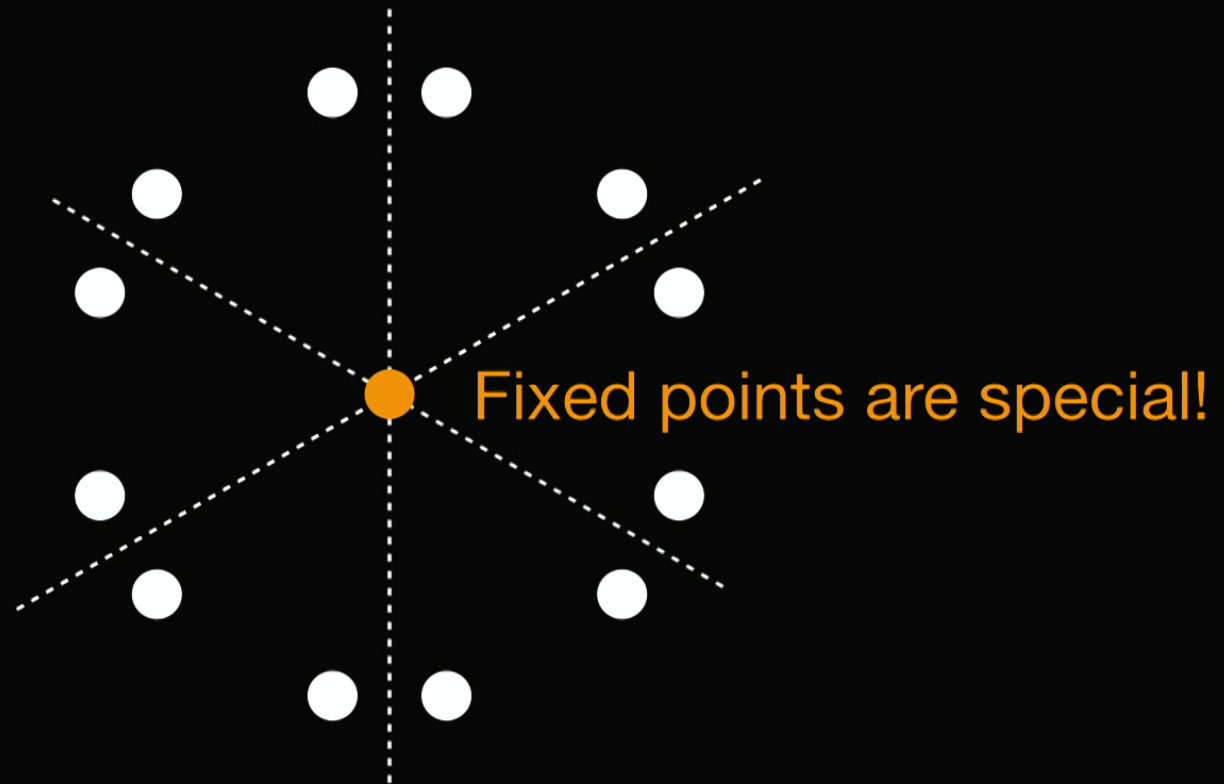


Rotation

Some more crystalline sym.

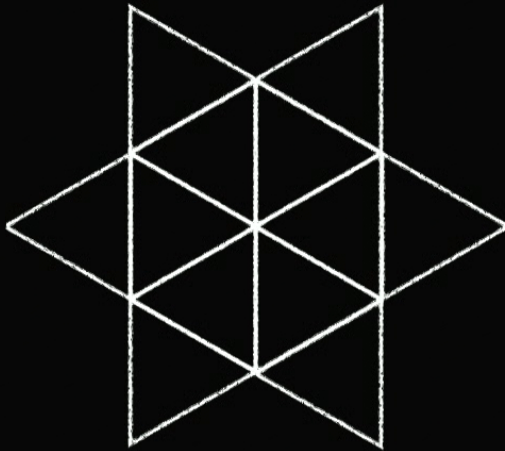


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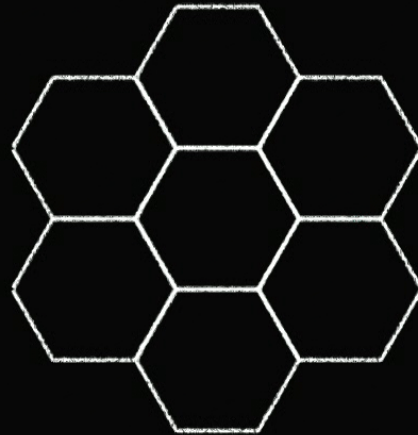


Lattices of fixed points

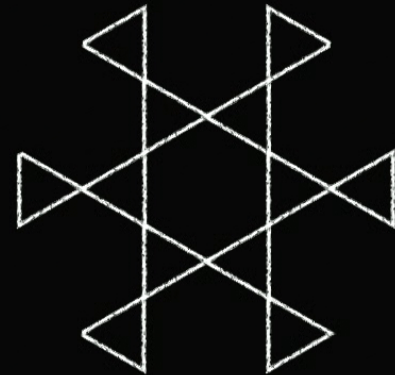
Same symmetries: C_6 rotation, mirror, and lattice translations



Triangular

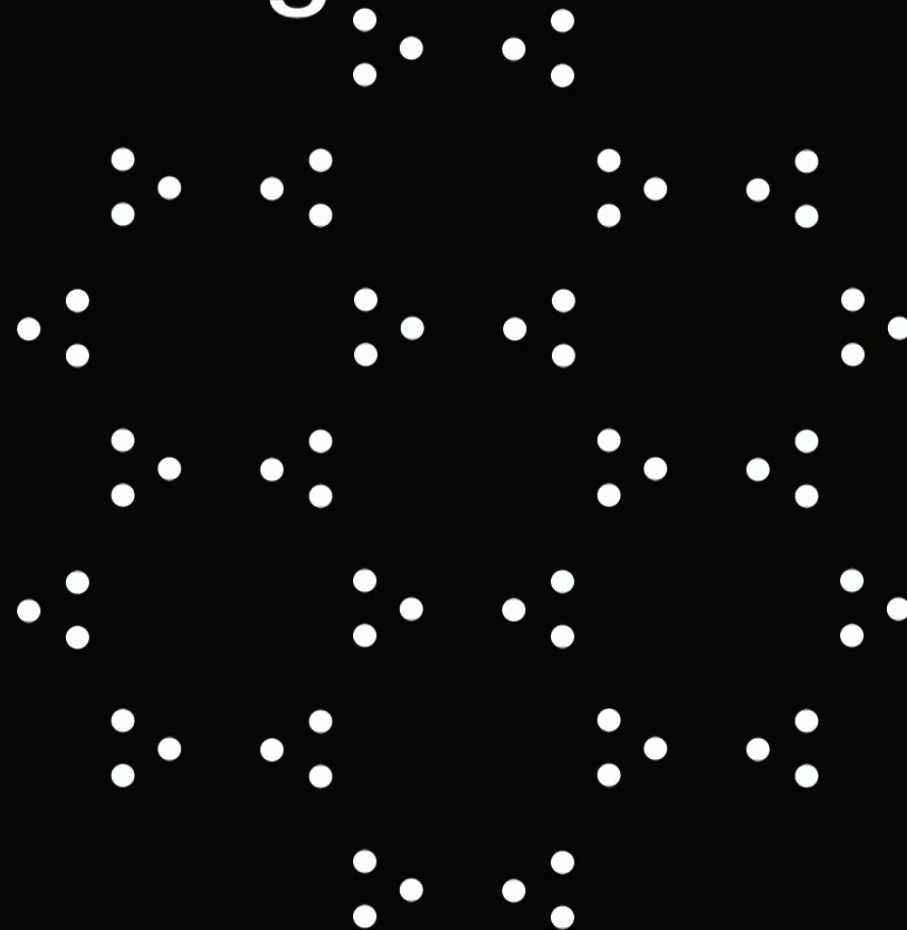


Honeycomb

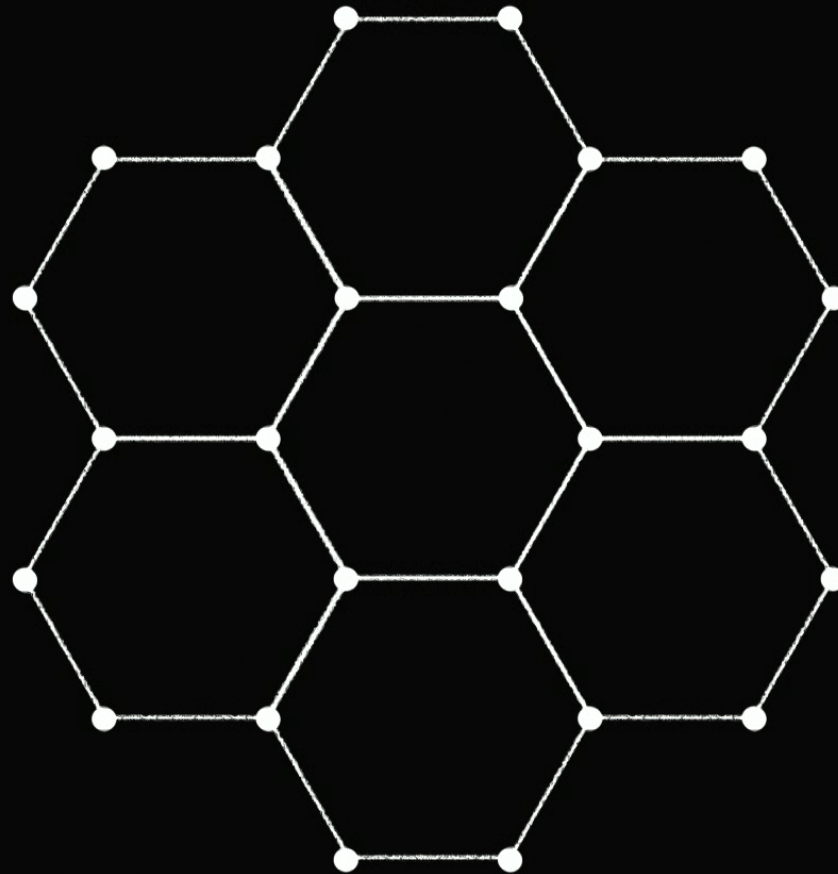


Kagome

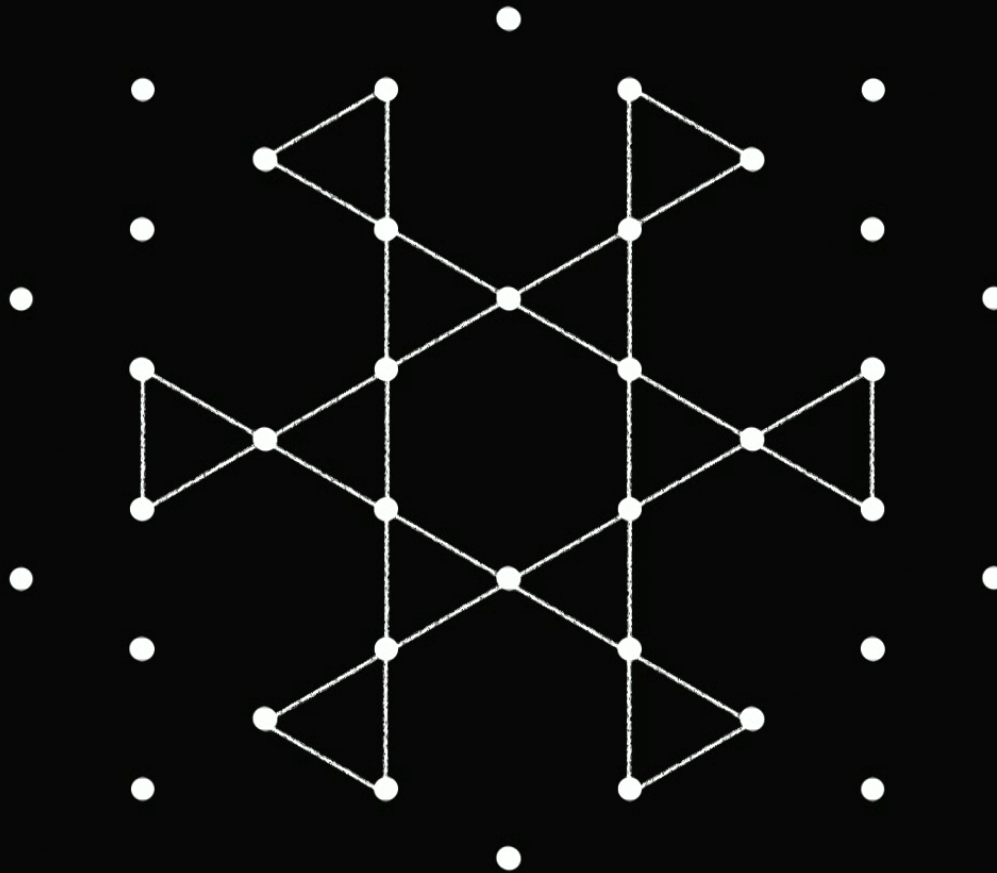
Moving sites around



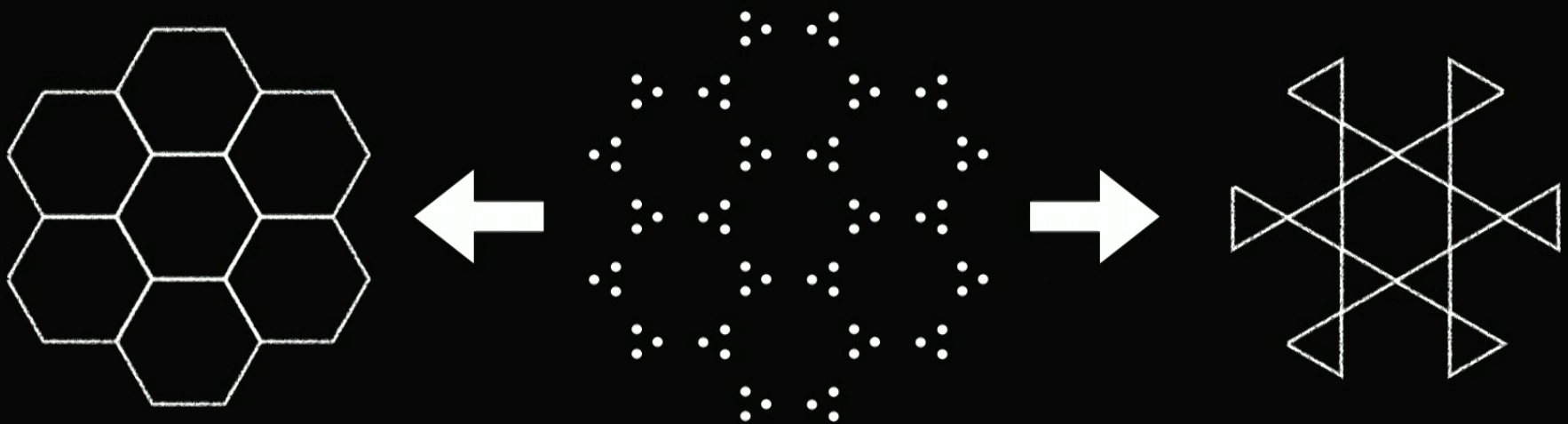
Moving sites around



Moving sites around



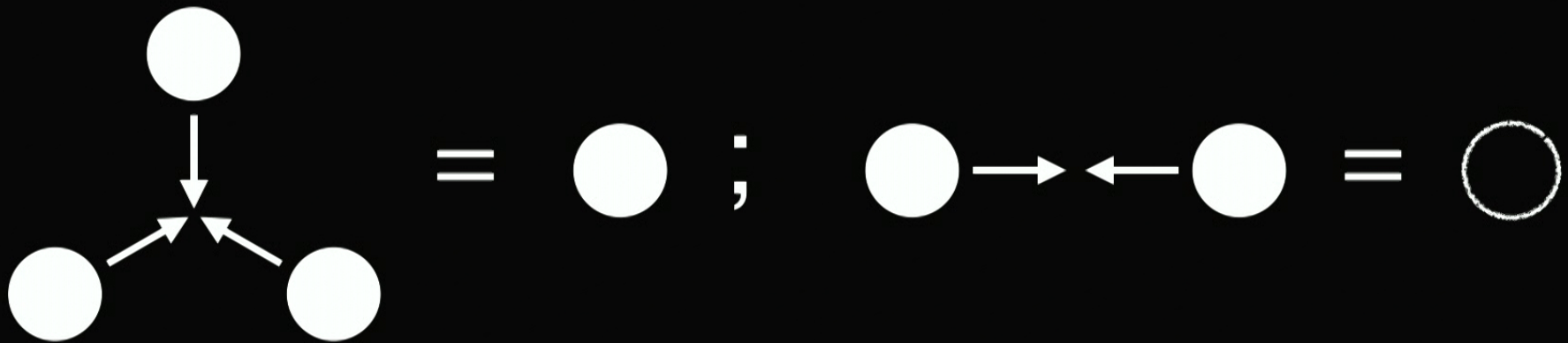
Moving sites around



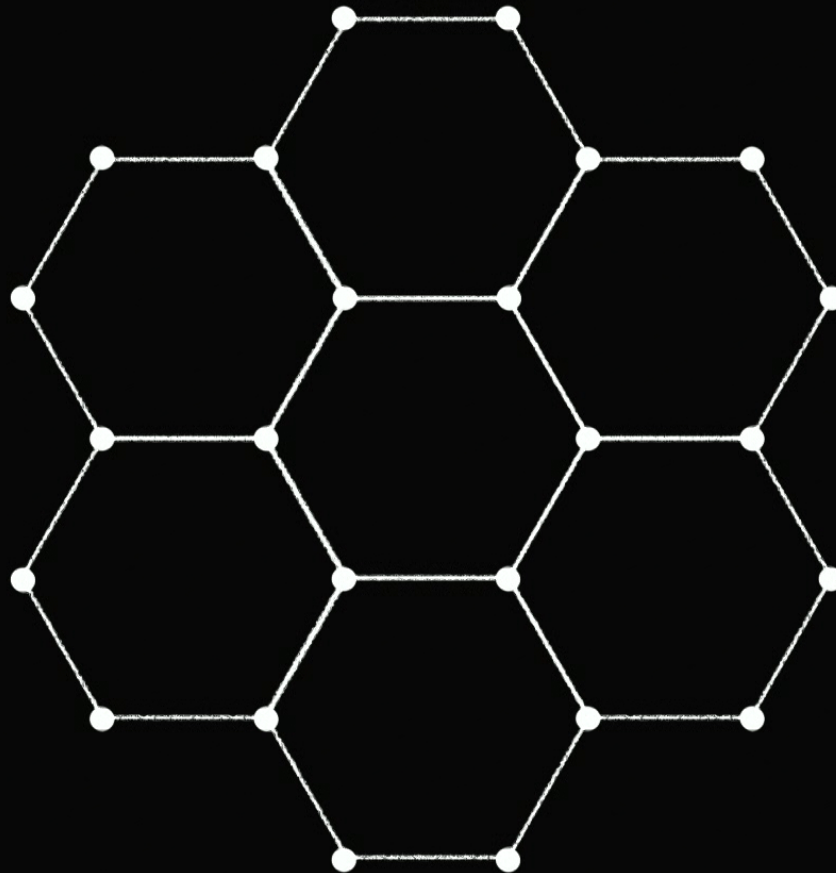
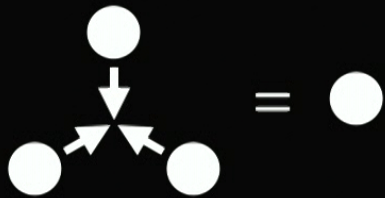
Are they the same lattice of *spins*?

Fusion of spins

● = half-integer ○ = integer

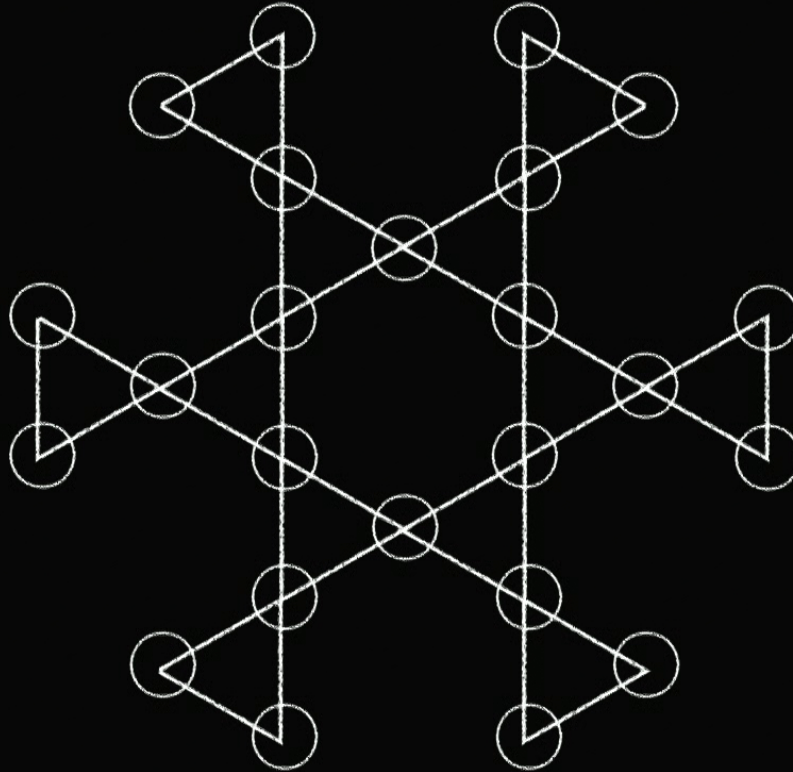


Moving *spins* around

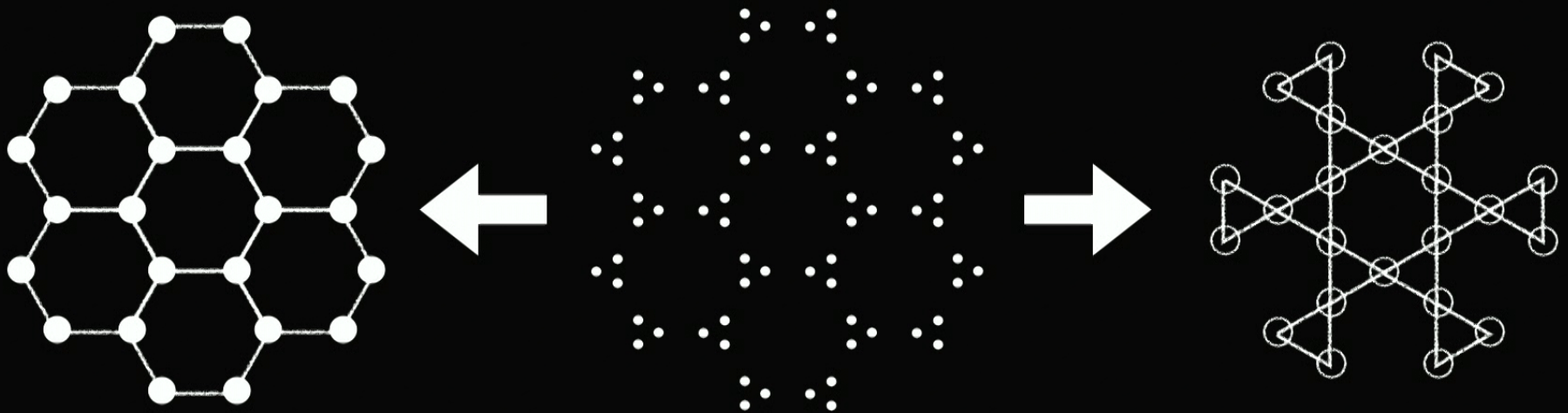


Moving *spins* around

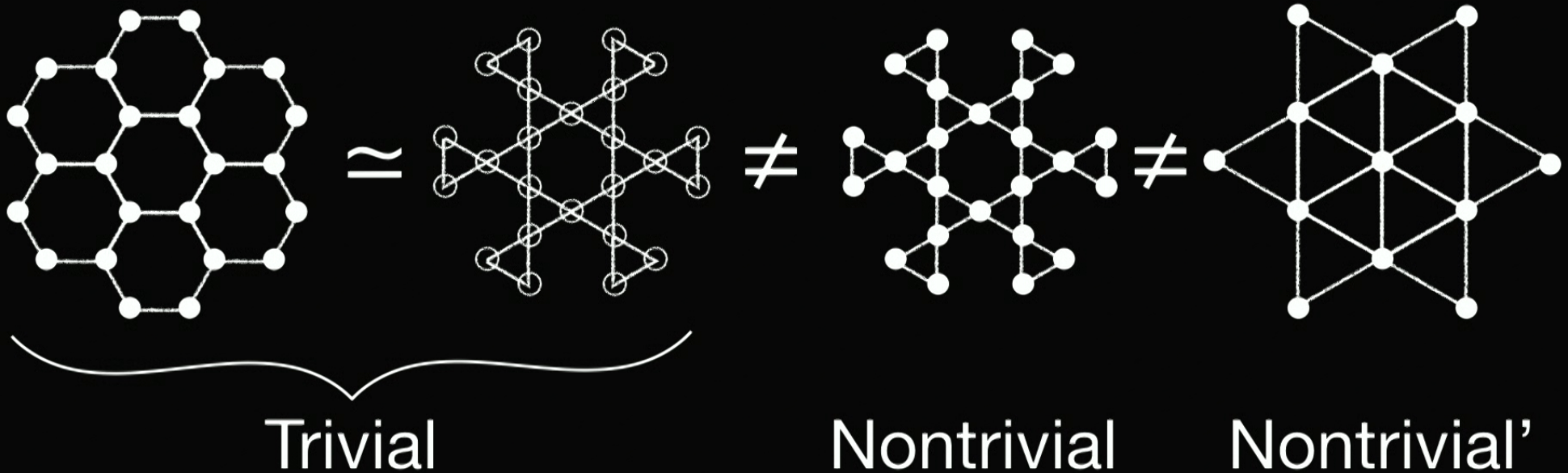
$$\bullet \rightarrow \leftarrow \bullet = \bigcirc$$



Lattice homotopy equivalence



Lattice homotopy equivalence



Note: we've gone beyond the "total count"

Lattice homotopy: systematics

[HCP, Watanabe, Jian, Zaletel PRL 2017]

- Lattice data: $(\Lambda, \{\omega_{\mathbf{x}}\})$
 - Λ : a sym. set of points in space (i.e. lattice sites)
 - $\omega_{\mathbf{x}} \in \mathbb{Z}_2 = H^2(\text{SO}(3), \text{U}(1))$ proj. rep. (i.e. integer vs half-integer spin)
- Composite: $(\Lambda_1, \{\omega\}_1) + (\Lambda_2, \{\omega\}_2)$
- Special lattices of fixed points $\Rightarrow$ finite set of generators
- LH-related lattice $\Rightarrow$ equivalence relations

Lattice homotopy: 2D

[HCP, Watanabe, Jian, Zaletel PRL 2017]

Lattice homotopy	Wallpaper group No. [20]
$\mathbb{Z}_2$	1, 4, 5, 13, 14, 15
$(\mathbb{Z}_2)^2$	3, 8, 12, 16, 17
$(\mathbb{Z}_2)^3$	7, 9, 10, 11
$(\mathbb{Z}_2)^4$	2, 6

Generalized version: 3D with $\mathbb{Z}_n$ projective rep.

Generalized LSM

Conjecture: lattice homotopy nontrivial $\Rightarrow$ LSM-type constraint on the quantum many-body ground state

- ▶ (Physicists') proof for a more restricted setting

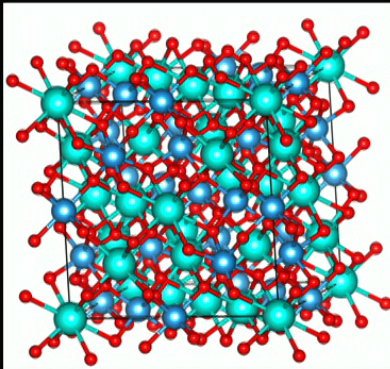
[HCP, Watanabe, Jian, Zaletel PRL 2017]

- ▶ Proved for general quantum magnets

[Else, Thorngren 1907.08204]

[Also, a large body of work on related problem of crystalline SPT:

Cheng...Bonderson, Hermele, Xie, Fu,
Else-Thorngren, Shiozaki, Xiong, Gomi,...]



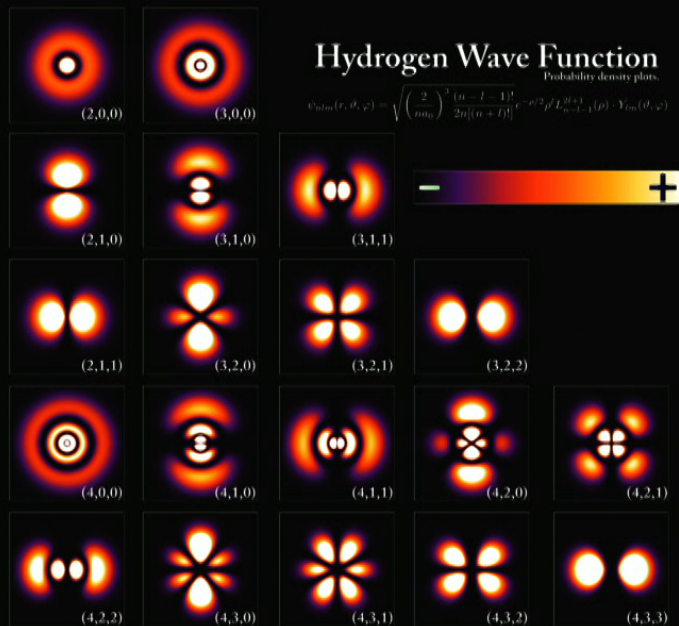
Upshot: this is lattice-homotopy nontrivial!

Outline aka take-homes

- ✓ Lieb-Schultz-Mattis theorem: no-go for “boring” phases
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Electronic insulators

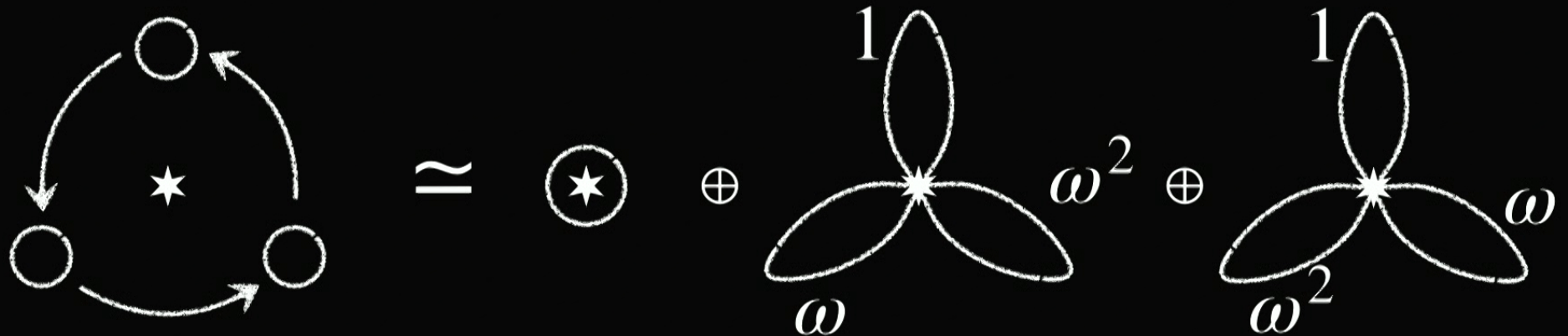
- Replace spin degrees of freedom by electronic orbitals



[Fig from Wiki]

Reduction in a crystal environment
(e.g. angular momentum defined mod n)

“Fusion” of atomic orbitals



$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \simeq \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}; \quad \omega = e^{i\frac{2\pi}{3}}$$

Lattice homotopy for atomic insulators

[Else, HCP, Watanabe PRB 2019]

[Related idea: Zak PRB 1981, Bradlyn et al Nature 2017]

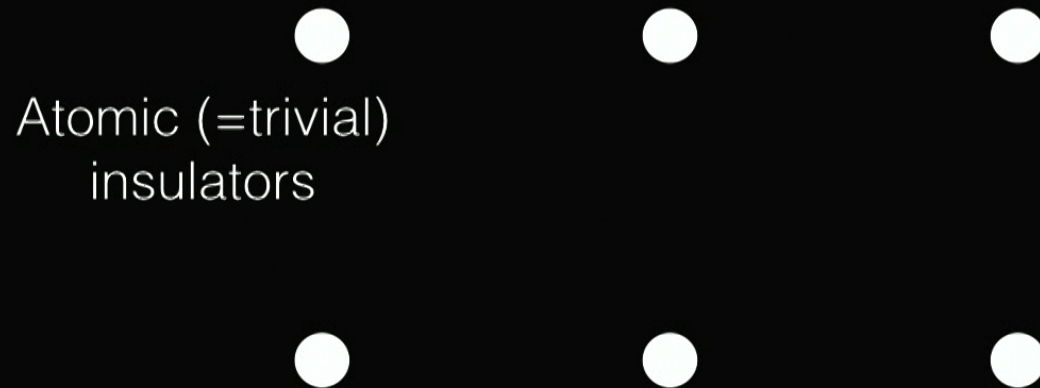
- Microscopic data: symmetries, lattice, and orbitals
- Equivalence from moving sites around and fusion (re-interpretation) of orbitals
- Output: finitely generated abelian group $\mathbb{Z}^d \times \mathbb{Z}_{n_1} \cdots$
 - Invariants for 1,651 magnetic space groups with or without spin-orbit: ~ 20 pages [HCP, unpublished]
[see also: Liu et al PRX 2019, Song et al, Science 2020]

Atomic insulators are product states

- They don't have any inherent quantum entanglement...
- BUT they provide a gateway to those that do!
- Specialization to electronic band theory
 - Non-interacting electrons described in momentum space
 - Focus on symmetry representations
 - The group becomes $\mathbb{Z}^d$, which is like a vector space

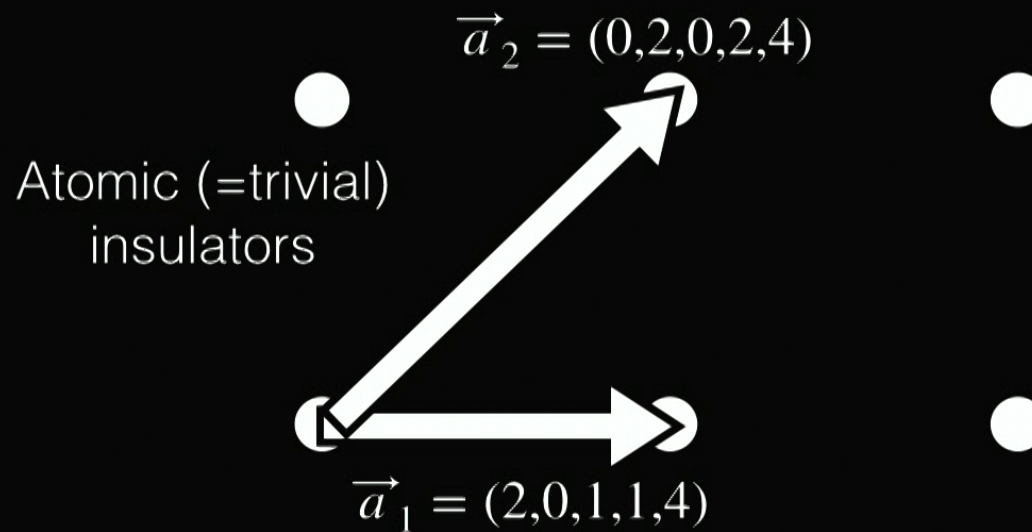
“Bootstrapping” from the trivial

[HCP, Vishwanath, Watanabe Nature Comm. 2017]



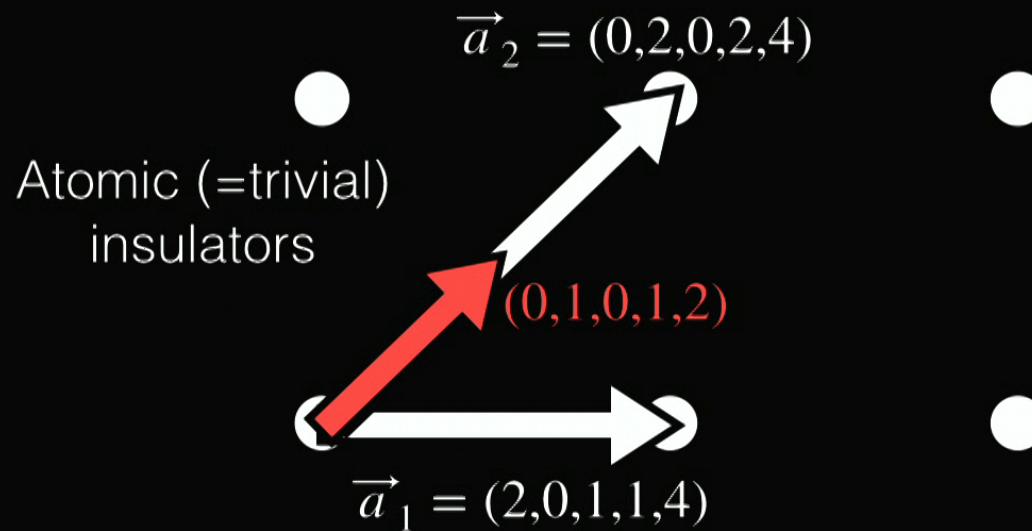
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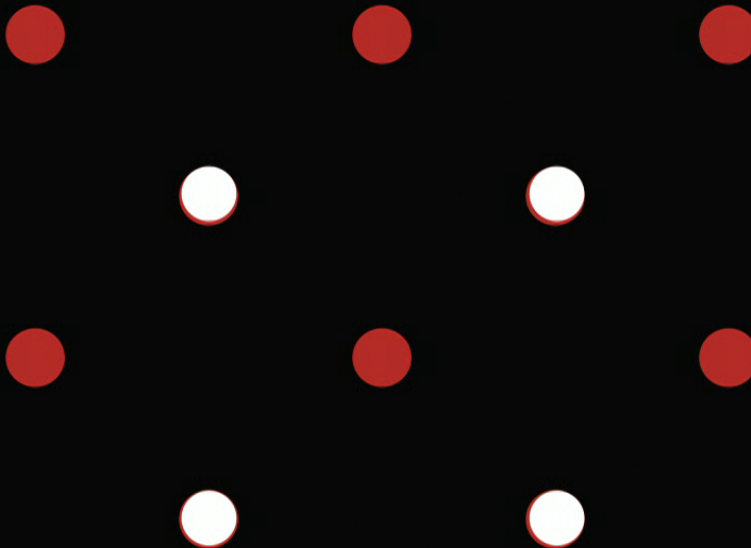


“Bootstrapping” from the trivial

[HCP, Vishwanath, Watanabe Nature Comm. 2017]

Nontrivial phases exposed
by symmetry data

Atomic (=trivial)
insulators

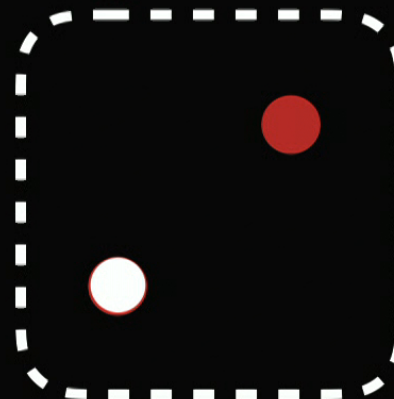


“Bootstrapping” from the trivial

[HCP, Vishwanath, Watanabe Nature Comm. 2017]

Nontrivial phases exposed
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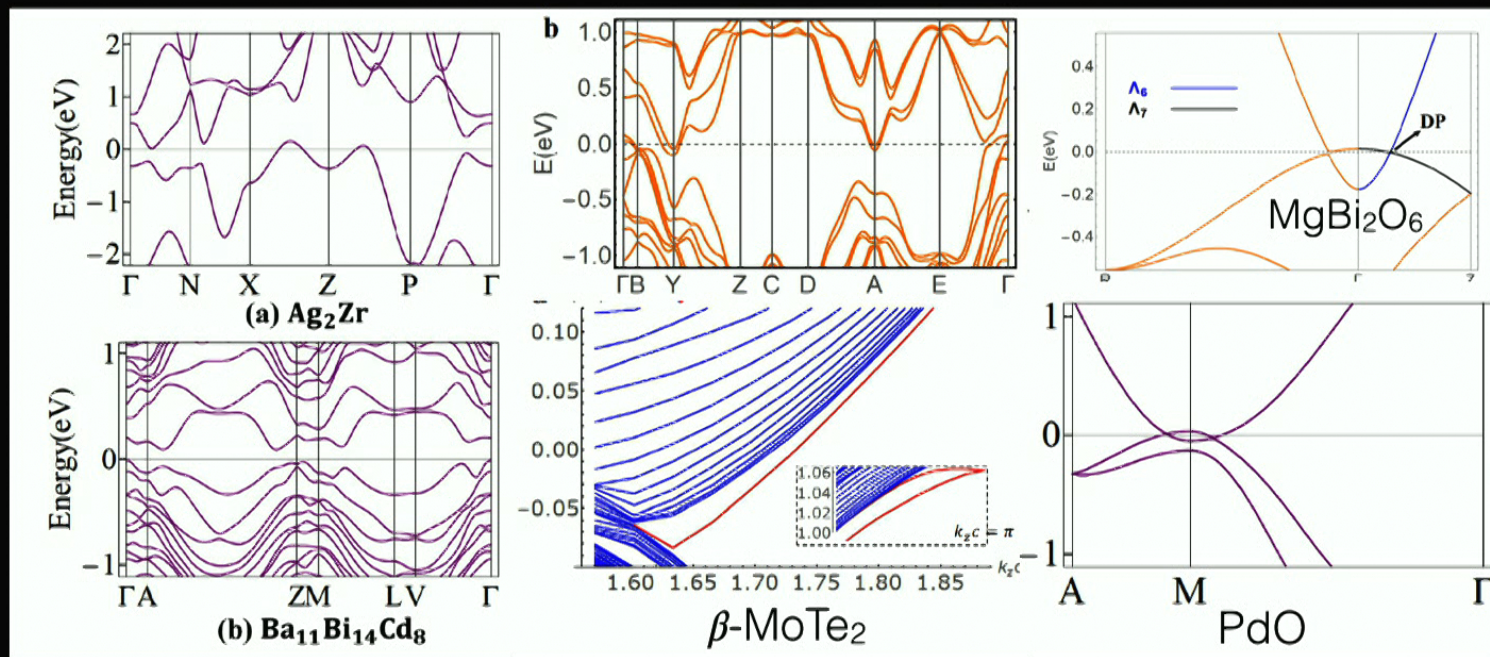
Quotient always finite

Uncovering topo. materials candidates

Chen, HCP, Neaton, Vishwanath, Nature Phys. 2018

Tang, HCP, Vishwanath & Wan, Nature Phys. 2019, Sci. Adv. 2019, Nature 2019

[also: Zhang et al., Nature 2019, Vergniory et al., Nature 2019]



Strong TIs

Higher-order TCIs

Dirac SM

Uncovering topo. materials candidates

Chen, HCP, Neaton, Vishwanath, Nature Phys. 2018

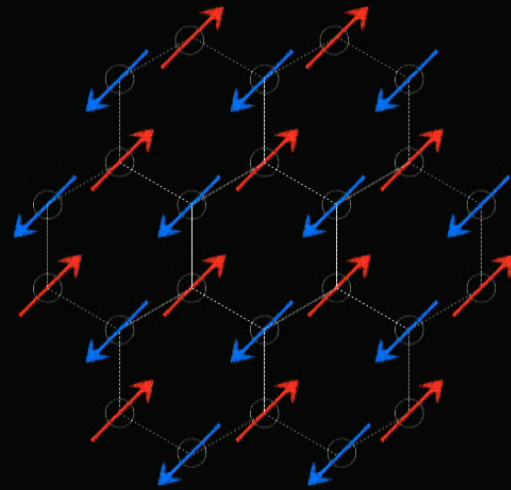
Tang, HCP, Vishwanath & Wan, Nature Phys. 2019, Sci. Adv. 2019, Nature 2019

SG	X_{BS}	Topological insulators	SG	X_{BS}	Topological crystalline insulators
2	$Z_2^2 \times Z_4$	Ag₂Fe	2	$Z_2^2 \times Z_4$	CsHg [256]
11	$Z_2^2 \times Z_4$	BBiLi	11	$Z_2^2 \times Z_4$	BaSb₂ [257], MoTe₂ [258], Al₄Cl₅₁Zr₁₂ [262], Al₄Na , As₄Ba₃Zn₂ [269], Ba₃Cd₂ , Cl₈NSc₅ [277], NbP₂ [278], LaSbSc [285], AsSY [286], GaPt₂ [287]
12	$Z_2^2 \times Z_4$	Ag₄K₂ , Ba₂Cd , Bi₄Pb , PdSe₆	12	$Z_2^2 \times Z_4$	Br₂TeW [396], CBrHgNS [397], Li₇Sn₃ [398], Mo₂S₂Sb [399], Ba₄La [400], AuCd [401], AuTi [402], Ag₂BiO₃ [403], Bi₃Sr₂ [404], Al₃Pd₅ [405], Al₃Pt₅ [406], BCl₆Sc₄ [407], Bi₉Ca₉Cd₄ [408], Bi₉Ca₉Zn₄ [409], Bi₉Cd₄Sr₉ [408], In₅S₁₃Y₄ [410], AlCaPd [411], BiK₂Sn [412], C₆₀K [413], Ag₃Sn [414], F₄NaTi [415], O₂Re [416], AgF₂ [417], AgAuF₇ [418], AgF₃K [419], AlPt₂ [420], Bi₃Ca₅ [421], Bi₃Sr₅ [422], Ca₅Sb₃ [423], GeNb₃Te₆ [424], GePd₂Y [425], N₃Nb₂ [426], Nb₃Si [427], PdSbZr [428], SiTa₃Te₆ [428], AuLu₂ [429], GeLa [430], GeLaPd₂ [430], GeLuPd₂ [431], LuPd₂Si [432], LuPt [433], LuPt₂Si [434], AgCa [435], AuCa [436], BiZr [437], Ga₃PdSr [438], Ga₅Zr₃ [439], GeSc [440], GeY [441], HfSb [442], K₃O₄Pd₂ [443], K₃O₄Pt₂ [444], K₄P₃ [445, 446], N₅NaTa₃ [447], PdY [448], SiY [449], AgC₈₂F₄ [453], Au₁₀Ca₄In₃ [454], Bi [455, 456], LaSb₂ [457], C₇Re₂Sc₅ [458], Ge₁₀La₇Li₈ [459], ReSi₂ [460], Ag₂La [461], Au₂La [461], In₂La [462], Ba₉In₄ [463], In₄Pd₁₇Se₄ [464], Pt₁₁Zr₉ [465], Pt₁₂Si₅ [466], Al₂₁Pt₈ [467], CsFO₃S [468], Ge₃Pd₂₁ [469], LaO₄Pd₂ [470], AgPPt₅ [471], AlPPt₅ [471], AsInPd₅ [472], AsPd₅Tl [473], AsPt₅Tl [473], As₂BaPd₂ [474], BaP₂Pd₂ [475], CaPb [476], CdPd [477], CdPd₅Se [478], CdPt [479], Cd₃Zr [480], FKNb₄O₅ [481], HgPd [482], HgPd₅Se [483], HgPt [484], Hg₂Pt [484], InPPd₅ [485], InPPt₅ [485], PPd₅Tl [485], PPt₅Tl [485], PdTi [486], Pd₅SeZn [487], SiSr [488], Sr [489], C₂Re [490], AsLa [491], LaSb [492], AlSc₂Si₂ [493], Au₂Ca₂Pb [494], Au₂InY₂ [495], B₂Ta₃ [496], B₄W [497], C₂B₂Y [498], Ga₂MgSc₂ [499], Ca₃Hg₂ [500], Ga₂Nb₃ [501], Ga₂Ta₃ [502], Ge₂Hf₃ [503], Hg₂Sr₃ [504, 505], InPd₂Y₂ [506], In₅Ti₂ [507], LiSi₂Y₂ [508], PbPd₂Y₂ [509], N₂Re [510], AgMgSb [511], AsNbSi [512], AsSiTa [513], BaMgSi [514], BiKMg [515], GeTeZr [516], MoNTa [517]
14	$Z_2 \times Z_4$	Ag₂Te	14	$Z_2 \times Z_4$	HgSr₃ [291], LaSbTe [292], BaGe [293], BaSi [294], B [301], Cd₂FSb₅Sr₅ [302], PbSr [303], Ca₈Ga₂Na₄ [308], Li [309], Ge₆Li₂Sr₄ [310], Ba₃Bi₄Li₄ [311], Ba₃Li₄S , Au₄Ti [312], O₄PbPd₂ [313], As₃CsZn₄ [314], As₃RbZi , AsGeNb [316], GeHfS [317], GeSeZr [317], HfSSi [317], Ba₂LiN [322], AsBa₂ [323], AsCa₂ [324], Ba₂Bi [325], Ba₂Sb [326], Bi [330], GePt₃ [331], Mo₃S₄ [332], BaSi₂ [333], BiTe [334], Bi , AsNaTe₂Zr₂ [340], As₃Cd , As₃Cd₄Na [341], As₃Cd₄ , ClZr [348], Hg [349], P [350], BrLa [351], CHf [352], InNbSe₂ [353], AgAsCa [4, 356], AgCaP , GeLiY [358], AsLuPd [358], B₂Zr [360], Pb₃SZr₆ [361]
15	$Z_2 \times Z_4$	MoP₄	15	$Z_2^2 \times Z_4$	
51	$Z_2^2 \times Z_4$	AlPt₂	51	$Z_2^2 \times Z_4$	
55	$Z_2 \times Z_4$	Bi₆In₂	55	$Z_2 \times Z_4$	
58	Z_4	Bi₂Hf	58	Z_4	
59	$Z_2 \times Z_4$	Ag₃Sb	59	$Z_2 \times Z_4$	
60	Z_4	Au₂Pt	62	Z_4	
62	Z_4	AsCd [68], FS , GeHfP , Ge₂W , P₂Zr [894], SiS , AlLaP , AgS₂T , Ga [100], AlLa [115], Ag₃Te , Be₂Zn , AsTeT , Br₂Hg , HfTe₄ , Ag₂S₄ , As₂Cd , BaGe₃ , B₄Y [11], HfSb₂ , Ag₅Cs , Ag₂Zr , CaGe₂	63	$Z_2 \times Z_4$	
63	$Z_2 \times Z_4$		63	$Z_2 \times Z_4$	
64	$Z_2 \times Z_4$		64	$Z_2 \times Z_4$	
65	$Z_2^2 \times Z_4$		65	$Z_2 \times Z_4$	
69	$Z_2^2 \times Z_4$		69	$Z_2^2 \times Z_4$	
71	$Z_2 \times Z_4$		71	$Z_2 \times Z_4$	
72	$Z_2 \times Z_4$		72	$Z_2 \times Z_4$	
87	$Z_2 \times Z_8$		87	$Z_2 \times Z_8$	
121	Z_2		121	$Z_2 \times Z_4$	
122	Z_2		122	$Z_2 \times Z_4$	
123	$Z_2 \times Z_4 \times Z_8$		123	$Z_2 \times Z_4$	
127	$Z_4 \times Z_8$		127	$Z_3 \times Z_3$	
129	$Z_2 \times Z_4$		129	$Z_3 \times Z_3$	
136	Z_4		136	$Z_3 \times Z_3$	
139	$Z_2 \times Z_8$		139	$Z_3 \times Z_3$	
191	$Z_6 \times Z_{12}$		191	$Z_6 \times Z_{12}$	
193	Z_{12}		193	Z_{12}	

Outline aka take-homes

- ✓ Lieb-Schultz-Mattis theorem: no-go for “boring” phases
 - A motivating example of lattice constraints
- ✓ Lattice homotopy: general framework & quantum magnets
 - Space-group generalization of Lieb-Schultz-Mattis
- ✓ Application to atomic insulators
 - Uncovering topologically nontrivial quantum materials

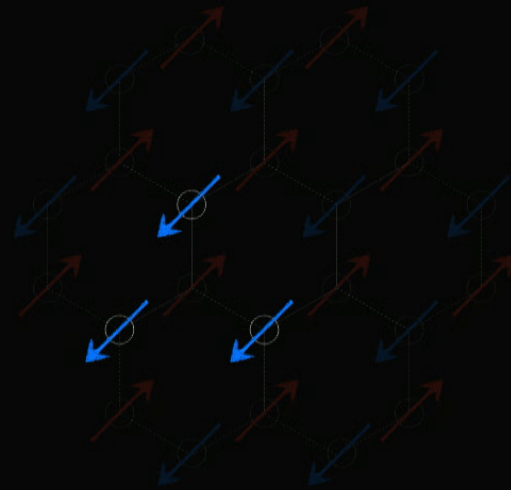
Topological materials: interplay between symmetries and locality



Real-space description for 2D topological insulator
with time-reversal symmetry

[Soluyanov-Vanderbilt 2011]

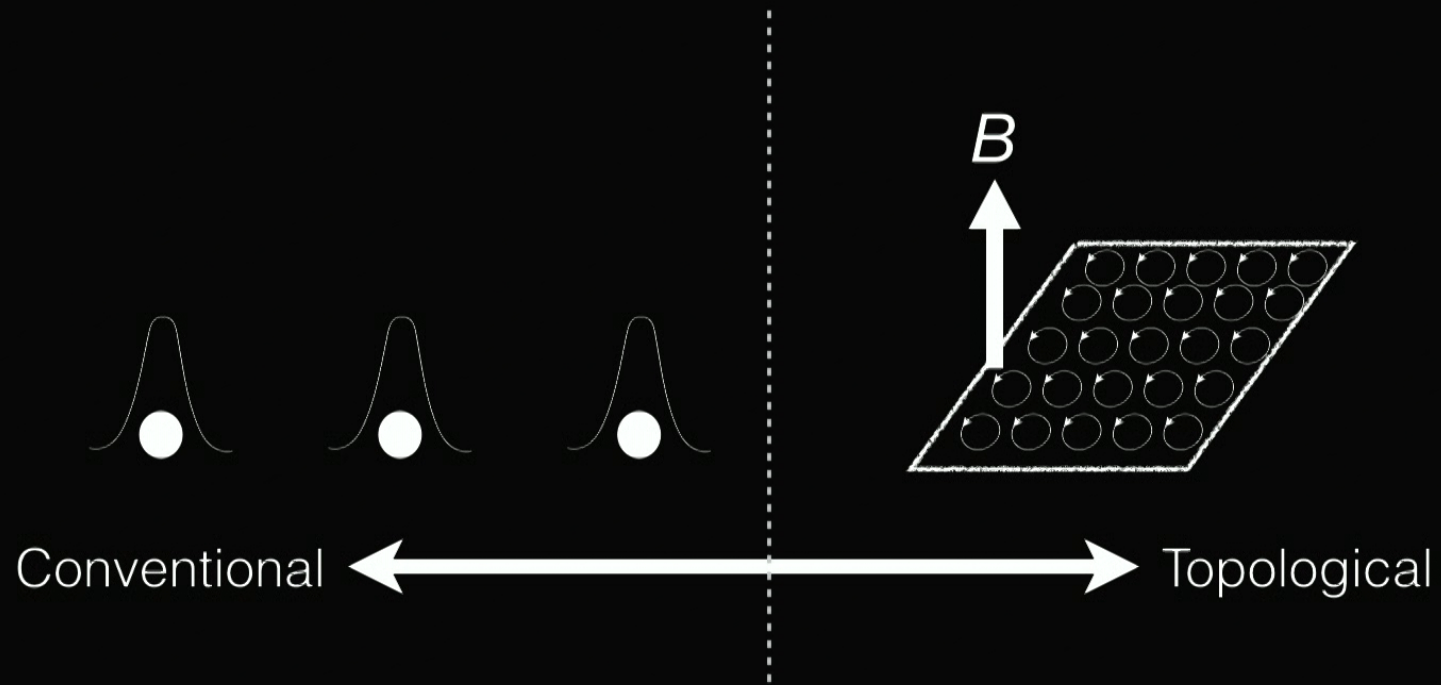
Topological materials: interplay between symmetries and locality



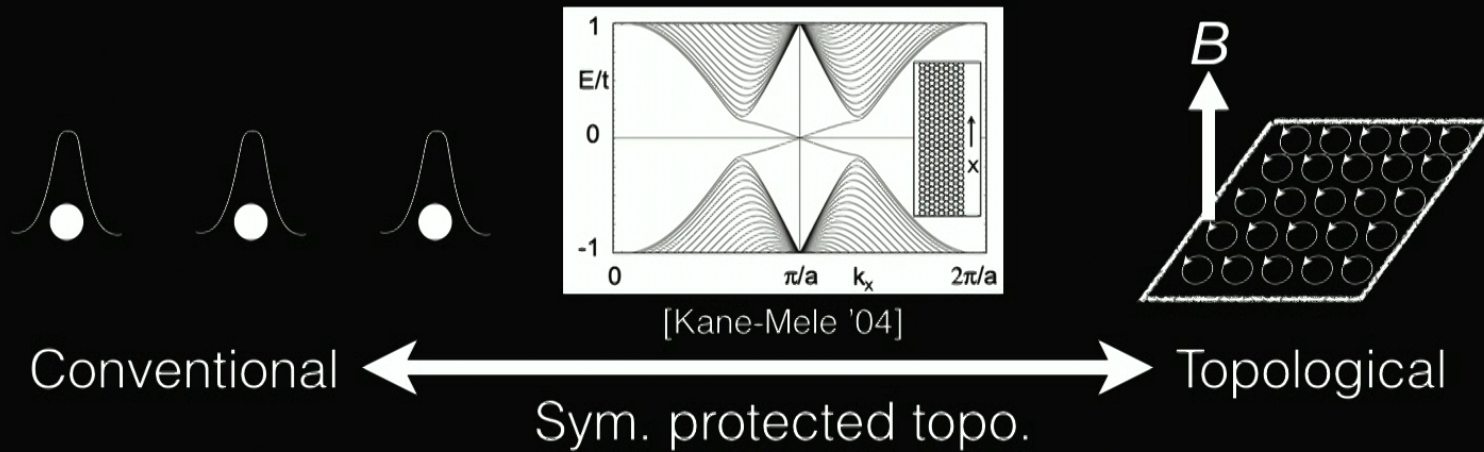
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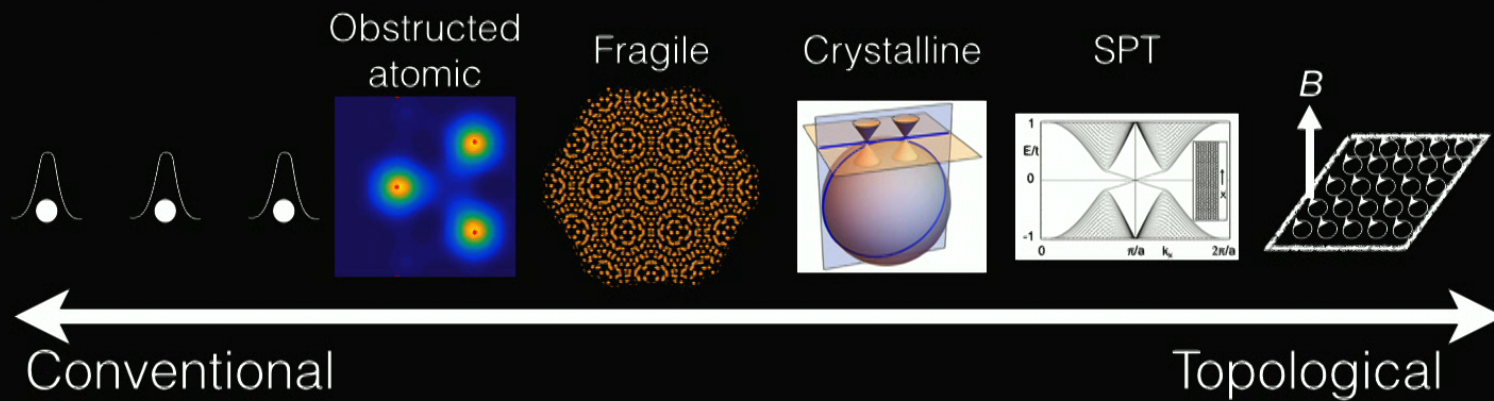
Lessons from the topo. materials



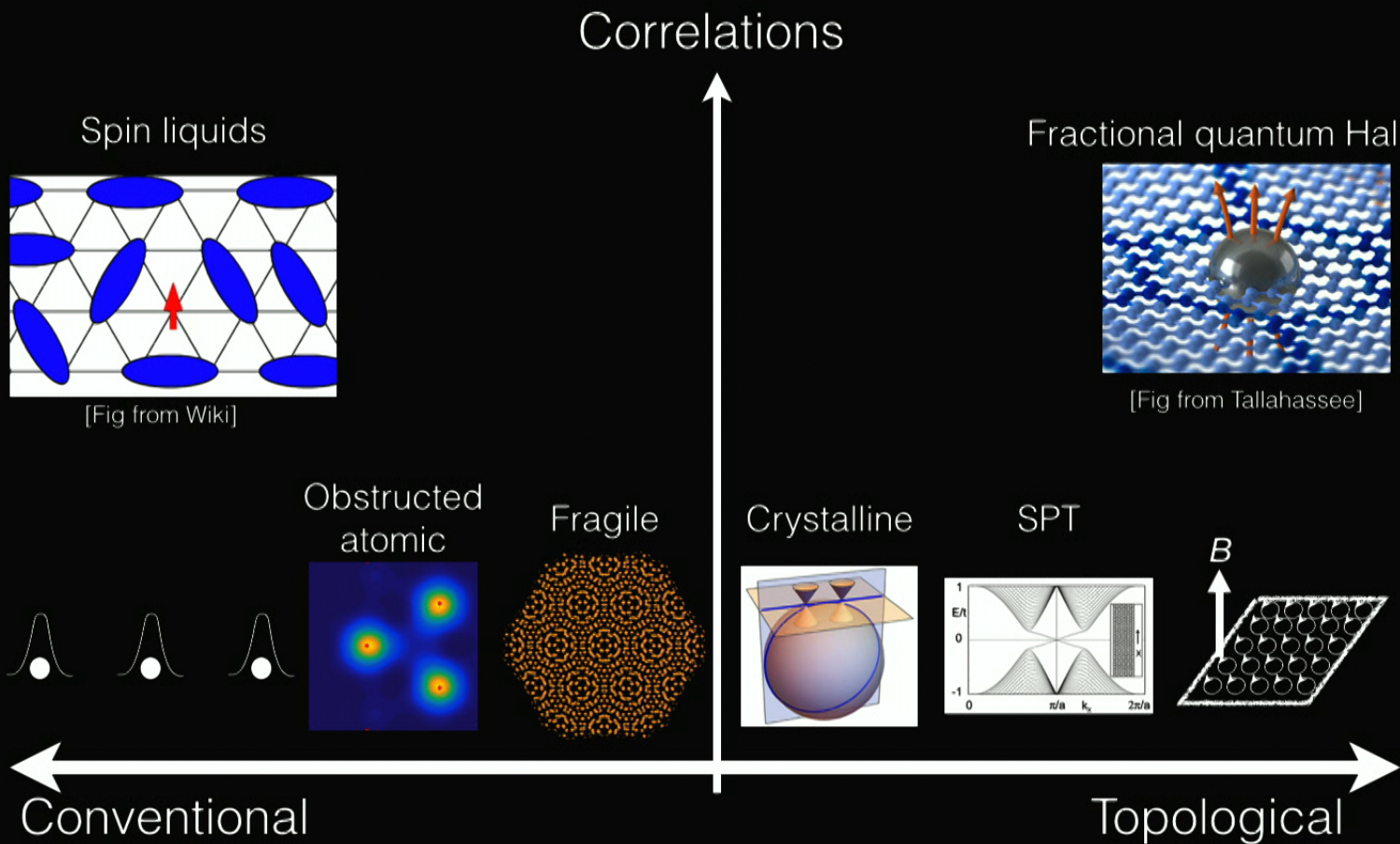
Lessons from the topo. materials



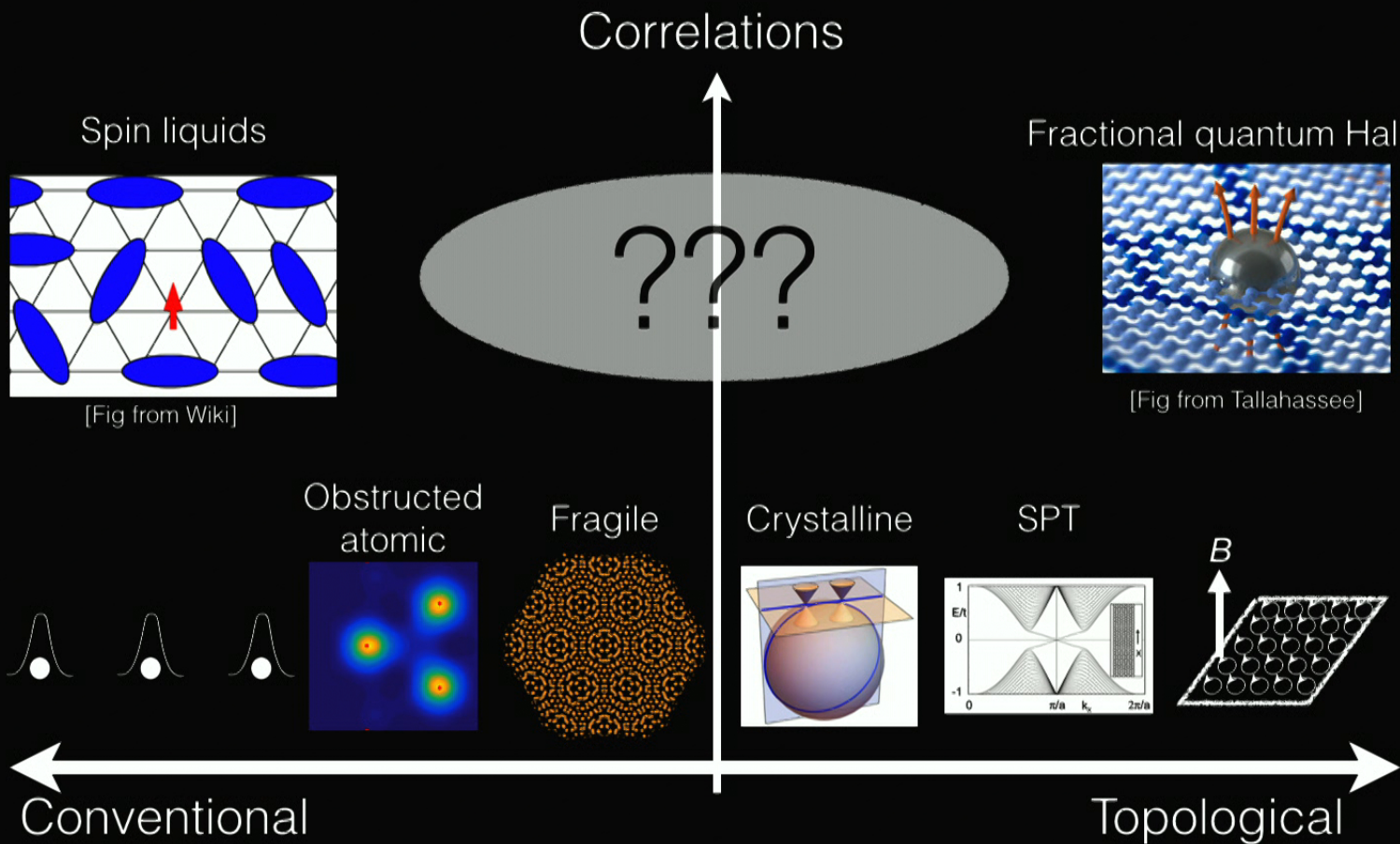
Lessons from the topo. materials



Lessons from the topo. materials



Lessons from the topo. materials



Acknowledgements

Lattice homotopy Symmetry indicators



M. Zaletel
(Berkeley)



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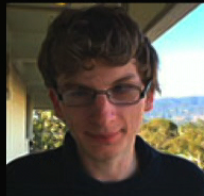
Materials discovery



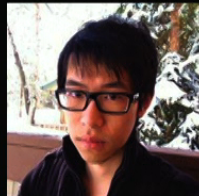
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