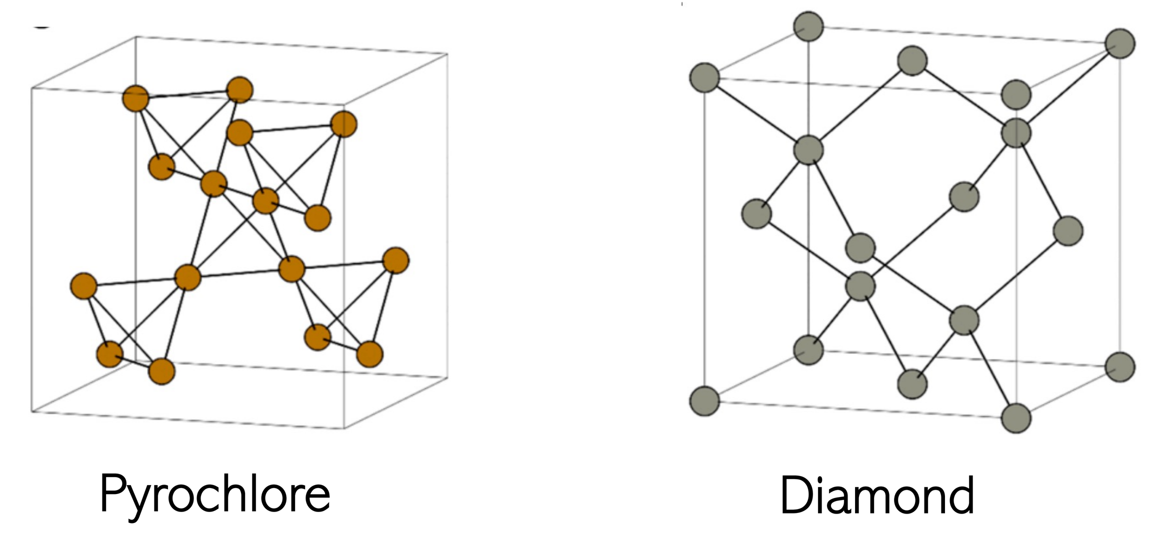
Towards a complete set of Lieb–Schultz–Mattis Theorems in 3D: application to the pyrochlore and diamond lattices*

Authors: Chunxiao Liu†, Weicheng Ye‡

† University of California, Berkeley ‡ University of British Columbia * work in progress.

Abstract

Lieb–Schultz–Mattis (LSM) theorem is a powerful statement about when the lattice symmetry of a quantum magnet forbids a trivial paramagnetic ground state. Two formalisms for the theorem have been established: one uses the notation of lattice homotopy [1] and the other uses the idea of quantum anomalies [2]. Here we discuss how these seemingly unrelated formalisms are unified, and how these ideas can be employed to obtain a set of complete LSM constraints in 3D lattice magnets. We will focus on the LSM theorem on the pyrochlore and diamond lattices, which host some of the prototypical spin liquids in 3D. We then go beyond the existing statement of the theorem by giving a detailed analysis of the microscopic origin of the LSM constraints. This analysis allows us to obtain and track the trivialization of the LSM constraints under the breaking of lattice symmetries. The principles and calculation methods presented here can be applied to all 3D lattice magnets.



LSM: a crash course

Definition: A trivial paramagnet (at $T = 0$) is a lattice magnet which has a unique, gapped, symmetric, short-range entangled ground state.

LSM theorems are conditions under which a lattice magnet *cannot* be a trivial paramagnet.

For $S = 1$ systems, a trivial paramagnetic phase can exist (the Haldane phase). Therefore, we will restrict ourselves to $S = 1/2$ systems from here on.

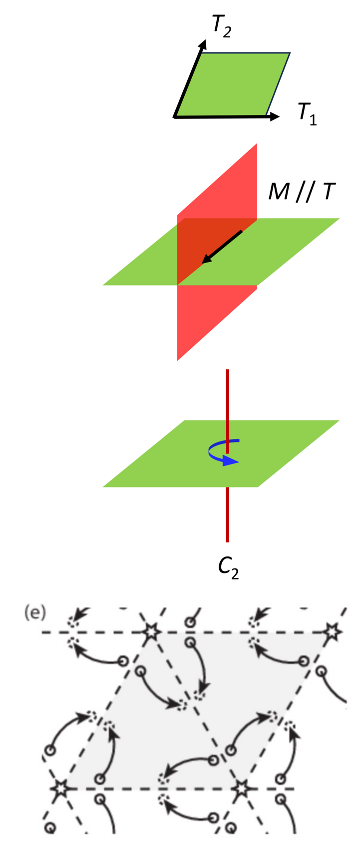
The LSM constraints are *consequences of lattice symmetry*. More precisely: interplay between onsite ($SO(3)$, or $O(2)$, or $\mathbb{Z}_2 \times \mathbb{Z}_2$) and lattice symmetry group G_{space}.

Complete set of LSM in 2D: lattice homotopy

Theorem (Complete LSM in 2D) For a lattice magnet of spin $S = 1/2$, with full lattice wallpaper group and onsite $SO(3)$ spin rotation symmetry. If there are odd numbers of spin-1/2's

1. per fundamental domain, or
2. per 1d unit cell defined by translation along a mirror axis, or
3. at a C_{2n} rotation center,

the ground state cannot be a trivial paramagnet.



Lattice homotopy (Key concept to prove the Theorem): classifies distinct lattices when symmetrically putting spins at high symmetry points (i.e. *irreducible Wyckoff positions*). These classes form an abelian group, denoted as A_{LH}.

Lattice homotopy for all 17 wallpaper groups. We have [1]

Wallpaper group	Lattice homotopy A_{LH}
1,4,5,15	$\mathbb{Z}_2$
2,6	$\mathbb{Z}_2^4$
3,8,12,16,17	$\mathbb{Z}_2^2$
7,9,10,11,13,14	$\mathbb{Z}_2^3$

A Quest in 3D

Two formalisms of the LSM theorem have been established: one uses the notation of lattice homotopy [1] and the other uses the idea of quantum anomalies [2]. In 2D two formalisms agree very well [3].

Question. what are some new 3D LSM theorems? How do the two notations match in 3D?

In this work, we answer this question for the pyrochlore/diamond lattice. These lattices are interesting because

- Heisenberg $S = 1/2$ on pyrochlore lattice: ground state not known!
- Many material candidates for QLSs: $Ce_2Zr_2O_7$, $Yb_2Ti_2O_7$, $LiYbSe_2$,...
- Large lattice symmetry and series of possible symmetry breaking:

$$I2 \subset I\bar{4} \subset I\bar{4}2d \subset I4_1/amd \subset Fd\bar{3}m$$
$$C2 \subset F222 \subset F23 \subset F\bar{4}3m \subset Fd\bar{3}m$$
$$C2 \subset P3_221 \subset R32 \subset R\bar{3}m \subset Fd\bar{3}m$$

LSM theorems can provide insights into the type of symmetric spin liquids compatible with a given low energy theory (spinon coupled to emergent gauge fields).

LSM Theorem for the 3D pyrochlore/diamond lattice

Using the concept of lattice homotopy, we obtain

LSM theorem for the pyrochlore lattice. If there are odd numbers of spin-$1/2$'s per pyrochlore site, a trivial paramagnet on the pyrochlore lattice is forbidden due to inversion symmetry i.

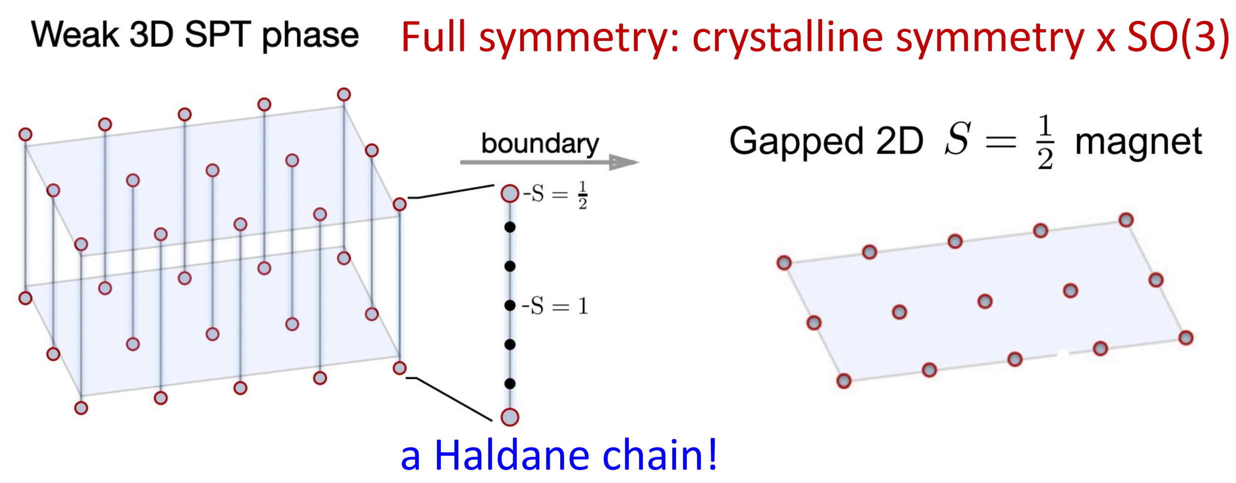
LSM theorem for the diamond lattice. If there are odd numbers of spin-$1/2$'s per diamond site, a trivial paramagnet on the diamond lattice is forbidden due to two orthogonal twofold rotation symmetry $C_2 \times C_2'$.

Note: LSM theorem does not apply to the breathing pyrochlore lattice.

LSM: a modern perspective

Claim (Non-technical version). All paramagnetic phases in d dim—trivial and nontrivial—can be realized as boundary of certain trivial paramagnetic phases in $d+1$ dim.

Claim (Technical version). A nontrivial paramagnet carrying LSM anomalies lives on the boundary of weak SPT of d-dim array of Haldane chains in $d+1$ dim. These weak SPT are protected by global $G_{\text{space}} \times SO(3)$ symmetry, classified by $\mathcal{H}^{d+1}(G_{\text{space}} \times SO(3), U(1))$ [2–4].



Criterion for LSM anomalies. LSM anomalies are mixed anomalies between lattice symmetry G_{space} and onsite $SO(3)$ symmetry. The anomalies must vanish upon breaking onsite $SO(3)$ to $SO(2)$ [3]. $\Rightarrow$ LSM anomalies live in

$$\mathcal{A} := \ker[\tilde{i}: \mathcal{H}^d(G_{\text{space}}, \mathbb{Z}_2) \to \mathcal{H}^d(G_{\text{space}}, U(1)_\rho)]. \quad (1)$$

3. Perfect matching between lattice homotopy and anomaly. In 2D, we have [3]

$$A_{\text{LH}} \cong \mathcal{A}. \quad (2)$$

LSM anomaly for the pyrochlore and diamond lattices

LSM anomalies are encoded in topological partition functions (TQFTs) that classify trivial paramagnets (SPT/'t Hooft anomaly) in $4+1$ dim, protected by $G_{\text{space}} \times SO(3)$:

$$Z_{\text{UV}} = e^{i\pi \int_{\mathcal{M}_5} \lambda[A_{\text{spatial}}] \cup \omega[A_{\text{spin}}]}, \quad (3)$$

where $\lambda \in \mathcal{H}^3(G_{\text{spatial}}, \mathbb{Z}_2)$, and $\omega \in \mathcal{H}^2(SO(3), U(1)) = \mathbb{Z}_2$.

Table 1. Correspondence between lattice homotopy and LSM anomalies for a series of space groups.

Space group G_{space}	A_{LH}	LSM anomaly
$Fd\bar{3}m$ (No. 227)	$\mathbb{Z}_2^4$	$A_i^2(A_m + A_i), A_iB_{\beta+\phi}, C_{n\gamma}, C_{s\psi}$
$F\bar{4}3m$ (No. 216)	$\mathbb{Z}_2^4$	$C_\gamma, C_{\gamma'}, C_{s\omega}, C_{s\psi}$
$F23$ (No. 196)	$\mathbb{Z}_2^4$	$C_\gamma, C_{\gamma'}, C_\omega + C_{\omega'}, C_\psi + C_{\psi'}$
$R\bar{3}m$ (No. 166)	$\mathbb{Z}_2^4$	$A_{x+y+z}B_{\beta+\phi}, A_iB_{\beta+\phi}, A_{x+y+z}A_i(A_m + A_i), A_i^2(A_m + A_i)$
$I4_1/amd$ (No. 141)	$\mathbb{Z}_2^4$	$A_i^2(A_m + A_i), A_iB_{\beta+\phi}, C_{n\gamma}, A_{c'}(A_{c'}^2 + B_\delta)$
$F222$ (No. 22)	$\mathbb{Z}_2^4$	$C_\gamma, C_{\gamma'}, A_c(A_c + A_{c'})A_{x+y}, A_cA_{c'}(A_c + A_{c'})$
$C2$ (No. 5)	$\mathbb{Z}_2^2$	$A_cB_{xy}, A_{x+z}B_{xy}$

Table 2. Details of the correspondence: Wyckoff positions and topological invariants for the space group Fd$\bar{3}$m (No. 227).

Wyckoff	Little group		Coordinates	LSM anomaly class λ				Topo. invariant
	Intl.	Schönflies		$B_{xy}A_i$	$A_i^2(A_i + A_\sigma)$	C_τ	$C_\psi[A_{C_2}, A_{C_2'}]$	
16d	$\bar{3}$m	D_{3d}	$(0,0,0)$	+	−	+	+	$\lambda(i,i,i)$
16d	$\bar{3}$m	D_{3d}	$(1/2,1/2,1/2)$	−	−	+	+	$\lambda(\tilde{i},\tilde{i},\tilde{i})$
8b	$\bar{4}$3m	T_d	$(1/8,1/8,1/8)$	+	+	+	−	$\prod_{\text{cyc}} \lambda(C_2, C_2', C_2')$
8a	$\bar{4}$3m	T_d	$(3/8,3/8,3/8)$	+	+	−	−	$\prod_{\text{cyc}} \lambda(\tilde{C}_2, \tilde{C}_2', \tilde{C}_2')$

Conclusion

(i) Using lattice homotopy, we stated the LSM theorems on a series of lattices. (ii) We found that all LSMs are associated with the intersection of two-fold axes, or 3D inversion—new types of LSM specific to 3D. (iii) We find the topological data for the LSM anomalies and identified them with lattice homotopy constraint on a series of lattices. (iv) These LSM constraints further restrict the type of quantum spin liquids as required by anomaly matching.

For future: (i) Anomaly matching (work in progress). (ii) Apply the general formalism to all 230 space groups and obtain full set of LSM in 3D (work in progress)!

References

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chunxiaoliu@berkeley.edu