Lieb-Schultz-Mattis constraints for 3D quantum paramagnets

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

Chunxiao Liu (刘春骁)
Laboratoire de physique des solides,
Université Paris-Saclay, CNRS

Laboratoire de physique des solides (LPS), Université Paris-Saclay

巴黎-萨克雷大学 固体物理实验室

université PARIS-SACLAY

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Laboratoire de physique des solides (LPS), Université Paris-Saclay
巴黎-萨克雷大学 固体物理实验室

Our theory group specializes in quantum transport, magnetism, topology, soft condensed matter, quasicrystals…

Outstanding colleagues in history:

- Jacque Friedel (one of the founders)
- Pierre-Gilles de Gennes (Nobel prize 1991)
- Albert Fert (Nobel prize 2007)

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

Chunxiao Liu[1*] **and Weicheng Ye**[2†]

1 Department of Physics, University of California, Berkeley, California, USA 94720
2 Department of Physics and Astronomy, and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, BC, Canada V6T 1Z1

Weicheng Ye
(U of British Columbia)

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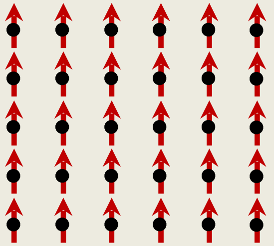
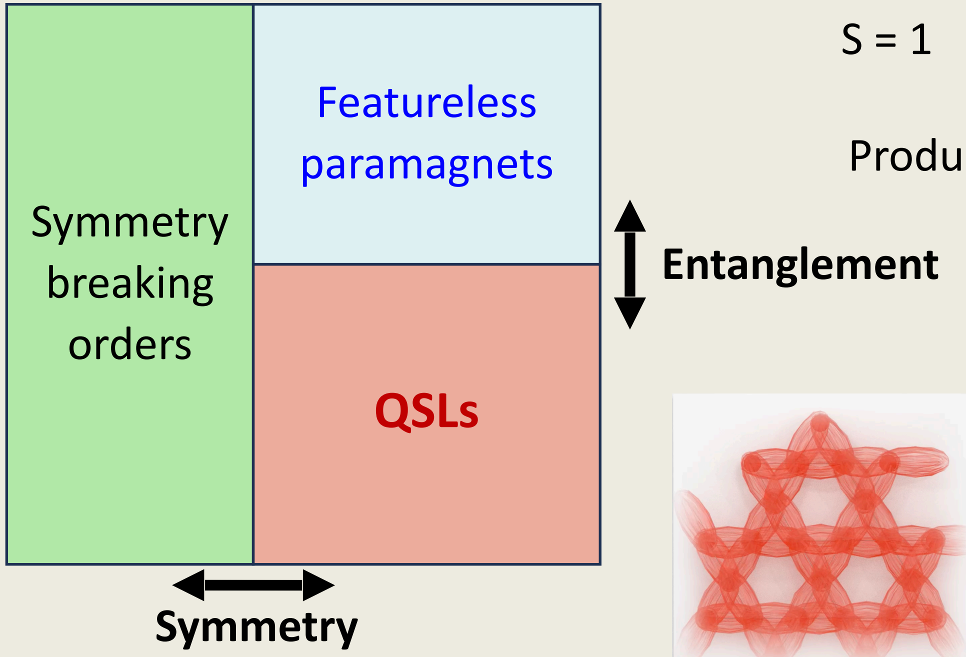
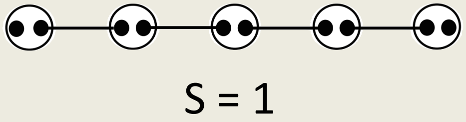
Quantum magnetism – a (crude) phase diagram

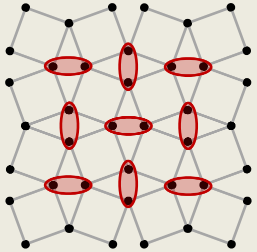
Phases of <u>ground states</u>:





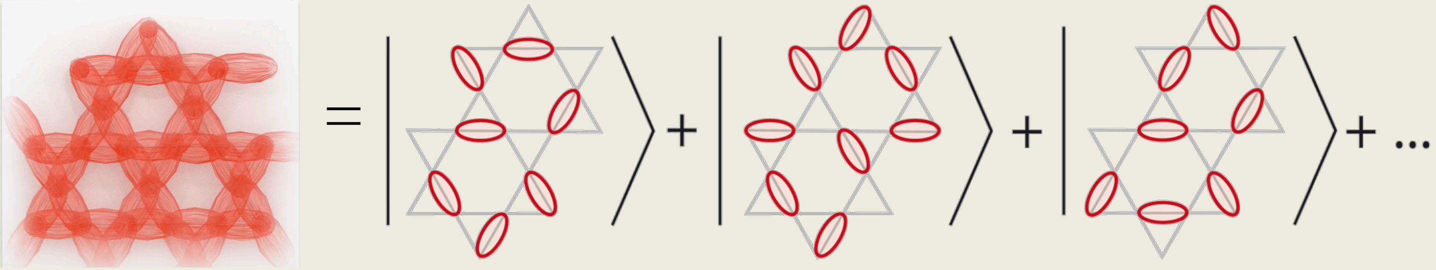


and



$= \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$ S = ½

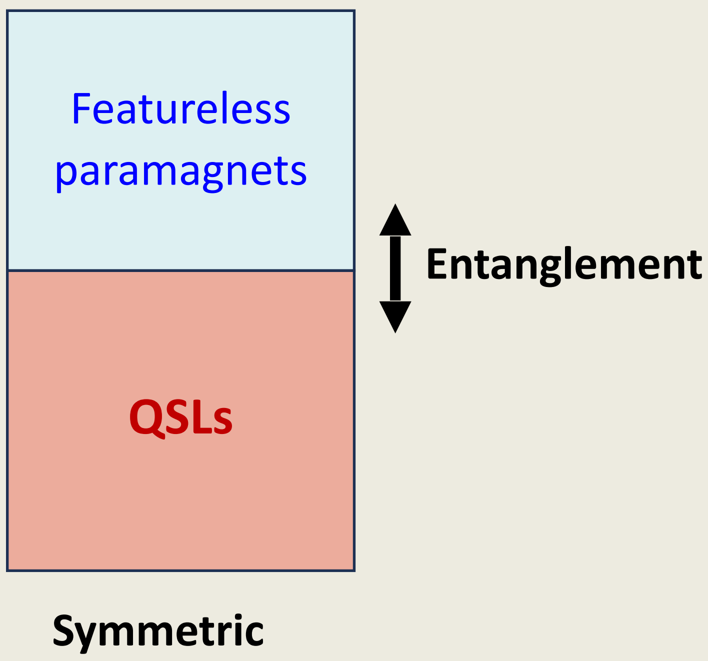
Product-like ground state – Short-range entangled



massive quantum superposition – Long-range entangled

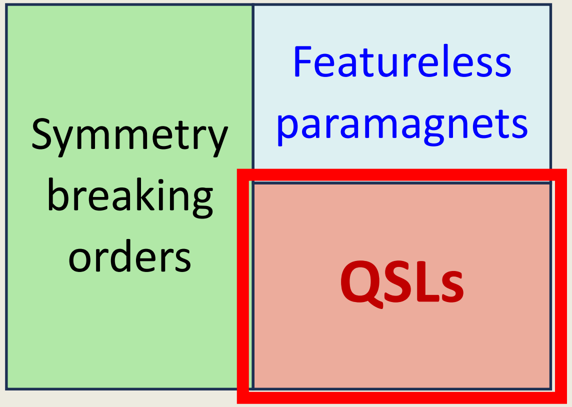
Quantum paramagnetism

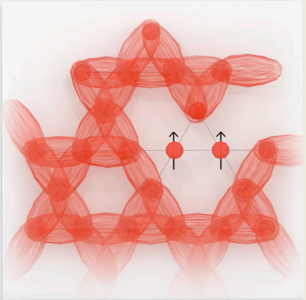
Phases of ground states:



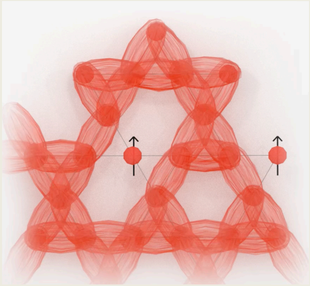
- A featureless paramagnet = a unique, symmetric, short-range entangled, gapped ground state. Includes all SPTs.
- A QSL is its complement (so has long-range entanglement). Includes all SETs.

Excitation of QSLs: spinon & gauge field

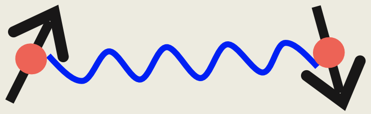




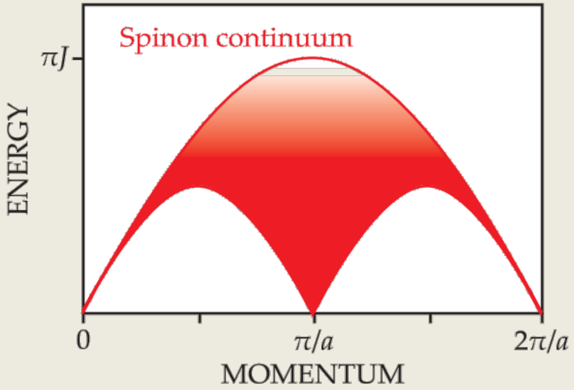
Breaking a singlet creates a $\Delta S = 1$ excitation



Behaves like 2 excitations carrying **fractional spins** $(\Delta S = 1/2)$ — **Spinons**

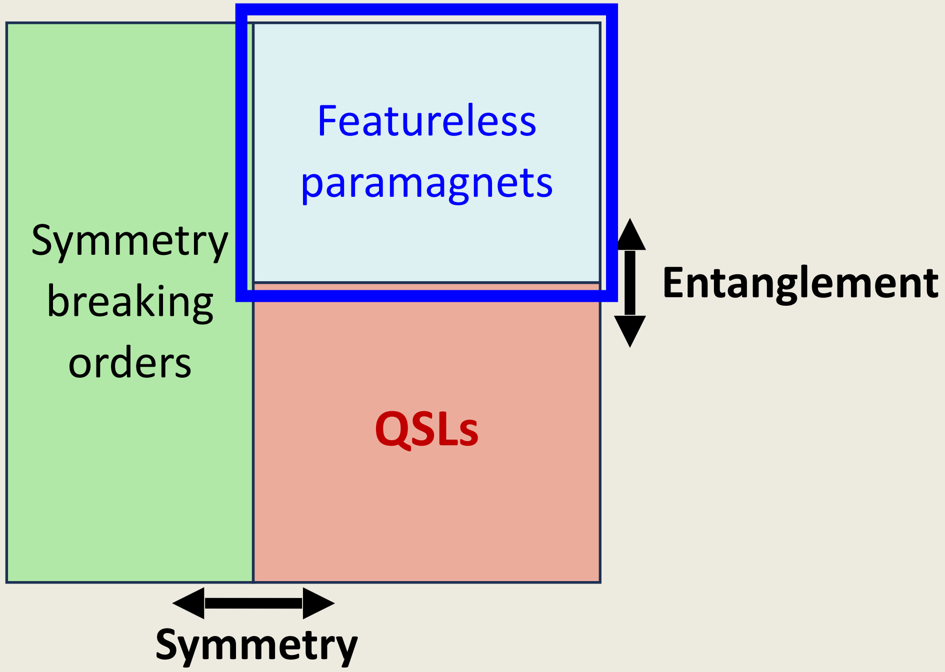


- **Excitations: spinons interacting via a gauge field**
- Allows to experimentally **detect** QSLs (e.g. in neutron scattering)



Central question

Phases of ground states:



Given: a lattice and a spin model.

Q: When can a featureless paramagnetic ground state exist?

Outline

Lieb–Schultz–Mattis (LSM) theorems

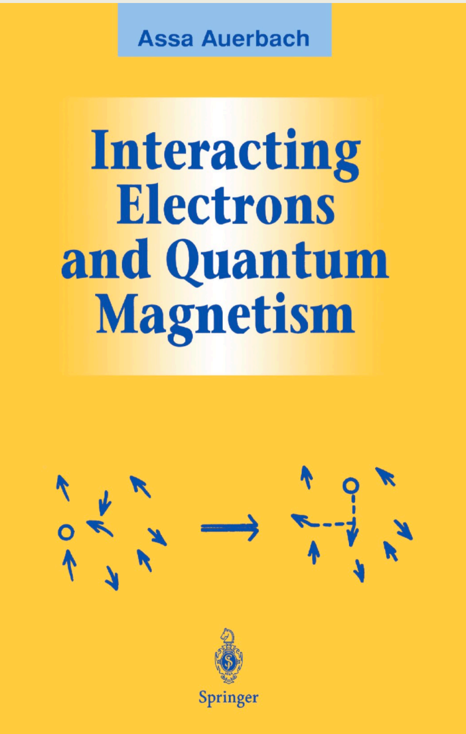
- In 1D and 2D
- In 3D

Topological theory of LSM

- Crystalline topological responses
- Applications (Triangular and pyrochlore lattice)

Original Lieb-Schultz-Mattis (LSM)

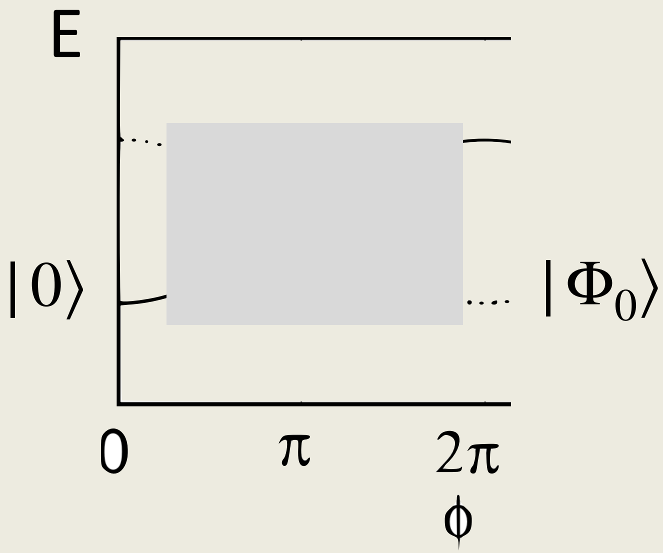
Lieb, Schultz, Mattis, Ann. Phys. '61



<u>Theorem (LSM)</u>.
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 – a history

Lieb, Schultz, Mattis, Ann. Phys. '61	d=1: translation LSM
Oshikawa, PRL '00; Hastings, PRB '04	All d: translation LSM
Cheng, Zaletel, Barkeshli, Vishwanath, Bonderson, PRX '16	d=2: translation topological response
Po, Watanabe, Jian, Zaletel, PRL '17	d=2: all lattice symmetry LSM
Else, Thorngren, PRB '20	General theory of topological response
Ye, Guo, He, Wang, Zou, Scipost '22	d=2: all lattice symmetry topological response
Our work!	d=3: all lattice symmetry LSM & topological response

LSM for 2D lattice magnets

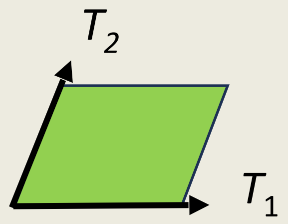
Theorem (LSM in 2D). Po, Watanabe, Jian, Zaletel, PRL '17

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

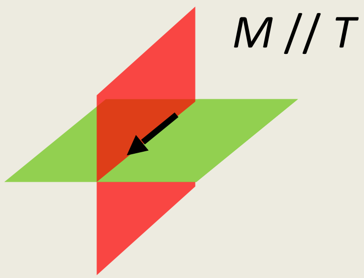
1. per 2d unit cell*, or
2. per 1d unit cell defined by translation along a mirror axis, or
3. at a C_2 rotation center.

*Translation, screw, glide

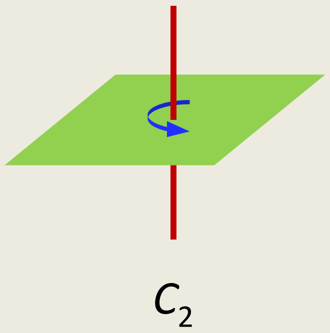
1.



2.



3.



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

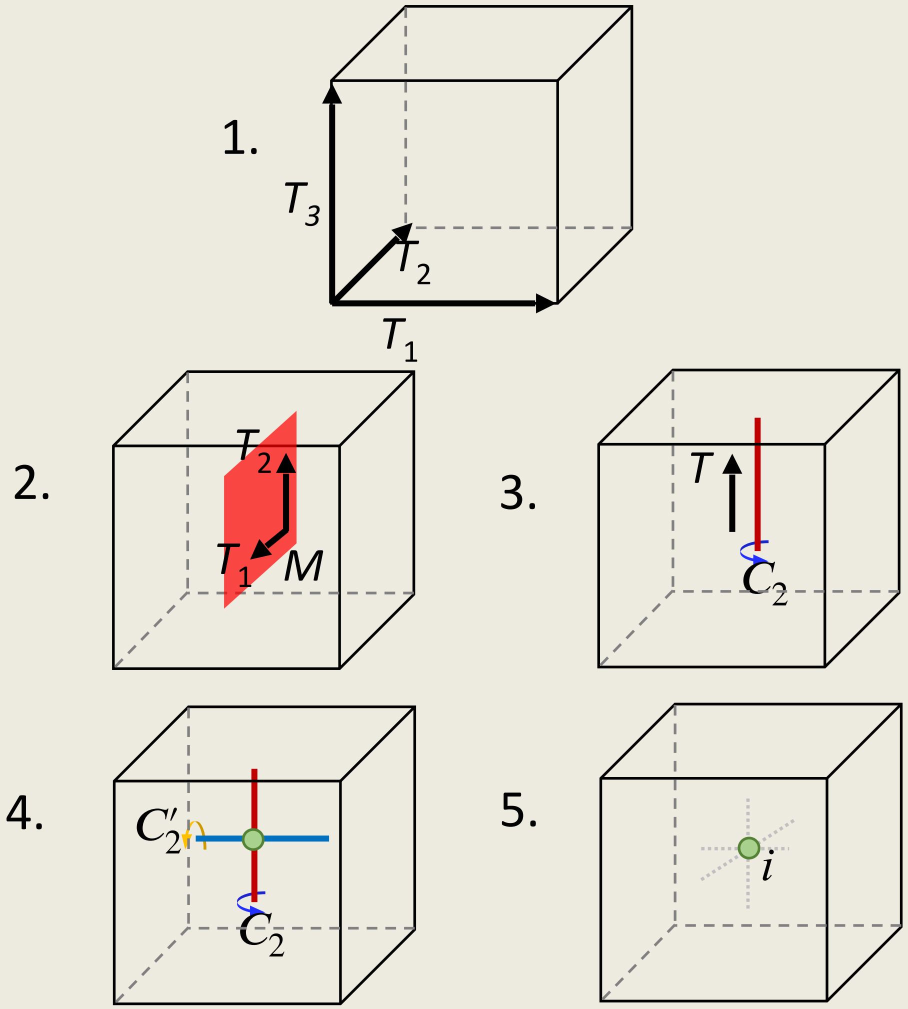
LSM for 3D magnets

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

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

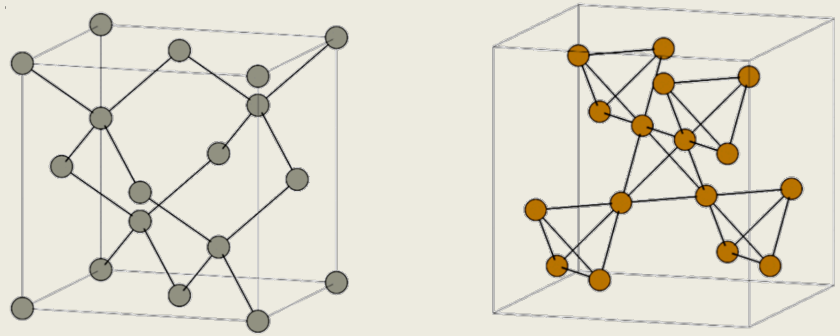
Assume the spin-1/2 lattice preserves lattice x SO(3) symmetry. Ground state *cannot be* a featureless paramagnet if the lattice has an odd number of spin-½'s

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.



Application:

The S=1/2 Heisenberg model *cannot* be a featureless paramagnet on the diamond or the pyrochlore lattice.



Overarching LSM

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

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]

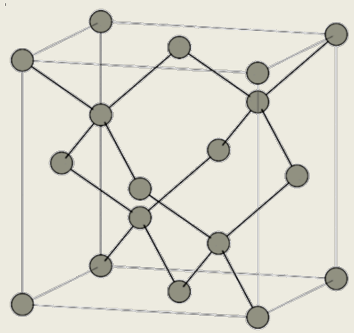
Multiplicity	Wyckoff letter	Site symmetry	Coordinates
4	e	1	(x,y,z) (-x,y+1/2,-z+1/2) (-x,-y,-z) (x,-y+1/2,z+1/2)
2	d	-1	(1/2,0,1/2) (1/2,1/2,0)
2	c	-1	(0,0,1/2) (0,1/2,0)
2	b	-1	(1/2,0,0) (1/2,1/2,1/2)
2	a	-1	(0,0,0) (0,1/2,1/2)

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)



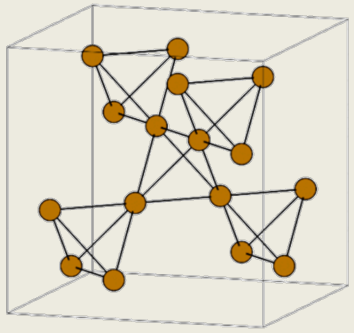


Table 232: IWPs and group cohomology at degree 3 of $Fd\bar{3}m$.

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

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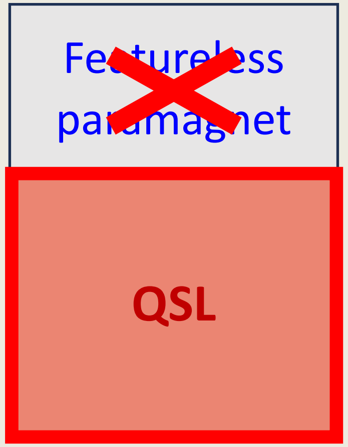
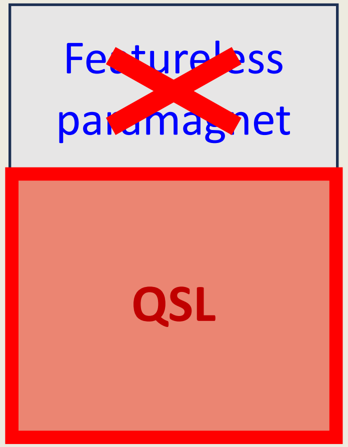
Topological theory of LSM

- Crystalline topological responses
- Applications (Triangular and pyrochlore lattice)



Topological crystalline response theory



— the topological theory behind LSM, that describes QSLs:

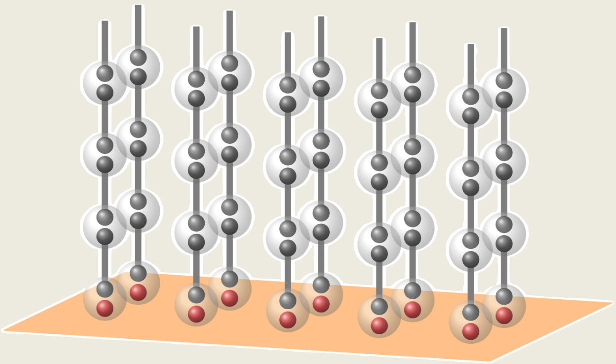
- G: crystallographic space group.
- A: gauge field of G.
- Topological Quantum Field Theory (TQFT):

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

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

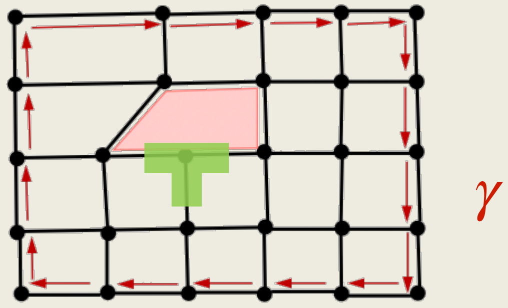
group cohomology

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



Topological crystalline response

= introducing a dislocation.



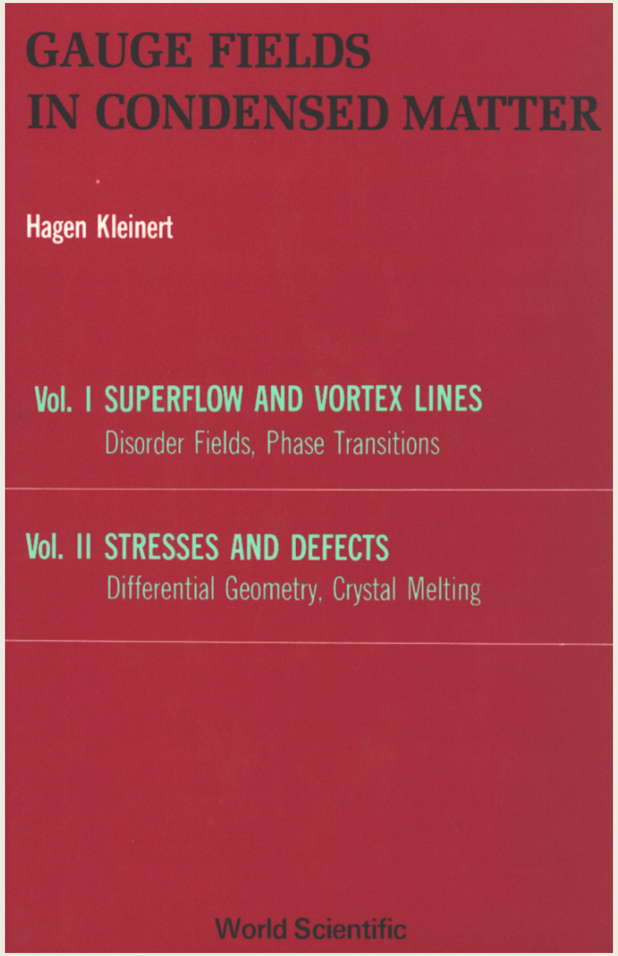
$$\partial_i u_j(\vec{r}) \to \partial_i u_j(\vec{r}) - \frac{a}{2\pi} R_{ij}(\vec{r})$$

Translation gauge field

Burgers vector

$$= \oint_{\gamma} \vec{R}$$

Dislocation = flux of R_{ij}



’t Hooft anomaly and anomaly inflow

‘t Hooft anomaly – two definitions: ‘t Hooft, ‘80

- *G* gauge symmetry in a classical system not preserved in the quantum system.
- Impossibility of having a unique, *G*-symmetric, SRE ground state.

Anomaly inflow: Callan, Harvey, '85

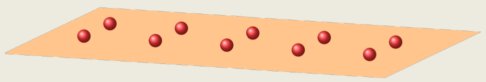
‘t Hooft anomaly can be cancelled by the boundary anomaly of a **TQFT** in one higher dimension.

- $Z[\mathscr{M}_{d+1}, A]$ not gauge invariant.
- $Z[\mathscr{M}_{d+1}] \neq 1.$

- $Z[\mathscr{M}_{d+2}, A]$ gauge invariant!
- $Z[\mathscr{M}_{d+2}] = 1$ exists!

A bulk-boundary correspondence for quantum magnets

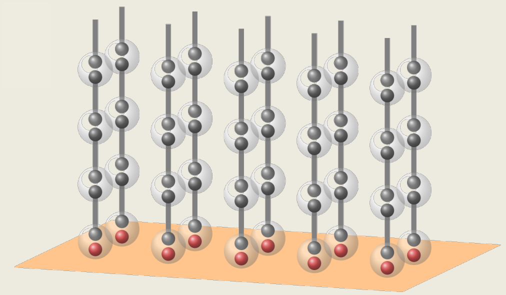
$Z[A]$ ***not*** faithful to



QSL in *d* spatial dim

- $Z[\mathscr{M}_{d+1}, A]$ not gauge invariant.
- $Z[\mathscr{M}_{d+1}] \neq 1.$

$Z[A]$ **is faithful to**



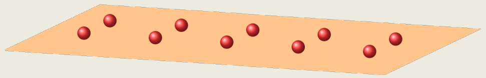
Trivial paramagnet in *d+1* spatial dim

QSL in *d* spatial dim

- $Z[\mathscr{M}_{d+2}, A]$ gauge invariant!
- $Z[\mathscr{M}_{d+2}] = 1$ exists!

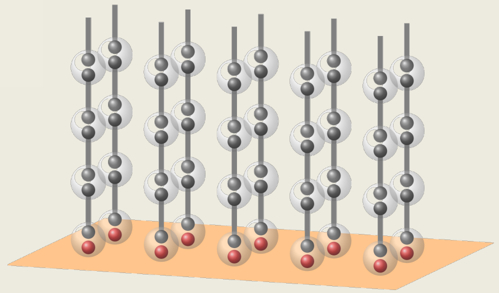
Topological crystalline response theory

$Z[A]$ ***not*** faithful to



QSL in *d* spatial dim

$Z[A]$ **is faithful to**



Trivial paramagnet in *d+1* spatial dim

QSL in *d* spatial dim

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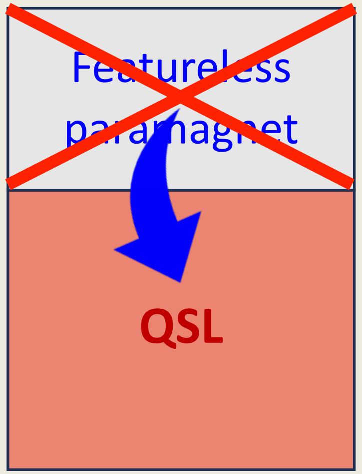
group cohomology

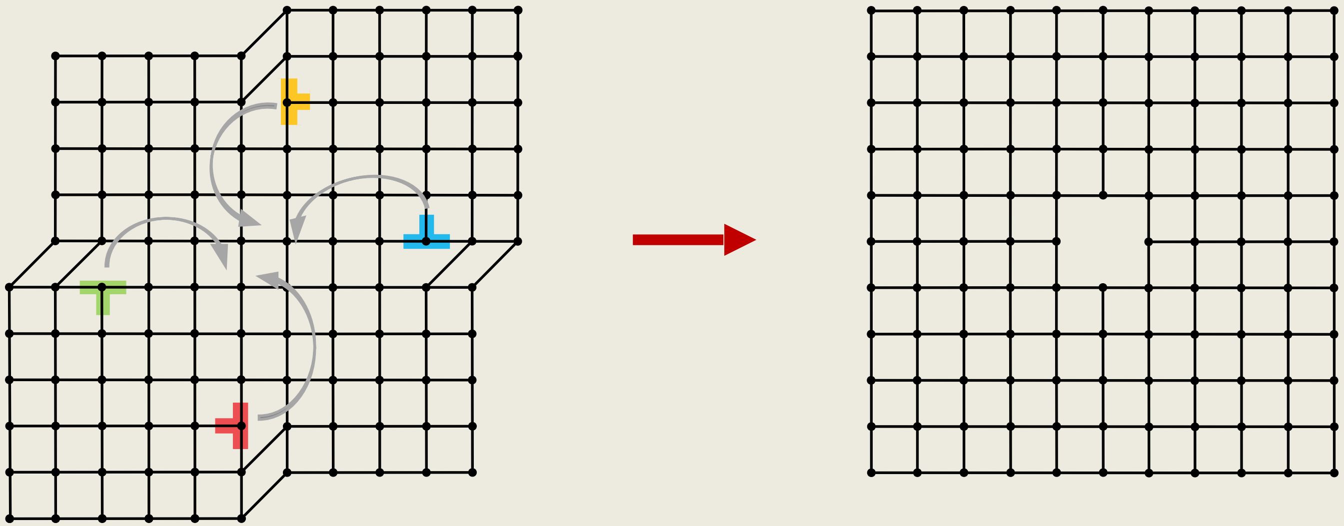
Cheng, Zaletel, Barkeshli, Vishwanath, Bonderson, PRX '16; Else, Thorngren, PRB '20

LSM as a topological crystalline response

<u>Theorem</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.



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



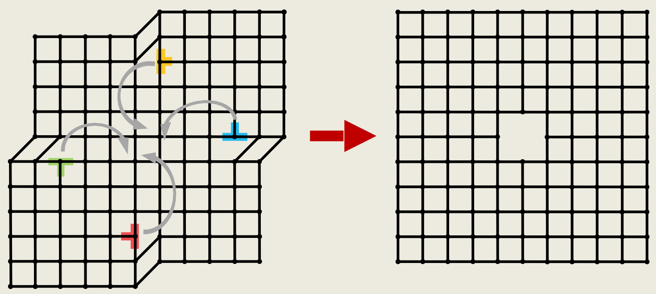
Wang, CL, Lu, PRB '24

Topological crystalline response – viewpoint 1

Theorem (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.

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

	$\mathbb{Z}^2$ (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

<u>Theorem (LSM)</u>. In a 2D lattice with spin-1/2's and translation x 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.

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

	$\mathbb{Z}^2$ (Translation)	$SO(3)$ (spin rotation)
Charge (linear or proj. rep)	momentum	spin-1/2 or spin-1
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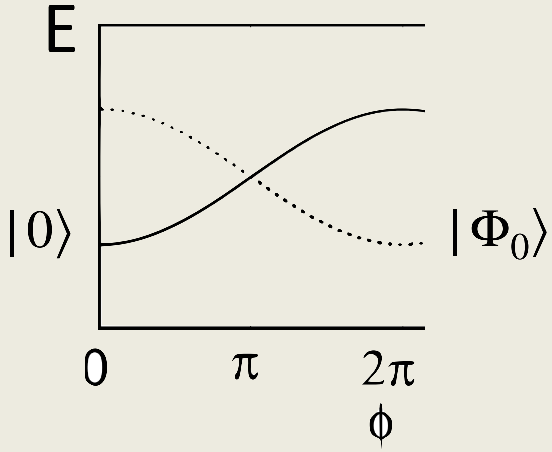

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Oshikawa, PRL '00;
Hastings, PRB '04

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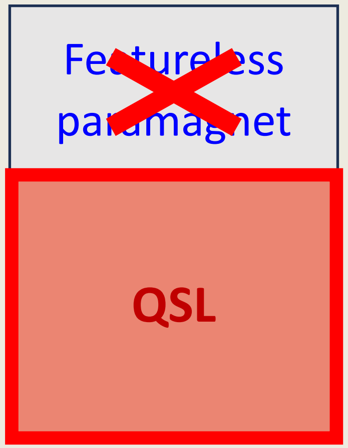
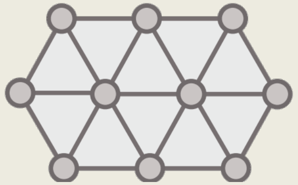


Application I – stability of DSL on triangular J1-J2

Numerics indicate a QSL g.s. with emergent U(1) gauge field and Dirac spinon (QED3), but it remains to show stability of QED3 on triangular lattice.

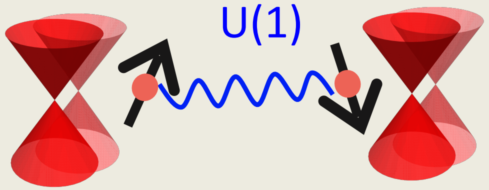
UV



Triangular lattice,

$S = 1/2,\ J_1/J_2 \approx 1/8$

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**

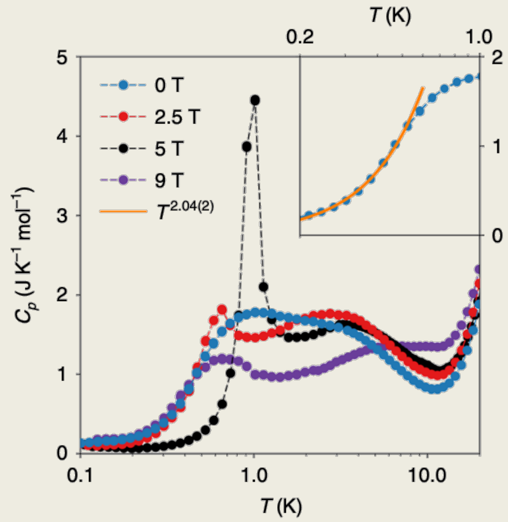
Song, He, Vishwanath, Wang, PRX '20

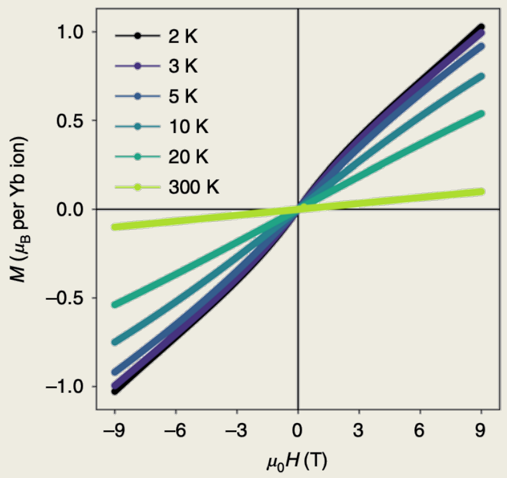
$$\Delta\mathscr{L} = \Phi_1\Phi_2\Phi_3 + h.c.$$

Monopoles irrelevant; DSL is **Stable** in triangular J1-J2!

Song, Wang, Vishwanath, He, Nat Comms '19.

Exp. advance: $NaYbO_2$ as a quantum paramagnet



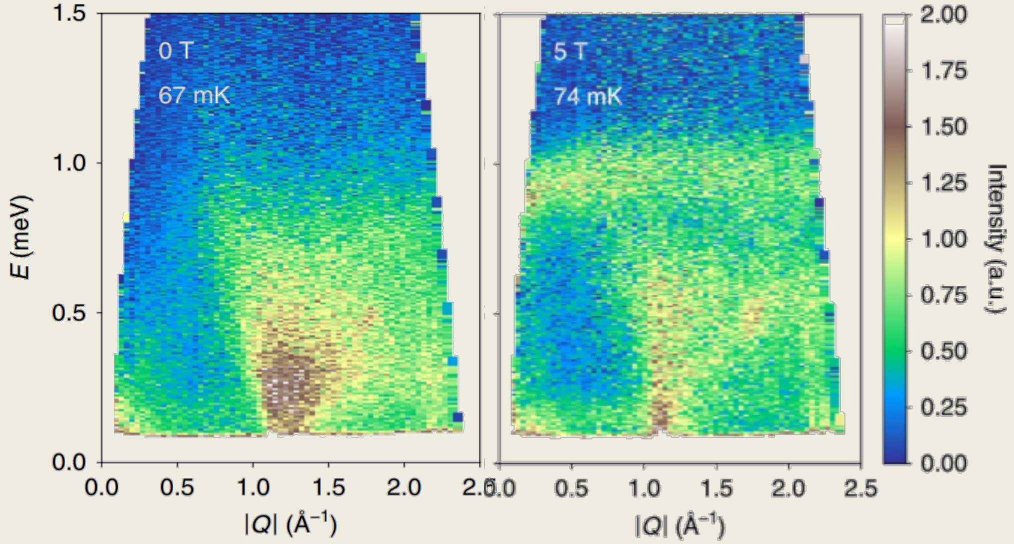


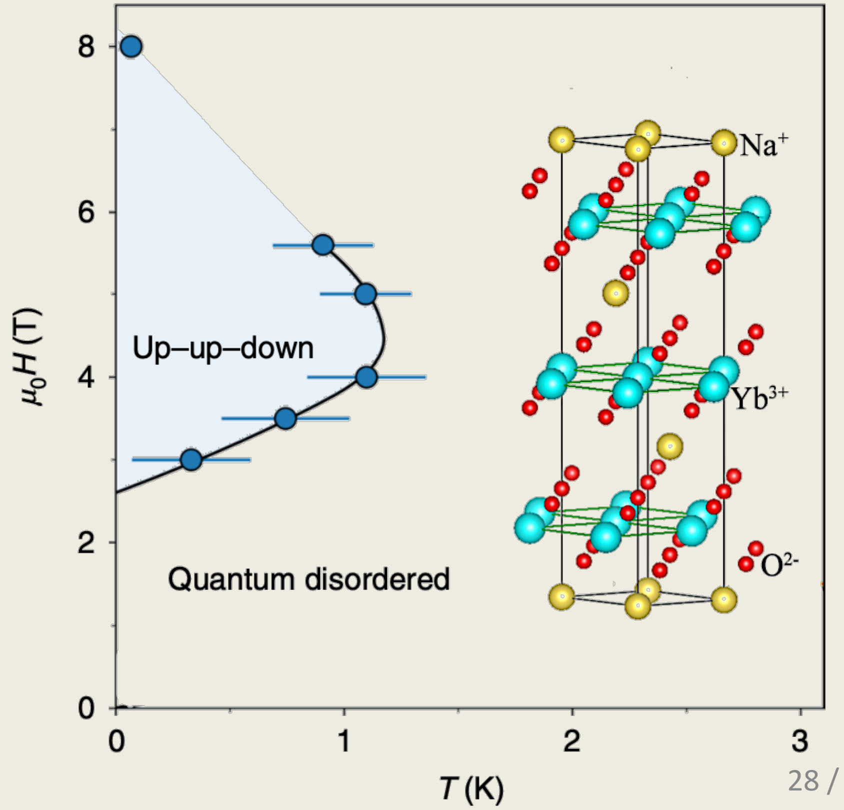
nature physics

29 July 2019

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

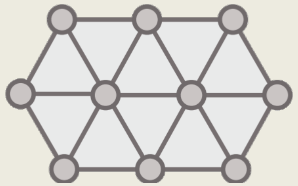
Bordelon, Kenney, CL, Hogan, Posthuma, Kavand, Lyu, Sherwin, Butch, Brown, Graf, Balents, Wilson





Application II – Stability of DSL in $NaYbO_2$

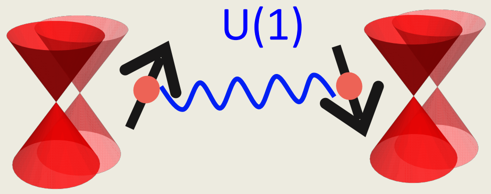
Topological crystalline response allows to determine the stability of DSL(s):



UV

(Triang. XXZ + SOC)

↓



IR

(DSL)

SciPost | SciPost Phys. 13, 066 (2022)

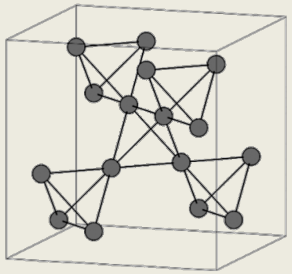
Topological characterization of Lieb-Schultz-Mattis constraints and applications to symmetry-enriched quantum criticality

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**."*

Background: Quantum spin ice on pyrochlore lattice

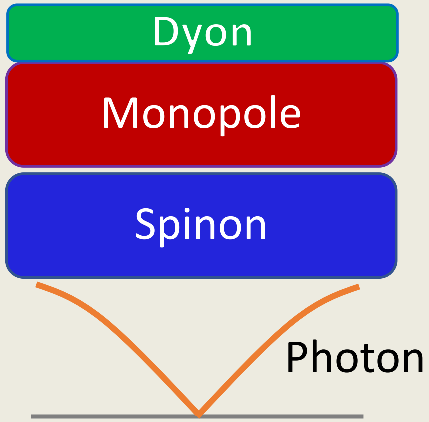
S = 1/2 XXZ model on pyrochlore has a QSL ground state, with emergent Maxwell photons:



UV

Pyrochlore lattice

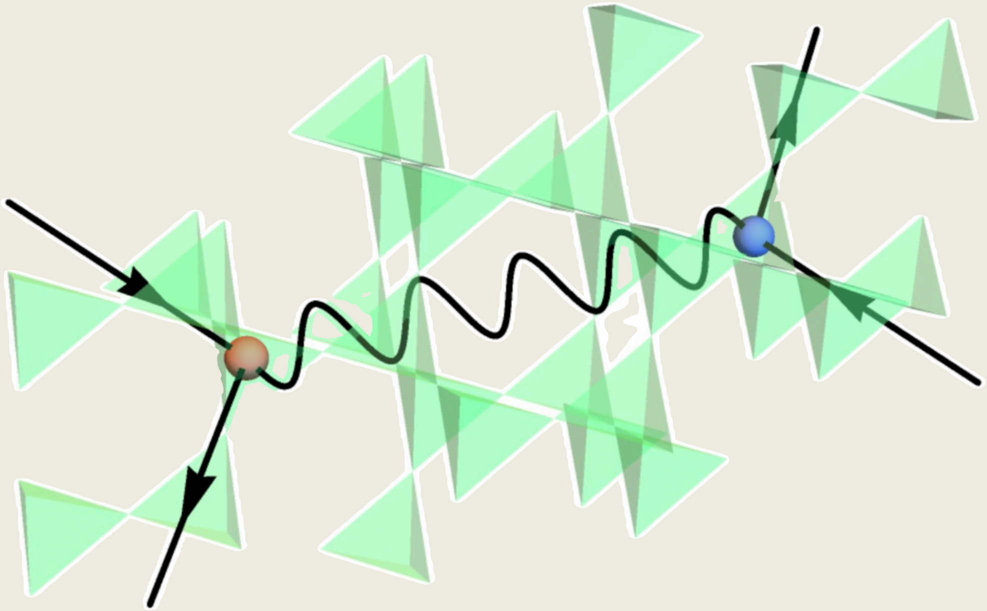
S = ½ *XXZ* model



IR

Emergent

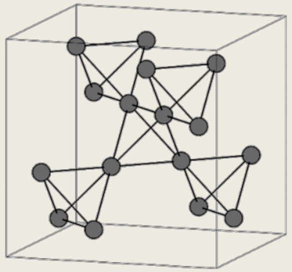
3+1D Maxwell



Hermele, Fisher, Balents, PRB '04

Application III – Monopole quantum numbers in QSI

Topological crystalline response allows to determine monopole properties:



UV

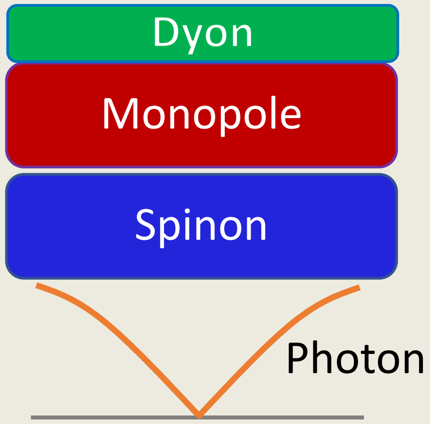
Pyrochlore lattice

S = ½ *XXZ* model

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

Topological crystalline response

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



Hermele, Fisher, Balents, PRB '04

IR

Emergent

3+1D Maxwell

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

Monopole quantum numbers (NEW!)

Nontrivial inversion & translation

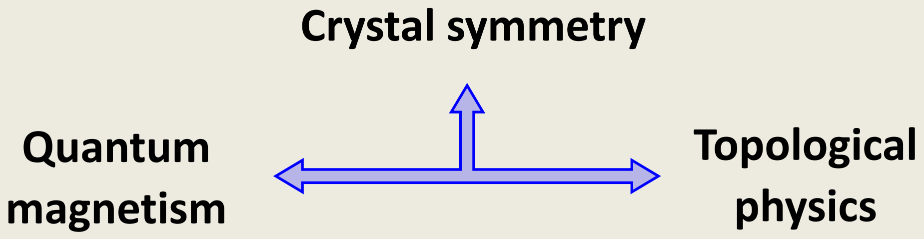
$$Z_e[A] = e^{i\pi(\omega_2^{\text{spin}} + \chi_1 B + \chi_2 B_\alpha)}$$

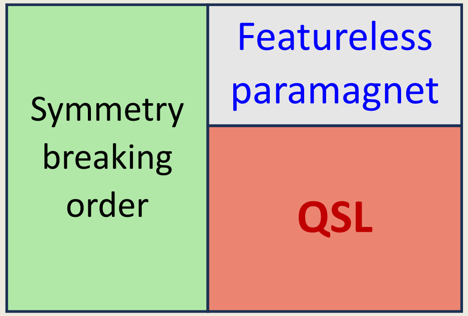
Spinon quantum numbers

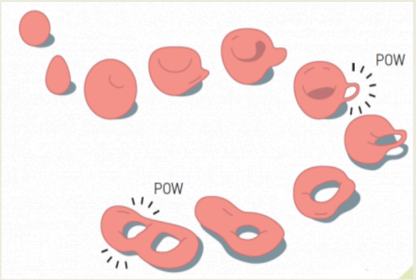
CL, Halász, Balents, PRB '21

Summary

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



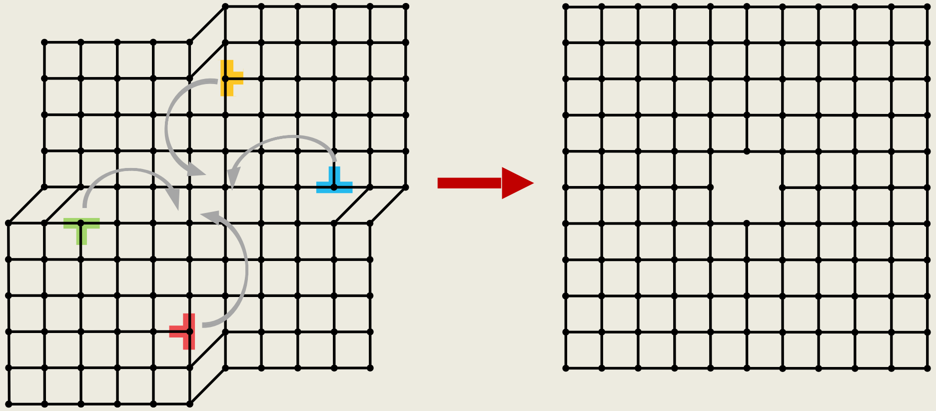




Challenges

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

Thank you for listening!