Lieb-Schultz-Mattis constraints for 3D quantum paramagnets

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LPS Orsay

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Crystallography, group cohomology, and Lieb–Schultz–Mattis constraints

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Weicheng Ye
(U of British Columbia)

GORDON AND BETTY MOORE FOUNDATION

DSL in triangular J_1-J_2 Heisenberg model

Triangular lattice,
S = ½, J_2/J_1~1/8

UV

IR

DSL (N=4 QED3)

Iqbal, Hu, Thomale, Poilblanc, Becca, PRB ‘16;
Zhu, Maksimov, White, Chernyshev, PRL ‘18;
Ferrari, Becca, PRX ‘19;
Hu, Zhu, Eggert, He, PRL ‘19;
Drescher, Vanderstraeten, Moessner, Pollmann, PRB ’23;
Wietek, Capponi, Läuchli, PRX ’24;
Gallegos, Jiang, White, Chernyshev, PRL ‘25…

	T_1	T_2	R	C_6	$\mathcal{T}$
$\Phi_1^\dagger$	$e^{i(-\pi/3)}\Phi_1^\dagger$	$e^{i(\pi/3)}\Phi_1^\dagger$	$-\Phi_3^\dagger$	Φ_2	Φ_1
$\Phi_2^\dagger$	$e^{i(2\pi/3)}\Phi_2^\dagger$	$e^{i(\pi/3)}\Phi_2^\dagger$	$\Phi_2^\dagger$	$-\Phi_3$	Φ_2
$\Phi_3^\dagger$	$e^{i(-\pi/3)}\Phi_3^\dagger$	$e^{i(-2\pi/3)}\Phi_3^\dagger$	$-\Phi_1^\dagger$	$-\Phi_1$	Φ_3
$\Phi_{4/5/6}^\dagger$	$e^{i(2\pi/3)}\Phi_{4/5/6}^\dagger$	$e^{i(-2\pi/3)}\Phi_{4/5/6}^\dagger$	$\Phi_{4/5/6}^\dagger$	$-\Phi_{4/5/6}$	$-\Phi_{4/5/6}$

Monopole quantum numbers associated with order-2 symmetries **determined by LSM constraints**

Song, He, Vishwanath, Wang, PRX ’20

$$\Delta\mathcal{L} = \Phi_1\Phi_2\Phi_3 + h.c.$$

Monopoles: irrelevant!

Song, Wang, Vishwanath, He, Nat comms ‘19.

Outline

Lieb–Schultz–Mattis (LSM) theorems

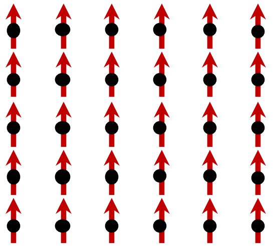
- In 1D and 2D
- In 3D

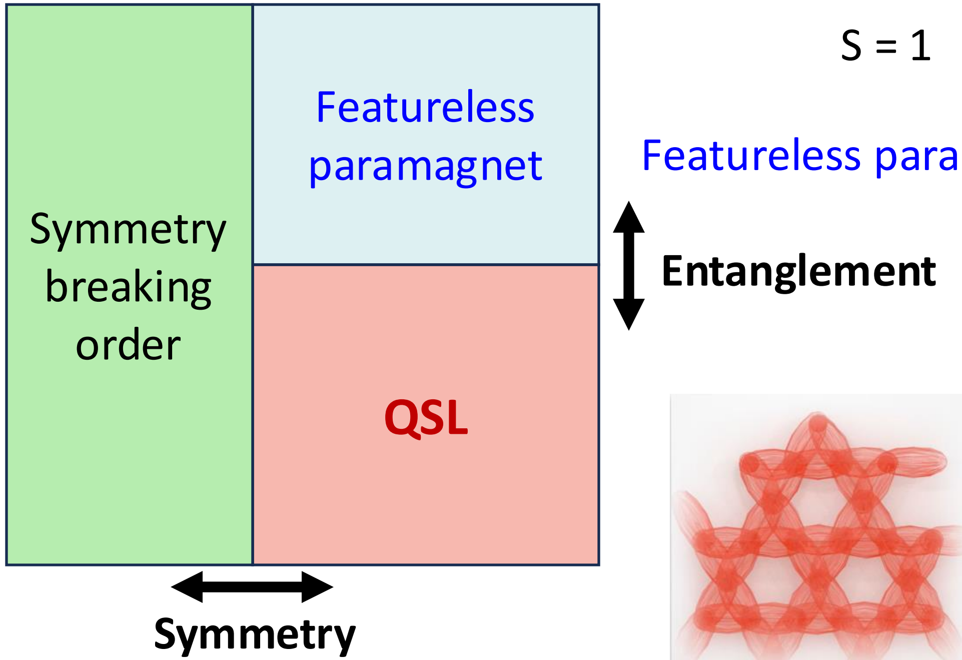
Topological theory of LSM

- Crystalline topological responses
- Applications (Triangular, pyrochlore…) and challenges

Quantum magnetism – a (crude) phase diagram

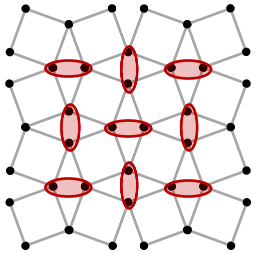
Phases of ground states:

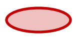




S = 1

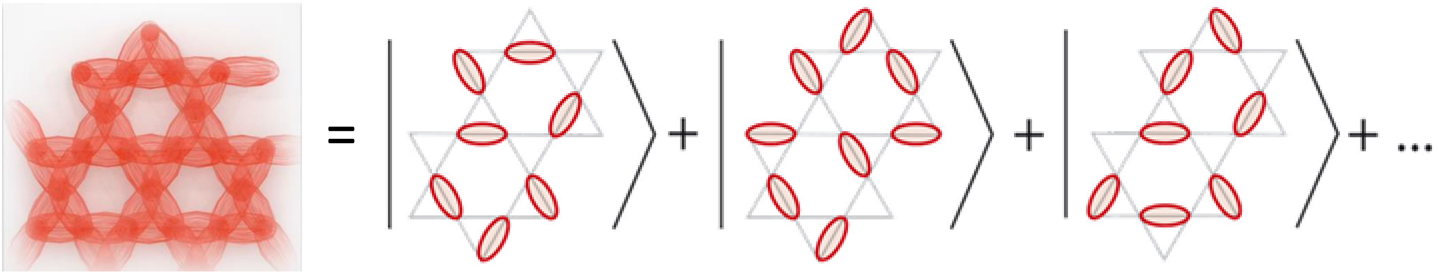
and



 $= \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$

S = ½

Featureless paramagnet: Product-like ground state – Short-range entangled



QSL: massive quantum superposition – Long-range entangled

Original Lieb-Schultz-Mattis (LSM)

Lieb, Schultz, Mattis, Ann. Phys. '61

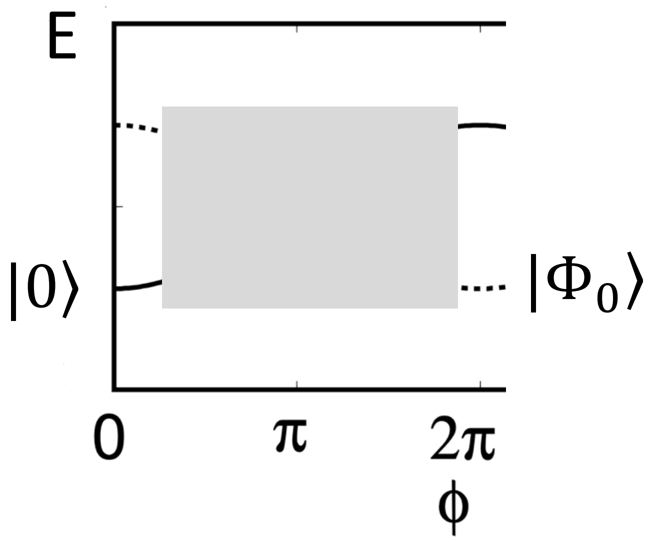
Thm. In a S=1/2 spin chain with translation symmetry and on-site SO(3) symmetry. If it has an odd number of spin-1/2's per unit cell, then the ground state cannot be a featureless paramagnet.

(unique, symmetric, SRE ground state)

Flux threading argument

Oshikawa, PRL '00; Hastings, PRB '04

Ground states before/after flux threading differ in crystal momentum:



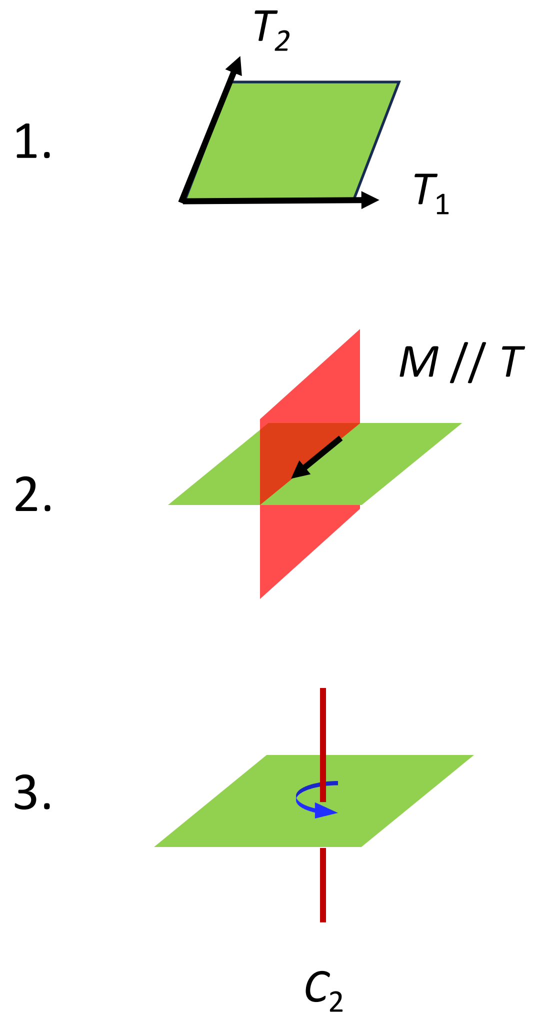
LSM for 2D lattice magnets

Theorem (LSM in 2D). Po, Watanabe, Jian, Zaletel, PRL '17

Assume the spin-1/2 lattice preserves lattice x SO(3)symmetry. The ground state cannot be a featureless paramagnet if the lattice has an odd number of spin-½'s

1. per 2d unit cell*, or
2. per 1d unit cell defined by translation along a mirror axis, or
3. at a C_2 rotation center.

*Translation, screw, glide



Application:

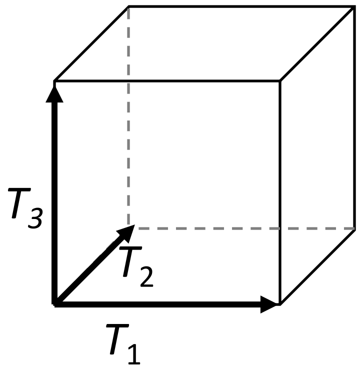
1. The S=1/2 Heisenberg model on the **triangular** lattice cannot be a featureless paramagnet.
2. A S=1/2 featureless paramagnet exists on the **honeycomb** lattice.

Kim, Lee, Jiang, Ware, Jian, Zaletel, Han, Ran, PRB '16

LSM for 3D magnets

CL, Ye, Scipost Phys. 18 (5), 161 (2025)

1.

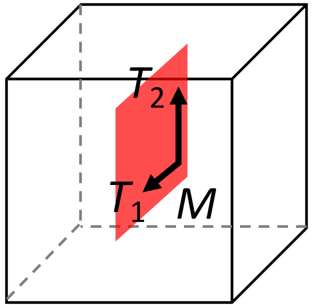


<u>"No-go" Theorem in 3D</u>

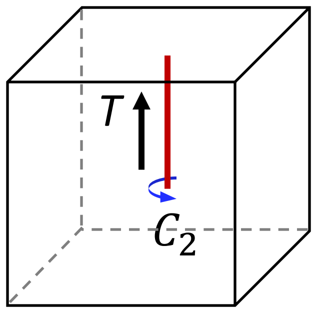
Assume the spin-1/2 lattice preserves lattice x SO(3)symmetry. Ground state cannot be a featureless paramagnet if the lattice has an odd number of spin-½'s

1. per <u>3D unit cell</u>, or
2. per <u>2D unit cell</u> spanned by two translations in a mirror, or
3. per <u>1D unit cell</u> defined by a translation/screw/glide along a C_2 axis, or
4. at the intersection of two C_2 axes, or
5. at a 3D inversion center.

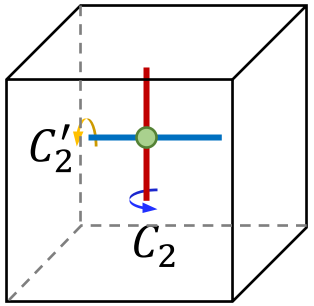
2.



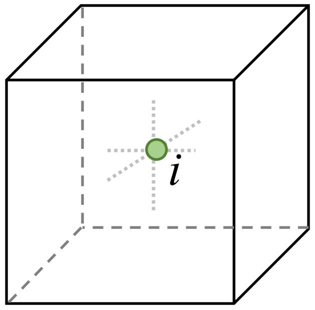
3.



4.

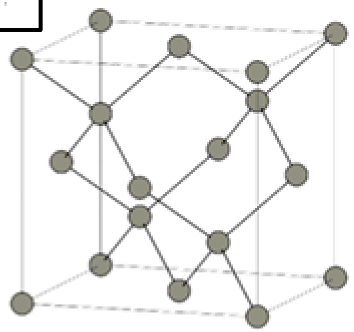


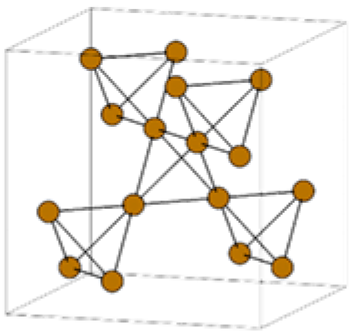
5.



Application:

The S=1/2 Heisenberg models cannot be a featureless paramagnet on either diamond or pyrochlore lattice.





Overarching LSM

CL, Ye, Scipost Phys. 18 (5), 161 (2025)

Statement (LSM).
A featureless paramagnet cannot exist when spin-1/2's sit at Z_2-Irreducible Wyckoff Positions.

Wyckoff Positions of Group $P2_1/c$ (No. 14) [unique axis b]

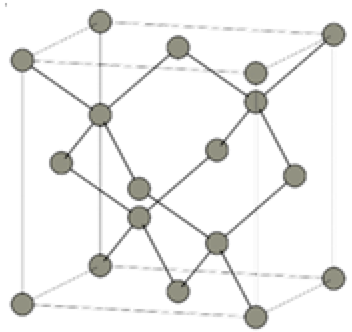
Multiplicity	Wyckoff letter	Site symmetry	Coordinates
4	e	1	(x,y,z) (-x,y+1/2,-z+1/2) (-x,-y,-z) (x,-y+1/2,z+1/2)
2	d	-1	(1/2,0,1/2) (1/2,1/2,0)
2	c	-1	(0,0,1/2) (0,1/2,0)
2	b	-1	(1/2,0,0) (1/2,1/2,1/2)
2	a	-1	(0,0,0) (0,1/2,1/2)

All Z_2-Irreducible Wyckoff Positions are listed in our paper:

Wyckoff position	Little group Intl.	Little group Schönflies	Coordinates	LSM anomaly class	Topo. inv.
2a	$\bar{1}$	C_i	$(0,0,0)$, $(0,1/2,1/2)$	$(A_i + A_x)B_\beta$	$\varphi_1[I]$
2b	$\bar{1}$	C_i	$(1/2,0,0)$, $(1/2,1/2,1/2)$	$A_x B_\beta$	$\varphi_1[T_1 I]$
2c	$\bar{1}$	C_i	$(0,0,1/2)$, $(0,1/2,0)$	$(A_i + A_x)(A_i^2 + B_\beta)$	$\varphi_1[T_2 I]$
2d	$\bar{1}$	C_i	$(1/2,0,1/2)$, $(1/2,1/2,0)$	$A_x(A_i^2 + B_\beta)$	$\varphi_1[T_1 T_2 I]$

Example: No. 227 (diamond/pyrochlore)

CL, Ye, Scipost Phys. 18 (5), 161 (2025)



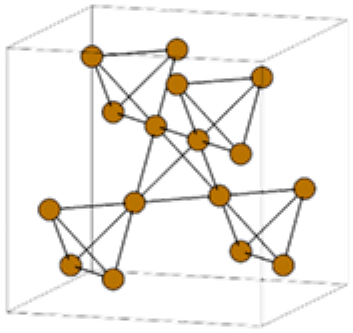


Table 232: IWPs and group cohomology at degree 3 of $Fd\bar{3}m$.

Wyckoff position	Little group		Coordinates	LSM anomaly class	Topo. inv.
	Intl.	Schönflies	$(0,0,0)+$ $(0,1/2,1/2)+$ $(1/2,0,1/2)+$ $(1/2,1/2,0)+$		
8a	$\bar{4}3m$	T_d	$(1/8,1/8,1/8)$, $(7/8,3/8,3/8)$	$C_\alpha + C_\gamma$	$\varphi_2[C_2, C_2']$
8b	$\bar{4}3m$	T_d	$(3/8,3/8,3/8)$, $(1/8,5/8,1/8)$	C_γ	$\varphi_2[T_3C_2, T_2C_2']$
16c	$\bar{3}m$	D_{3d}	$(0,0,0)$, $(3/4,1/4,1/2)$, $(1/4,1/2,3/4)$, $(1/2,3/4,1/4)$	$A_i(A_i^2 + A_iA_m + B_{xy+xz+yz})$	$\varphi_1[I]$
16d	$\bar{3}m$	D_{3d}	$(1/2,1/2,1/2)$, $(1/4,3/4,0)$, $(3/4,0,1/4)$, $(0,1/4,3/4)$	$A_iB_{xy+xz+yz}$	$\varphi_1[T_1T_2I]$

Summary of Part 1

- LSM: crystal symmetry-based criteria for *when a featureless paramagnet cannot exist at $T = 0$.*
- Applicable to SOC, but only to half-integer spins
- 1D, 2D, 3D now complete!
- 3D: five criteria *(0D + 0D + 1D + 2D + 3D)*
- Tables for 230 space groups also available

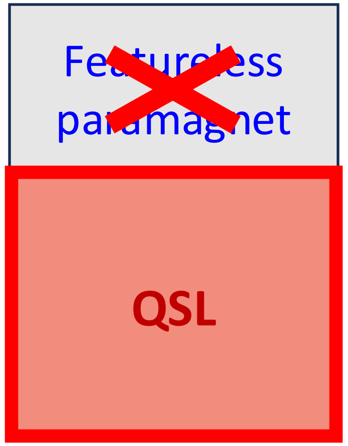
Outline

Lieb–Schultz–Mattis (LSM) theorems

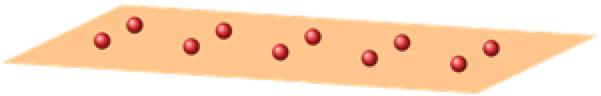
- In 1D and 2D
- In 3D

Topological theory of LSM

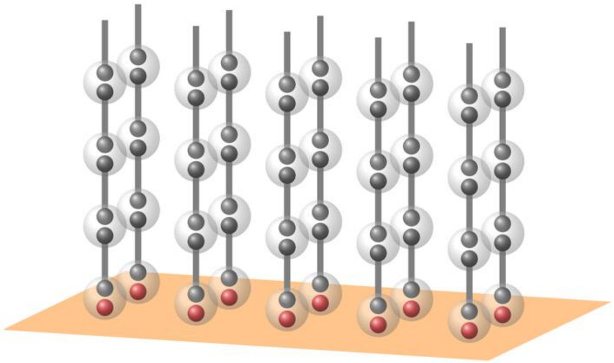
- Crystalline topological responses
- Applications (Triangular, pyrochlore…) and challenges



A bulk-boundary corresp. for quantum magnets



QSL in *d* spatial dim



Featureless paramagnet
in *d+1* spatial dim

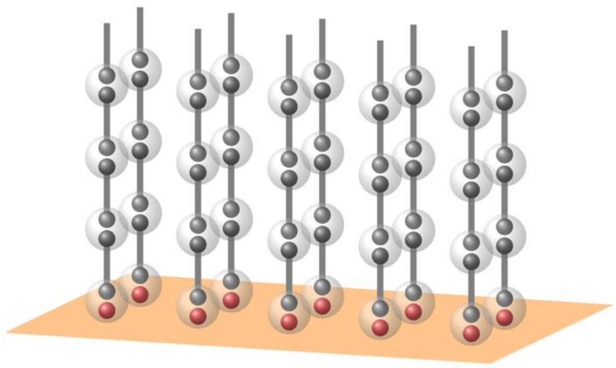
QSL in *d* spatial dim

Cheng, Zaletel, Barkeshli, Vishwanath, Bonderson, PRX '16;
Else, Thorngren, PRB '20

Topological crystalline response theory

- G: crystallographic space group.
- A: gauge field of G.
- Topological Quantum Field Theory (TQFT):

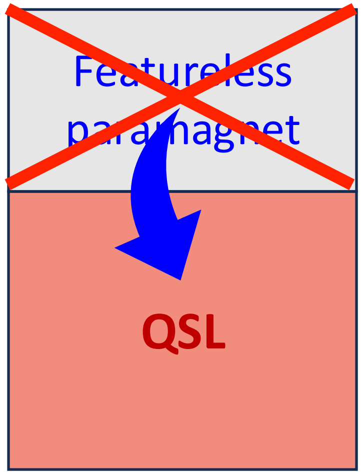
$$Z[A] = e^{i\pi \int_{\mathcal{M}_{d+2}} \lambda[A] \cup \omega_2^{spin}}$$



$Z[A]$
$\in \boldsymbol{H}^{\boldsymbol{d+2}}(\boldsymbol{G} \times \boldsymbol{SO}(\boldsymbol{3}), \boldsymbol{U}(\boldsymbol{1}))$
group cohomology

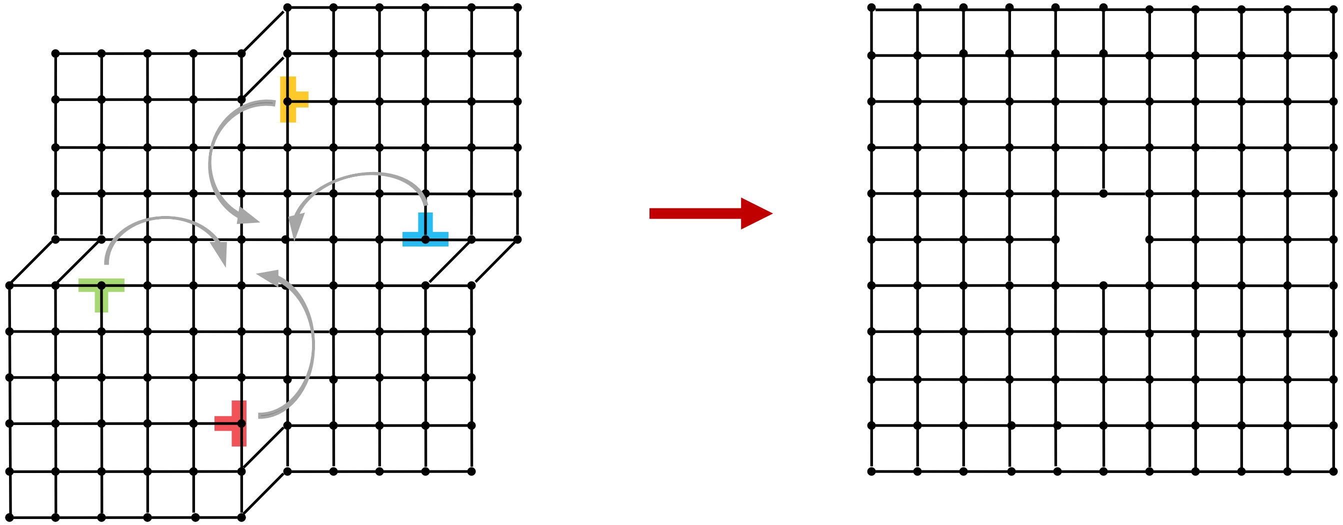
Dijkgraaf, Witten, Comm. Math. Phys., '90

LSM as a topological crystalline response



<u>Thm</u>(LSM). In a 2D lattice with odd number of spin-1/2's and translation x SO(3) symmetry, fusing four dislocations **leaves no dislocations behind, but traps a spin-1/2.**

$$Z[A] = e^{i\pi \int_{\mathcal{M}_4} A_x \cup A_y \cup \omega_2^{spin}}$$



Wang, CL, Lu, PRB '24

Topological crystalline response – viewpoint 1

Thm(LSM). In a 2D lattice with odd number of spin-1/2's and translation x SO(3) symmetry, fusing four dislocations leaves no dislocations behind, but traps a spin-1/2.

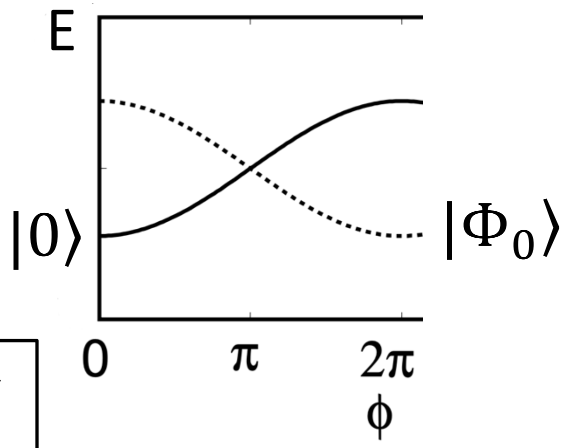
$$Z[A] = \mathrm{e}^{i\pi \int_{\mathcal{M}_4} A_x \cup A_y \cup \omega_2^{spin}}$$

	$G = \mathbb{Z}^d$ (Translation)	SO(3) (spin rotation)
Charge (linear or proj. rep)	momentum	spin-1/2 or spin-1
Topological defect (group element)	dislocation	2π flux

Topological crystalline response – viewpoint 2

Flux threading argument for LSM

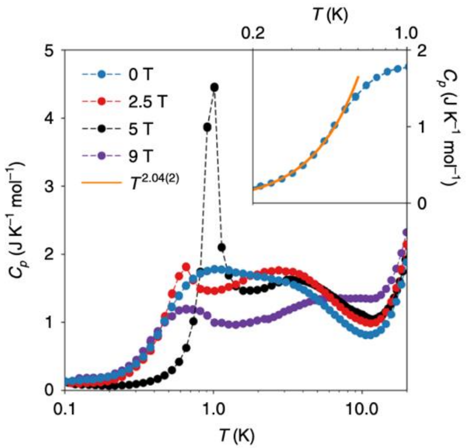
Oshikawa, PRL '00; Hastings, PRB '04

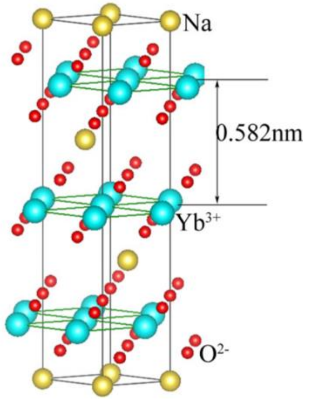


$$Z[A] = e^{i\pi\int_{\mathcal{M}_4} A_x \cup A_y \cup \omega_2^{spin}}$$

	$G = \mathbb{Z}^d$ (Translation)	SO(3) (spin rotation)
Charge (linear or proj. rep)	momentum	spin-1/2 or spin-1
Topological defect (group element)	dislocation	2π flux

$NaYbO_2$ as a Dirac spin liquid candidate





Triangular lattice

S = ½ with SOC

UV

IR

DSL (N=4 QED3)

nature physics

29 July 2019

Field-tunable quantum disordered ground state in the triangular-lattice antiferromagnet $NaYbO_2$

Bordelon, Kenney, CL, Hogan, Posthuma, Kavand, Lyu, Sherwin, Butch, Brown, Graf, Balents, Wilson

SciPost

SciPost Phys. 13, 066 (2022)

Topological characterization of Lieb-Schultz-Mattis constraints and applications to symmetry-enriched quantum criticality

Weicheng Ye[1,2], Meng Guo[1,3], Yin-Chen He[1], Chong Wang[1] and Liujun Zou[1]

*"… our exhaustive search finds 3 realizations of DSL. **for all three realizations**, symmetries of $NaYbO_2$ are sufficient to **forbid** all relevant operators of DSL."*

Symmetry fractionalization in pyrochlore QSI

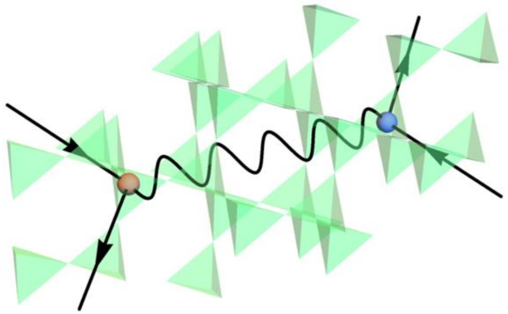
Pyrochlore lattice

S = ½ *XXZ* model

Hermele, Fisher, Balents, PRB '04

UV

$$Z[A] = e^{i\pi \int_{\mathcal{M}_5} \lambda[A] \cup \omega_2^{spin}}$$



3+1D Maxwell

IR

$$Z_m[A] = e^{i\pi\, (A_i^2 + B)}$$

Inv. + trans.

$$Z_e[A] = e^{i\pi(\omega_2^{spin} + \chi_1 B + \chi_2 B_\alpha)}$$

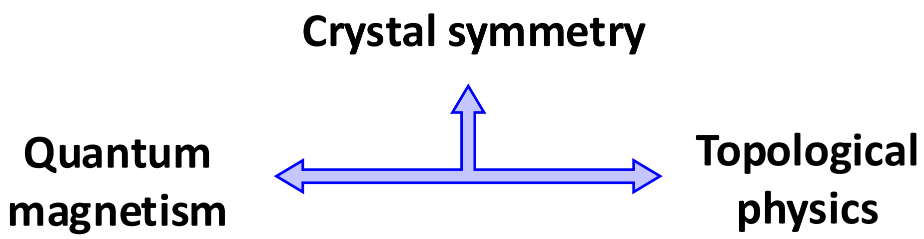
(spinon) Trans. + rotation

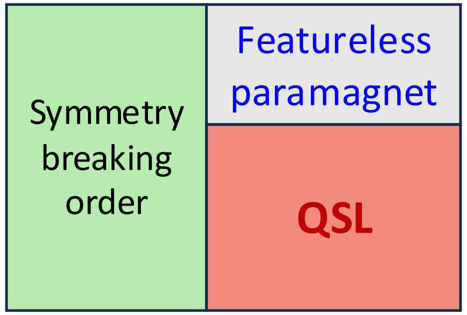
CL, Halász, Balents PRB '21

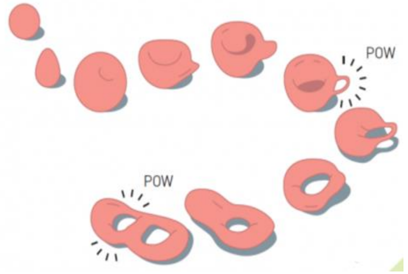
Symmetry fractionalization

Summary

- Lieb-Schultz-Mattis criteria for featureless paramagnets
- Topological crystalline response for QSLs







Challenges

Use crystalline defects to probe QSLs

- Topological framework established
- But *exactly how* unclear yet!

Realistic systems with disorder

- Some results established (translation)
- *Needs generalization to other symmetries*

Kimchi, Nahum, Senthil, PRX '18