Characterizing 3D quantum paramagnets with Lieb-Schultz-Mattis constraints

arXiv:2410.03607

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LPTMC
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Crystallography, Group Cohomology, and Lieb–Schultz–Mattis Constraints

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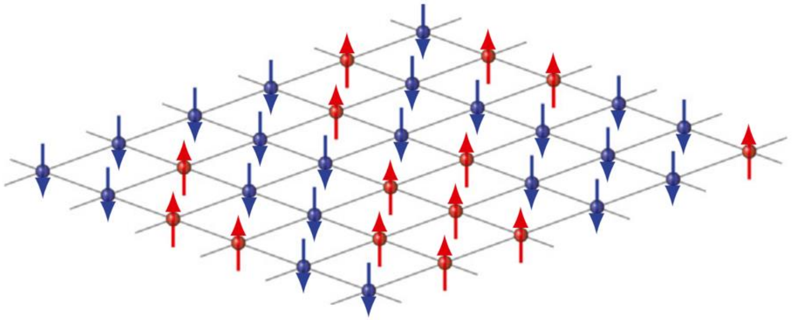
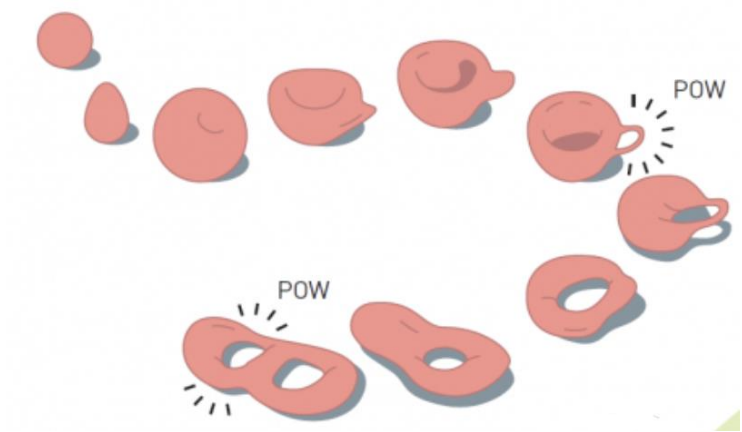
Weicheng Ye

(U of British Columbia)

Two main themes of my research:





1. Quantum magnetism in lattice spin systems
(Since my PhD in 2015)

2. Topological phases of matter
(Since my Postdoc in 2021)

In this talk, I will tell my efforts to study 1 using 2.

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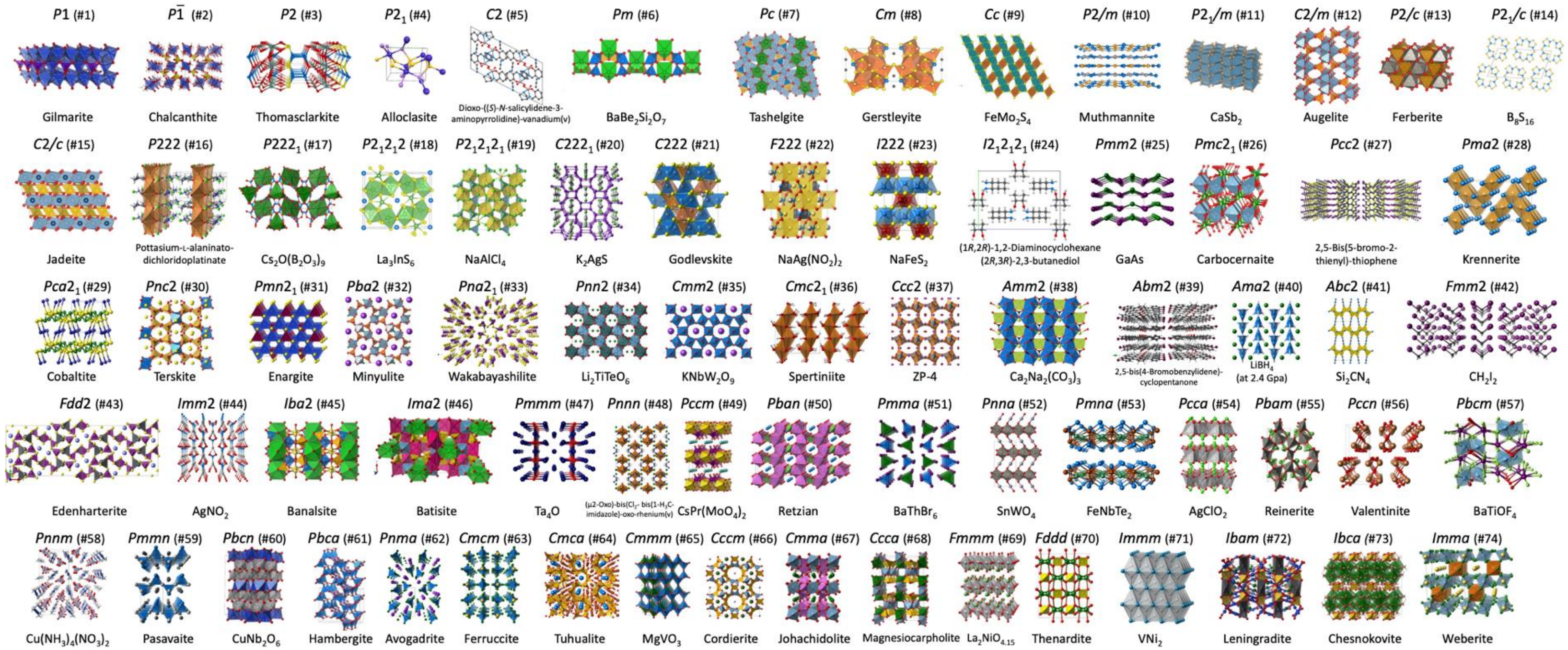
Crystallography, Group Cohomology, and Lieb–Schultz–Mattis Constraints

Chunxiao Liu[1] and Weicheng Ye[2]

Crystallographic group = Symmetry of crystals:



Frank Hoffmann, The Space Group List Project

Symmetry in physics

SSB 1	Symmetric 1
SSB 2	Symmetric 2
SSB 3	Symmetric 3
SSB 4	…
…	
Symmetry breaking	Symmetry preserving
`Group Theory 1.0`	**`Group Theory 2.0`**

Q: **`Group Theory 2.0`**?

- Symmetry classifies phases

Q: crystalline symmetries?

- Symmetry and response

$$\mathcal{L}_0 \rightarrow \mathcal{L}_0 - A_\mu j^\mu$$

Q: consistency principle?

- Choice of symmetry depends on the theory

Translation $\rightarrow Z_2$: $\phi \rightarrow -\phi$

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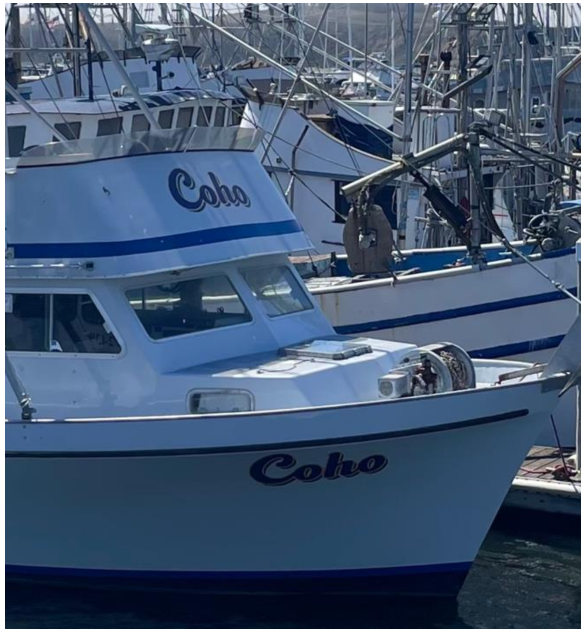
Group Theory 2.0

Crystallography, $\boxed{\text{Group Cohomology,}}$ and Lieb–Schultz–Mattis Constraints

Chunxiao Liu[1] and Weicheng Ye[2]



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Main results

A correspondence between high symmetry points in crystals and their topological data.

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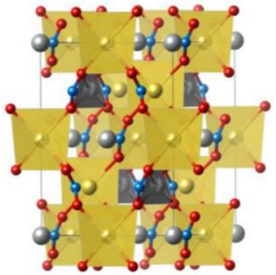


Wyckoff position	Little group	Coordinates	LSM anomaly class $\lambda \in H^3(G, \mathbb{Z}_2)$	Topological invariant
1a	D_2	$(0, 0, 0)$	$(A_c + A_{c'} + A_x)(A_c + A_y)(A_{c'} + A_z)$	$\varphi_2[C_2, C_2']$
1b	D_2	$(1/2, 0, 0)$	$A_x(A_c + A_y)(A_{c'} + A_z)$	$\varphi_2[T_1C_2, T_1C_2']$
1c	D_2	$(0, 1/2, 0)$	$(A_c + A_{c'} + A_x)A_y(A_{c'} + A_z)$	$\varphi_2[T_2C_2, C_2']$
1d	D_2	$(0, 0, 1/2)$	$(A_c + A_{c'} + A_x)(A_c + A_y)A_z$	$\varphi_2[C_2, T_3C_2']$
1e	D_2	$(1/2, 1/2, 0)$	$A_xA_y(A_{c'} + A_z)$	$\varphi_2[T_1T_2C_2, T_1C_2']$
1f	D_2	$(1/2, 0, 1/2)$	$A_x(A_c + A_y)A_z$	$\varphi_2[T_1C_2, T_1T_3C_2']$
1g	D_2	$(0, 1/2, 1/2)$	$(A_c + A_{c'} + A_x)A_yA_z$	$\varphi_2[T_2C_2, T_3C_2']$
1h	D_2	$(1/2, 1/2, 1/2)$	$A_xA_yA_z$	$\varphi_2[T_1T_2C_2, T_1T_3C_2']$

Lattice data

Topological data

Group Theory 2.0

Connection!

Plan of talk

Quantum magnetism

- a phase diagram

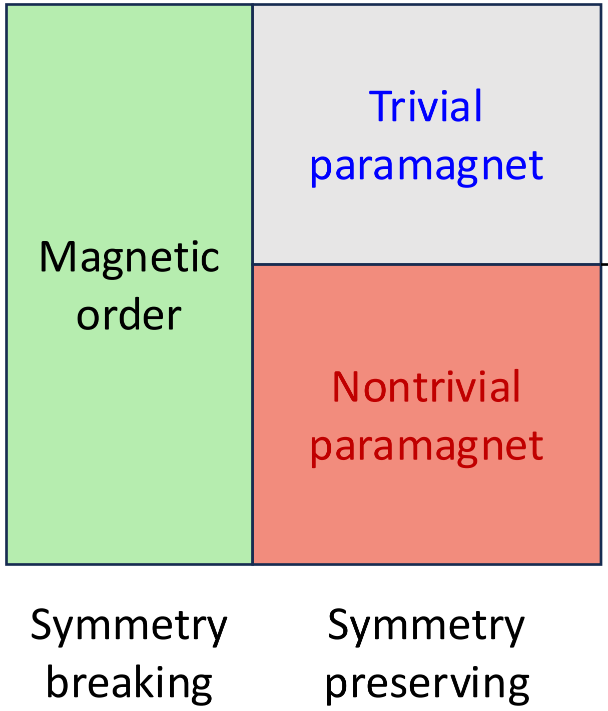
Lieb-Schultz-Mattis (LSM) theorems

- a history
- new results in 3D

LSM and topological responses

- crystalline fields and responses
- case study: QSLs

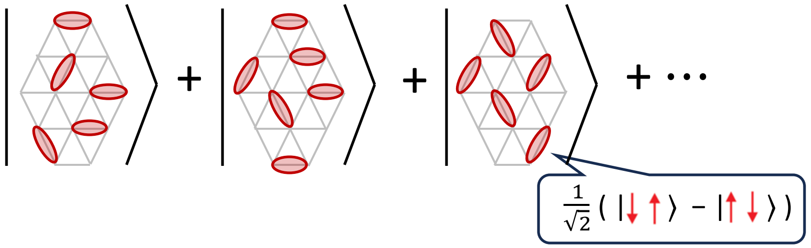
Quantum magnetism



S = 1 chain: $H = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$

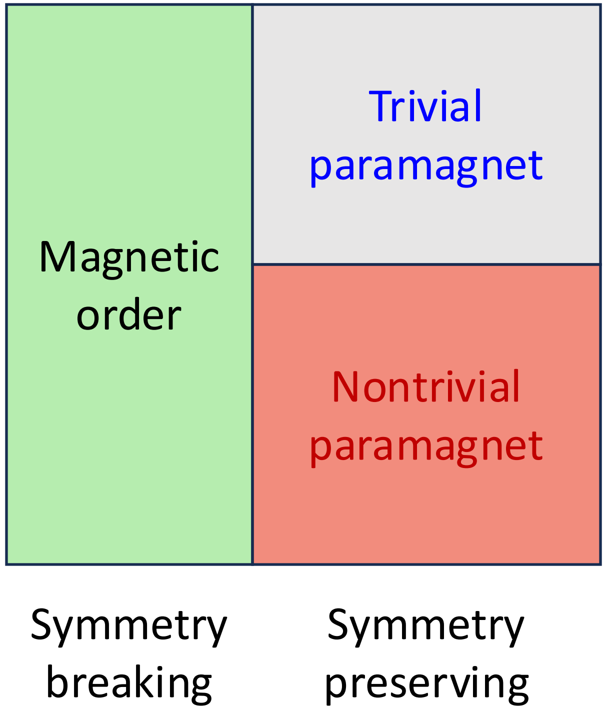
S = 1/2 chain

$|\mathrm{RVB}\rangle =$



P.Anderson, F.D.M.Haldane

Quantum paramagnetism



“insulator”

“liquid”

- A trivial paramagnet = a unique, symmetric, short-range entangled, gapped ground state.
- A nontrivial paramagnet is its complement (so has long-range entanglement).

Q: When can a trivial paramagnet exist at $T = 0$?

Plan of talk

Quantum magnetism

- a phase diagram

Lieb-Schultz-Mattis (LSM) theorems (When a **trivial paramagnet** cannot exist)

- a history
- new results in 3D

LSM and topological responses

- crystalline fields and responses
- case study: QSLs

Original Lieb-Schultz-Mattis (LSM)

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

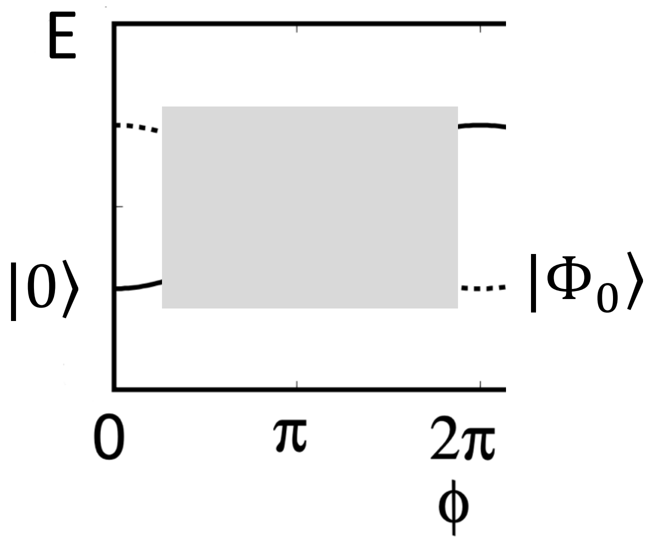
Thm. In a spin chain with translation symmetry and on-site SO(3) symmetry. If there are odd numbers of spin-1/2's per unit cell, then the ground state cannot be a trivial paramagnet.

(unique, symmetric, gapped 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

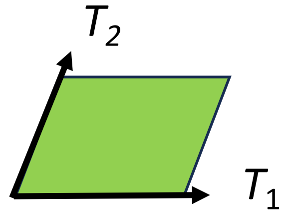
<u>Theorem (LSM in 2D).</u> Po, Watanabe, Jian, Zaletel, PRL '17

Assume the magnet preserves lattice x SO(3) symmetry. No trivial paramagnetic ground state can exist if the lattice has an odd number of spin-½'s

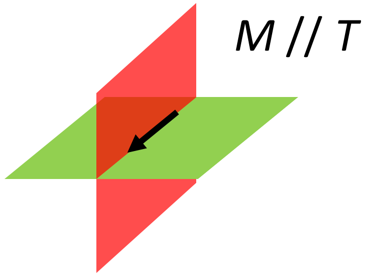
Translation, screw, glide

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

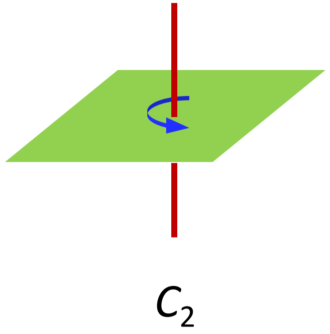
1.



2.



3.



Direct application:

1. The S=1/2 J_1-J_2 model on the triangular lattice cannot be a trivial paramagnet.
2. A S=1/2 trivial paramagnet exists on the honeycomb lattice.

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

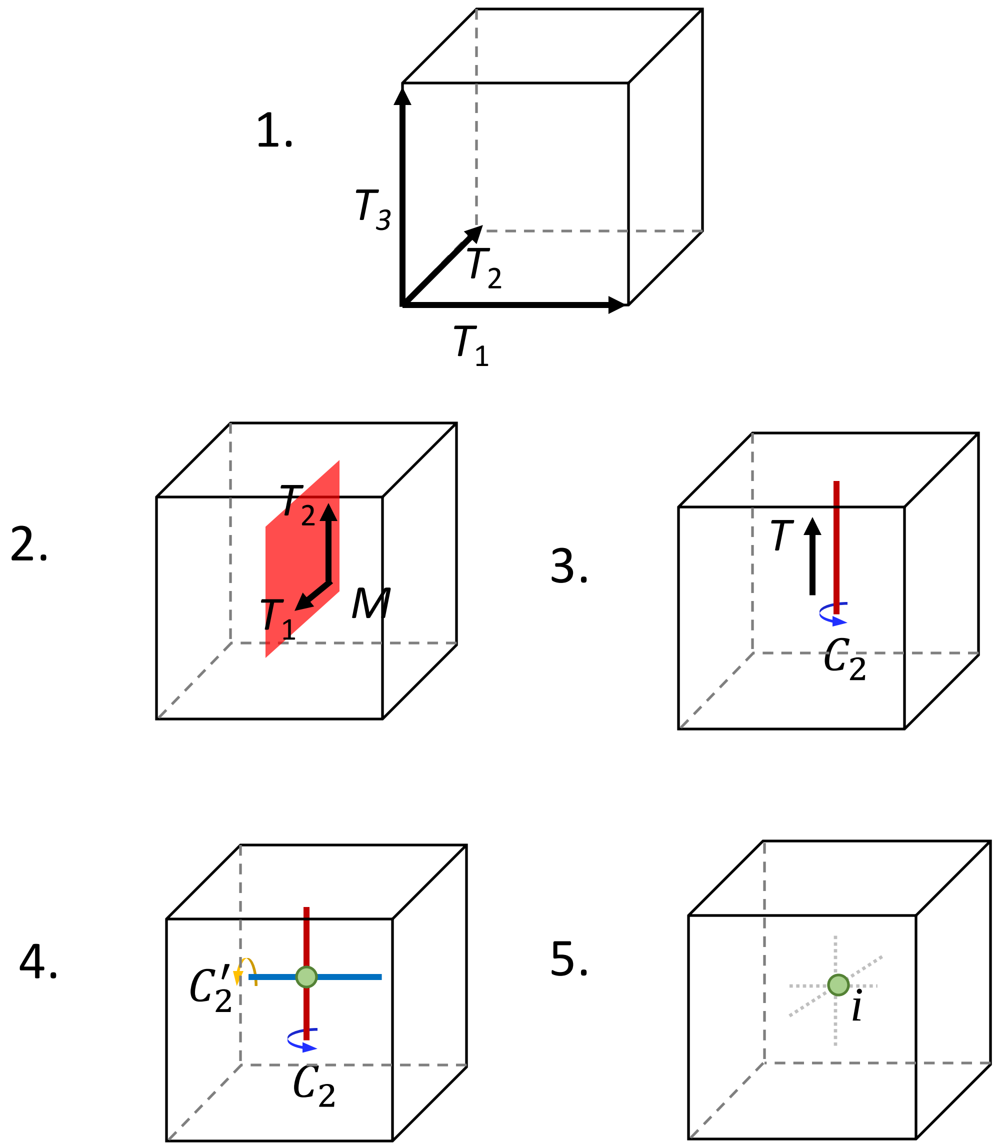
The complete LSM theorems in 3D

CL, Ye, arXiv:2410.03607

<u>Theorem (LSM in 3D).</u>

Assume the magnet preserves lattice x SO(3) symmetry.
No trivial paramagnetic ground state can exist
if the lattice has an odd number of spin-½'s

1. per **3d unit cell***, or
2. per **2d unit cell*** on a mirror plane, or
3. per **1d unit cell** along a C_2 axis, or
4. intersection of two C_2 axes, or
5. at a 3D **inversion center.**

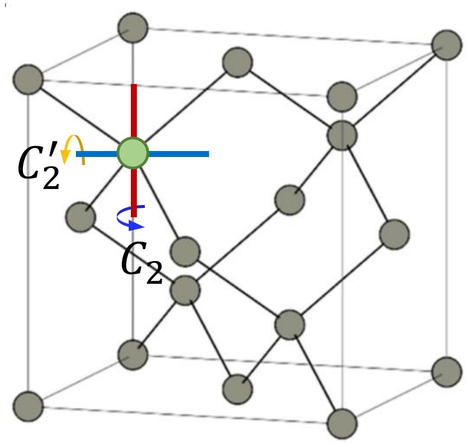


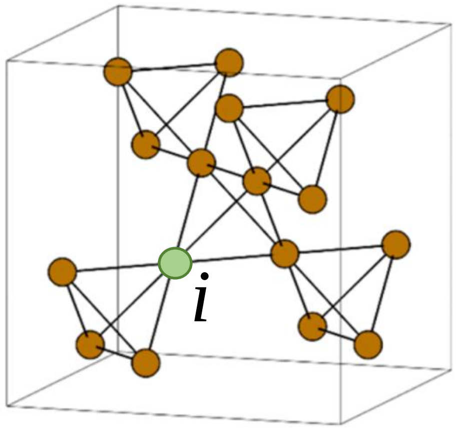
3D LSM – application

CL, Ye, arXiv:2410.03607

1. The S=1/2 Heisenberg/XXZ model on the diamond lattice cannot be a trivial paramagnet.

2. The S=1/2 Heisenberg/XXZ model on the pyrochlore lattice cannot be a trivial paramagnet.





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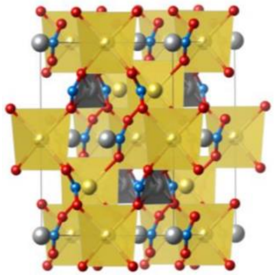

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1h	D_2	$(1/2,1/2,1/2)$	$A_xA_yA_z$	$\varphi_2[T_1T_2C_2, T_1T_3C_2']$

Lattice data

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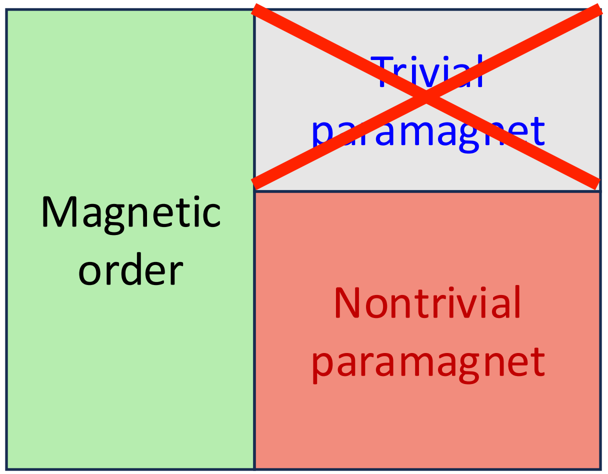
- new results in 3D

LSM and topological responses

- crystalline fields and responses
- case study: QSLs



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Crystallography, $\boxed{\text{Group Cohomology,}}$ and Lieb–Schultz–Mattis Constraints

Chunxiao Liu[1] and Weicheng Ye[2]

Topological response theory to crystalline symmetries!

Response theory – a crash course

In a *charge transport experiment:*

- Fixed total charge
- Apply an electric field
- Attach leads (source & drain)
- Measure current
- Quantized conductivity

Formally:

- U(1) symmetry
- Couple with a U(1) gauge field
- Perturb U(1) symmetry
- Write down response theory
- Topological response

For every symmetry there is a response theory.

To study response, need to first break that symmetry!

Apply a translation gauge field

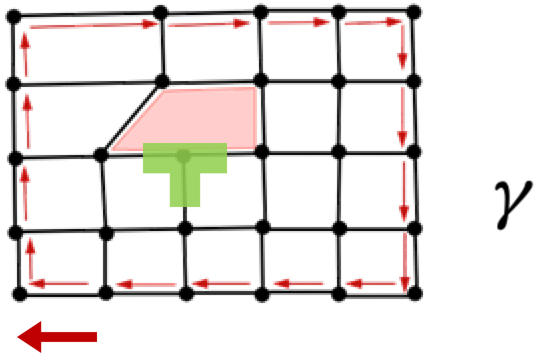
= introducing a dislocation.

Origin of gauge freedom: coordinates label up to integers

$$\partial_i u_j(\vec{r}) \to \partial_i u_j(\vec{r}) - \frac{a}{2\pi} R_{ij}(\vec{r}) \qquad \tfrac{1}{2\pi} R_{ij} \in \mathbb{Z}$$

Dislocation = flux of the translation gauge field.

$\oint_\gamma \vec{R}$ gives the Burgers vector for dislocations contained in γ.

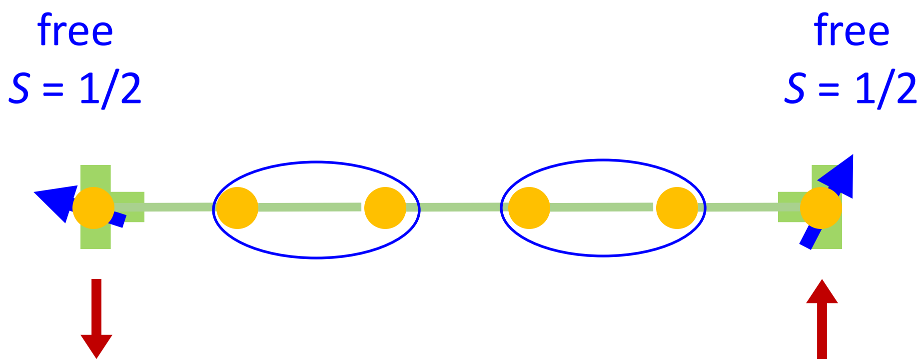


Burgers vector for dislocation associated with broken T_y

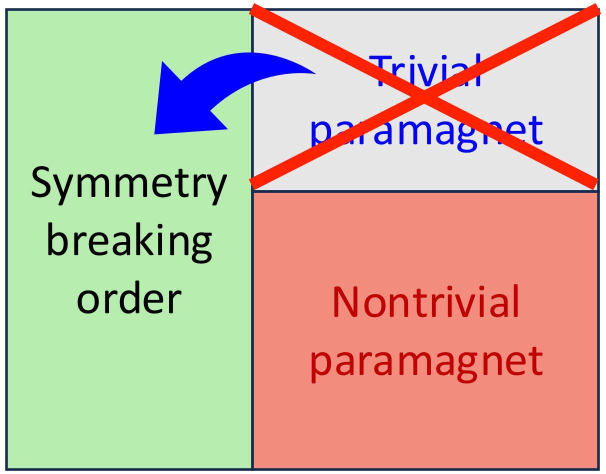
Manjunath, Barkeshli, PRR '21;
Field Theory of Multiscale Plasticity, Hasebe, '23

Crystalline response – 1D example

Boundary can have a (free) spin-1/2:



Burgers vector associated with broken T_x



Symmetry:
$\mathbb{Z} \times SO(3)$

1D LSM can be reformulated as a crystalline response theory:

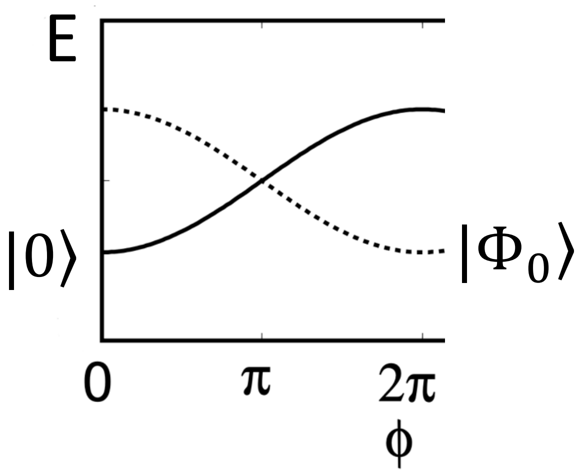
In a spin-1/2 chain with translation x SO(3) symmetry, a dislocation (boundary) binds a spin-1/2.

Written as

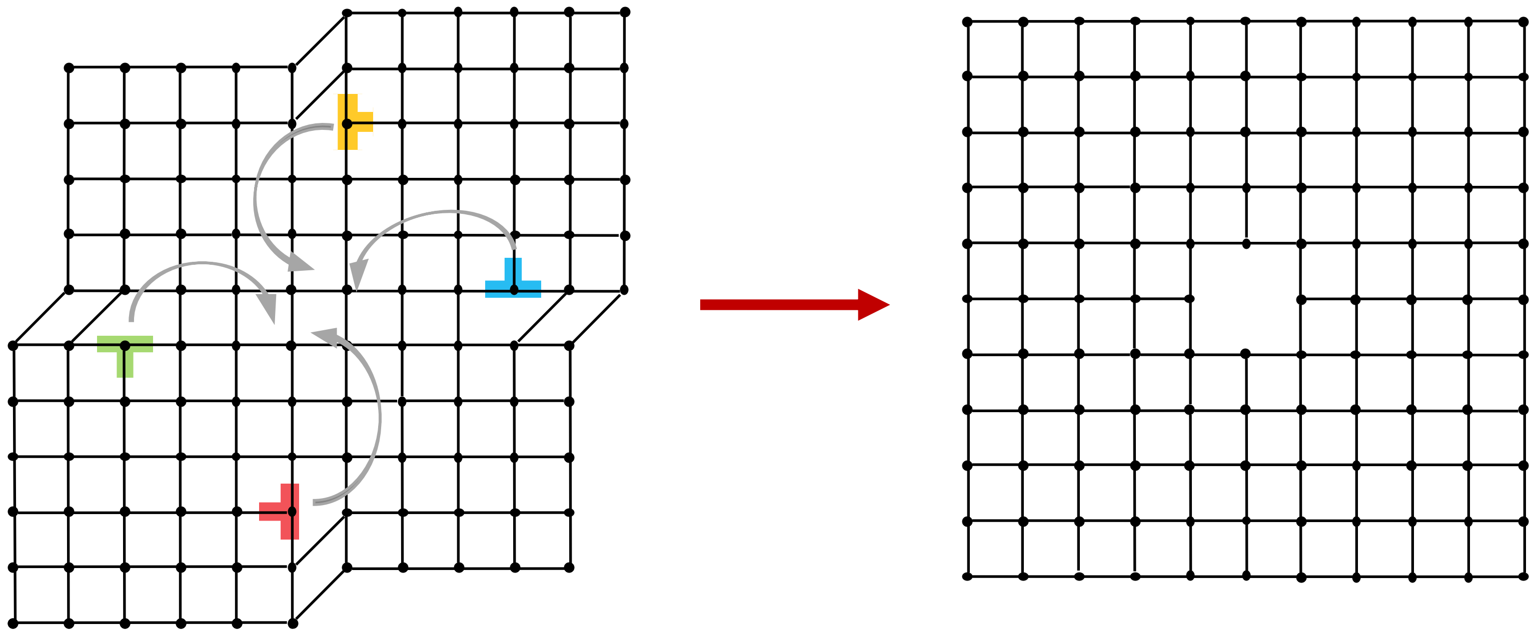
$$Z_{1\mathrm{D}} = e^{i\pi \int_{\mathcal{M}_3} A_x \cup \omega_2^{\mathrm{spin}}}$$

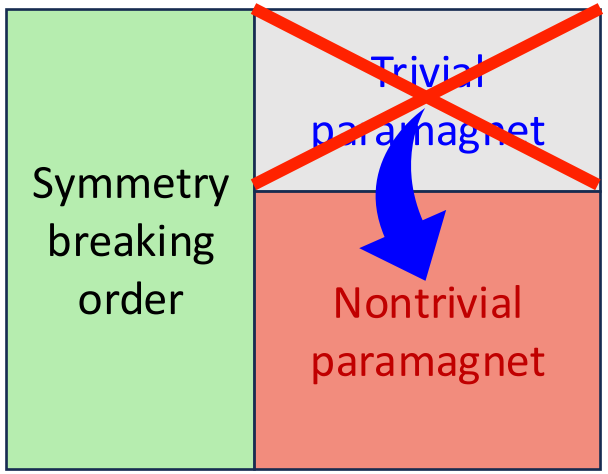
This complements the flux threading argument:

SO(3) defect binds crystal charge!
(=flux) (=momentum)



Crystalline response – 2D example





Symmetry:
$\mathbb{Z}^2 \times SO(3)$

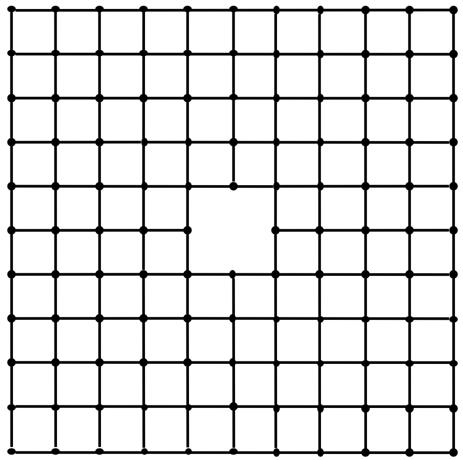
Wang, **CL**, Lu, PRB '24

2D LSM can be reformulated as a crystalline response theory:

In a 2D lattice magnet with spin-1/2 and translation x SO(3) symmetry, fusing four dislocations leaves no dislocations behind, but traps a spin-1/2.

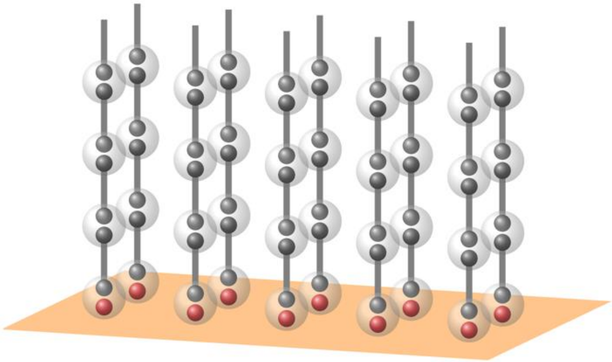
Written as

$$\boxed{Z_{2\mathrm{D}} = e^{i\pi \int_{\mathcal{M}_4} A_x \cup A_y \cup \omega_2^{\mathrm{spin}}}}$$

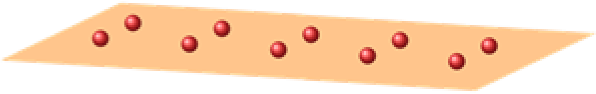


Bulk-boundary correspondence for quantum paramagnets

A nontrivial paramagnets in ***d*** dim can exist at the boundary of certain ***trivial*** paramagnet in ***d*+1** dim.



Trivial in *d*+1 spatial dim



Nontrivial in *d* spatial dim

Nontrivial is not trivial.

Trivial is not trivial.

P.Anderson, F.D.M.Haldane

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

Topological crystalline response – general theory

Global symmetry: $G \times SO(3)$

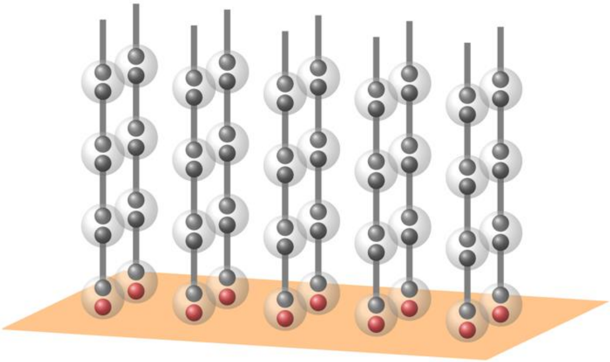
(Group Theory 1.0)

$$\boxed{Z = e^{i\pi \int_{\mathcal{M}_{d+2}} \underline{\lambda} \cup \underline{\omega_2^{\text{spin}}}}}$$

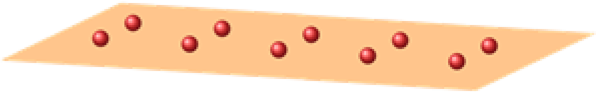
(Group Theory 2.0)

$\underline{\lambda \in H^d(G, \mathbb{Z}_2)}$

S=1/2 or S=1



Trivial in *d*+1 spatial dim



Nontrivial in *d* spatial dim

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

Plan of talk

Quantum magnetism

- a phase diagram

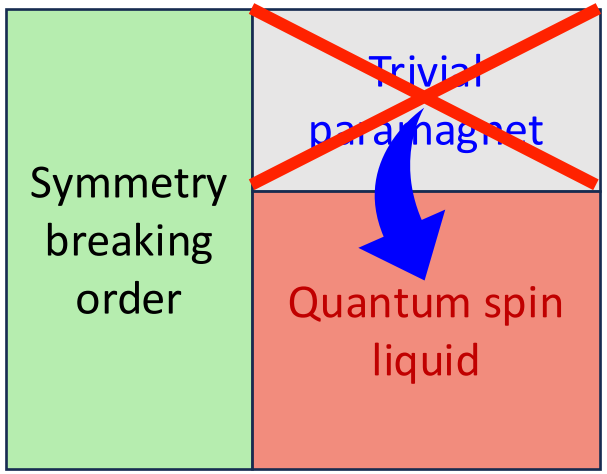
Lieb-Schultz-Mattis (LSM) theorems

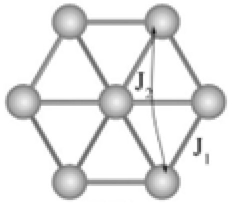
- a history
- new results in 3D

LSM and topological responses

- crystalline fields and responses
- case study: QSLs

Quantum spin liquids





Triangular lattice

S = ½ J_1-J_2 model

Numerical evidence

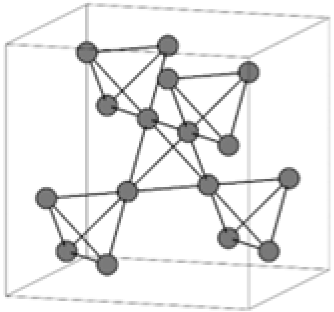
Dirac spin liquid

(2+1D QED3)

Iqbal, Hu, Thomale, Poilblanc, Becca, PRB '16; Iaconis, **CL**, Halász, Balents, Scipost '18; Wietek, Capponi, Läuchli, PRX '24…

UV

IR



Pyrochlore lattice

S = ½ *XXZ* model

Exact mapping
$S_i^{\pm} \sim e^{\pm i\, A_i}, S_i^z \sim E_i$

Quantum spin ice

(3+1D Maxwell)

Hermele, Fisher, Balents, PRB '04

Dirac spin liquid in triangular lattice magnet

nature physics

29 July 2019

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

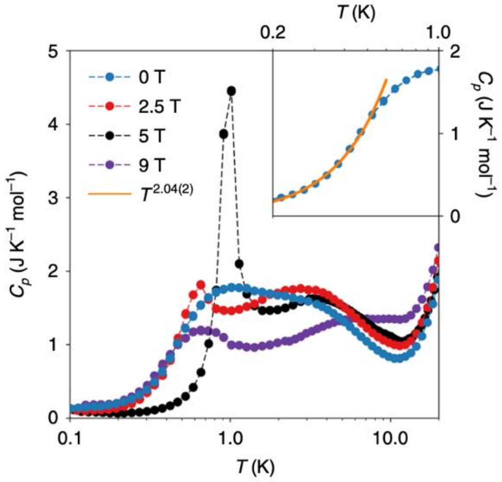
Bordelon, Kenney, CL, Hogan, Posthuma, Kavand, Lyu, Sherwin, Butch, Brown, Graf, Balents, Wilson

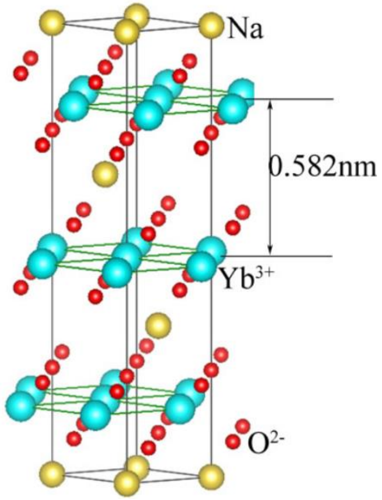
SciPost

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]





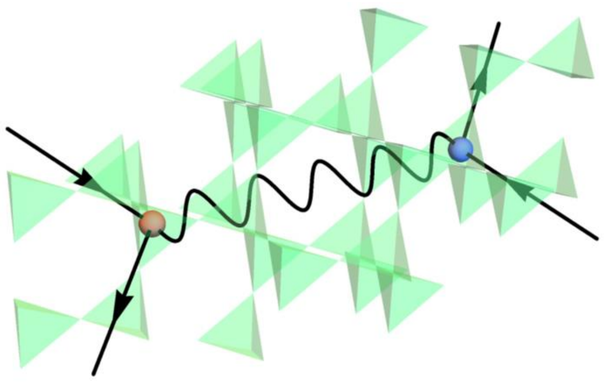
$NaYbO_2$

"… As a concrete example, we find that a DSL can be stable in a recently proposed candidate material, $NaYbO_2$."

$NaYbO_2$: a promising candidate for Dirac spin liquid!

Anomaly matching for quantum spin ice

Pyrochlore lattice



UV

IR

symmetry fractionalization

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

$$Z_m = \exp\left(i\pi(A_i^2 + B_{xy+xz+yz})\right)$$

Inversion translation

CL, Ye, arXiv:2410.03607

$$Z_e = \exp\left(i\pi w_2^{SO(3)} + i\chi_1 B_{xy+xz+yz} + i\chi_{\overline{C}_6 S} B_\alpha)\right)$$

(spinon) Translation rotation

CL, Halász, Balents PRB '21

Mathematics

CL, Ye, arXiv:2410.03607

https://gap-packages.github.io/hap/tutorial/chap8_mj.html

8.6-2 Mod 2 cohomology rings of 3-dimensional crystallographic groups

For a crystallographic group G, we

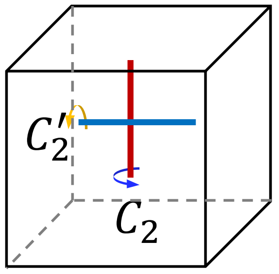
- proved that the cohomology ring $H^*(G,F)$ is finitely generated;
- obtained the mod-2 cohomology ring $H^*(G,Z_2)$;
- obtained explicit 1-, 2-, and 3-cocycle functions;
- give a mathematical criterion for LSM anomalies;
- identified topological invariants for the cocycles.

```
gap> SpaceGroupCohomologyRingGapInterface(30);
==========================================
Mod-2 Cohomology Ring of Group No. 30:
Z2[Ac,Am,Ax,Bb]/<R2,R3,R4>
R2:  Ac.Am  Am^2  Ax^2+Ac.Ax
R3:  Am.Bb
R4:  Bb^2
==========================================
LSM:
2a Ac.Bb+Ax.Bb
2b Ax.Bb
true
```

Topological invariants

CL, Ye, arXiv:2410.03607

Wyckoff position	Little group	Coordinates	LSM anomaly class $\lambda \in H^3(G, \mathbb{Z}_2)$	Topological invariant
1a	D_2	$(0,0,0)$	$(A_c + A_{c'} + A_x)(A_c + A_y)(A_{c'} + A_z)$	$\varphi_2[C_2, C_2']$
1b	D_2	$(1/2,0,0)$	$A_x(A_c + A_y)(A_{c'} + A_z)$	$\varphi_2[T_1C_2, T_1C_2']$
1c	D_2	$(0,1/2,0)$	$(A_c + A_{c'} + A_x)A_y(A_{c'} + A_z)$	$\varphi_2[T_2C_2, C_2']$
1d	D_2	$(0,0,1/2)$	$(A_c + A_{c'} + A_x)(A_c + A_y)A_z$	$\varphi_2[C_2, T_3C_2']$
1e	D_2	$(1/2,1/2,0)$	$A_xA_y(A_{c'} + A_z)$	$\varphi_2[T_1T_2C_2, T_1C_2']$
1f	D_2	$(1/2,0,1/2)$	$A_x(A_c + A_y)A_z$	$\varphi_2[T_1C_2, T_1T_3C_2']$
1g	D_2	$(0,1/2,1/2)$	$(A_c + A_{c'} + A_x)A_yA_z$	$\varphi_2[T_2C_2, T_3C_2']$
1h	D_2	$(1/2,1/2,1/2)$	$A_xA_yA_z$	$\varphi_2[T_1T_2C_2, T_1T_3C_2']$



$$\varphi_2(\lambda)[g_1, g_2] := \sum_{\text{cyc}} \lambda(g_1, g_2, g_2)$$

Lattice

Topological response

Connection!

Summary:

LSM theorems for 3D magnets

S=1/2 on high sym. pts. ⇒ no trivial paramagnet allowed

Topological crystalline responses

Crystalline defects carry free spin-1/2's

Anomaly matching for quantum spin liquids

Stability of Dirac QSL in triangular compound $NaYbO_2$

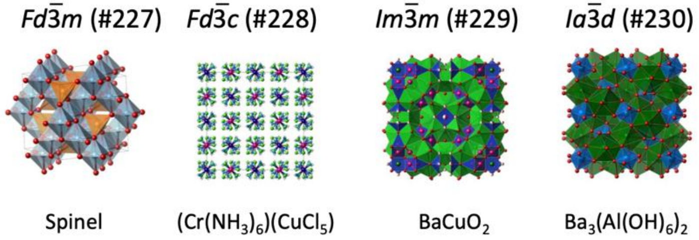
Symmetry fractionalization in U(1) QSL on pyrochlore

For Future:

Anomaly matching for more quantum spin liquids

Group cohomology -> Equivariant cohomology

Extending Lieb-Schultz-Mattis (hyperbolic, quasicrystal…)



Crystallography

Quantum magnetism ⟵ Group Cohomology ⟶ **Topological physics**

Magnetic order	Trivial paramagnet
	Nontrivial paramagnet