
Frustrated magnets and spin liquids

I P h T



s a c l a y

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Outline

- ❑ Frustration in **classical** spin models
 - Frustrated Ising models
 - Pyrochlore lattice & spin ice
 - 3-component spins and non-planar structures

- ❑ Frustration in **quantum** spin models
 - Antiferromagnetic long ranged order
 - Examples of spin gap materials

- ❑ Spin liquids
 - Zero modes on the kagome lattice and spin wave theory
 - Short-range RVB spin liquids, spinons and fractionalization

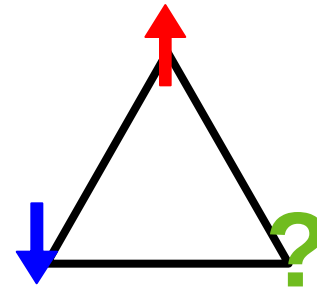
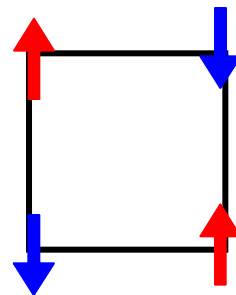
Classical spins

The simplest magnetic frustration – classical Ising models

$$E = + \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \quad \sigma_i^z = \pm 1$$

- Antiferromagnetism on a square and triangular lattice.

Satisfaction (M. Jagger 1965) and *frustration*.



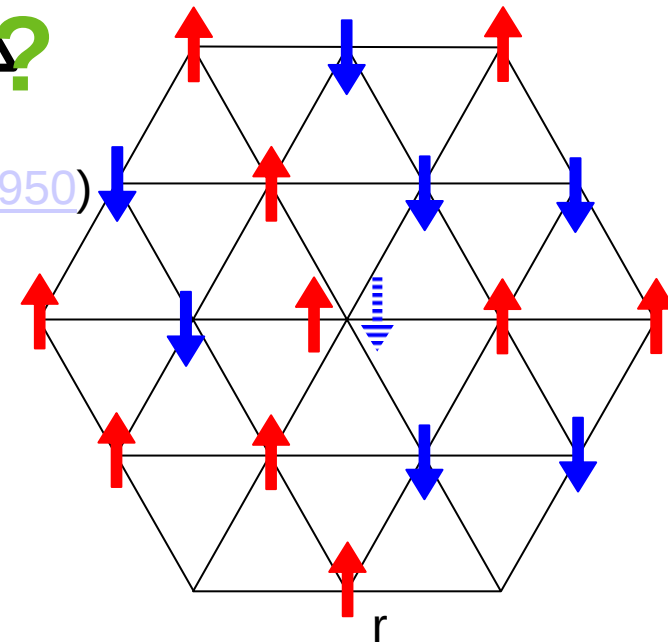
- Extensive entropy at $T=0$ for the Ising model (Wannier [1950](#))

$$S(0) = R \frac{2}{\pi} \int_0^{\pi/3} \ln(2 \cos \omega) d\omega = 0.3383R.$$

- Power law spin-spin correlations at $T=0$.

- Effect of perturbations ?

Example: (quantum) transverse field
Moessner & Sondhi [2001](#).



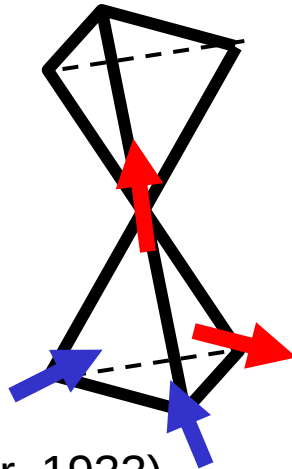
Ising(-like) spins on a frustrated 3d lattice & spin ice

Bramwell and Gingras, Science [2001](#) + refs. therein

- Pyrochlore lattice: corner-sharing tetrahedron

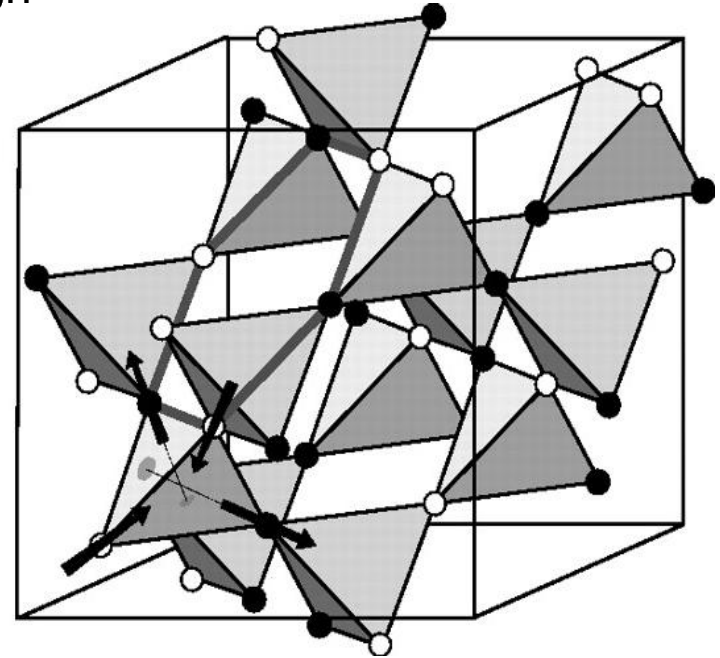
- Strong easy axis anisotropy

→ spins must point toward the center of a tetrahedron



“2 in & 2 out”

= ice rules (Bernal & Fowler, 1933)



- Examples: $\text{Ho}_2\text{Ti}_2\text{O}_7$, $\text{Dy}_2\text{Ti}_2\text{O}_7$, $\text{Ho}_2\text{Sn}_2\text{O}_7$

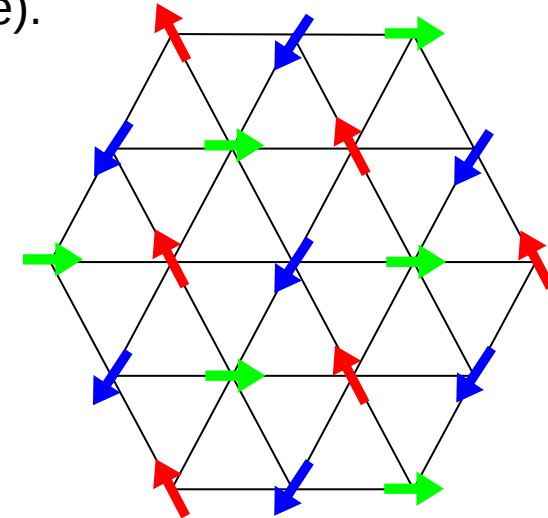
- Extensive entropy (measured by Ramirez, Nature [1999](#)), $S_0 \sim 1/2 R \ln(3/2)$

- Power law spin-spin correlations ($1/r^3$), seen in neutron scattering

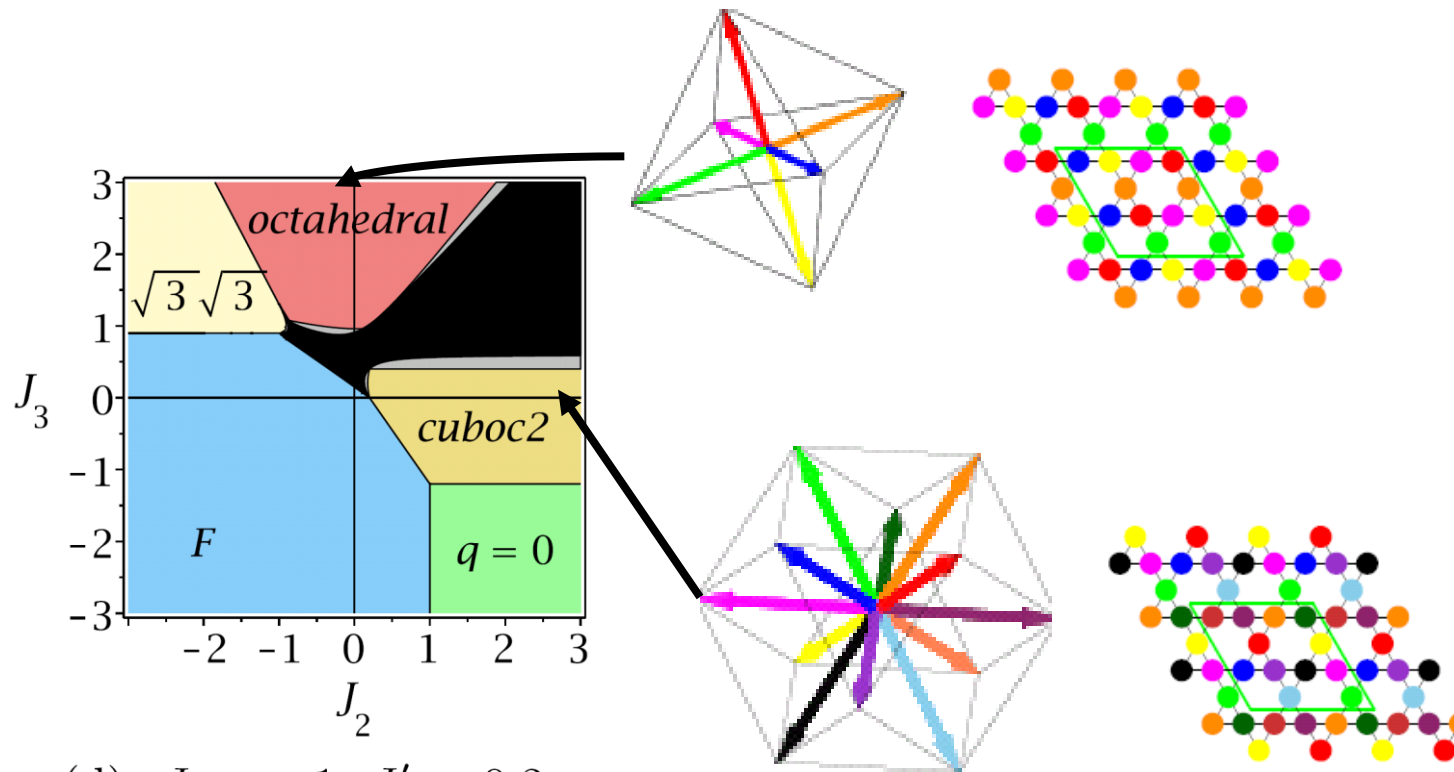
- Exotic excitations: “monopoles” (=half spin flips!). Castelnovo *et al.* Nature [2008](#)

Classical $O(3)$ models: non-collinear (and non-planar) structures

□ **Triangular** lattice: three sublattice (120° degree) Néel for Heisenberg (or XY) spins. Degeneracy: *global* rotations (different from the Ising case).



□ **Kagome** lattice with competing J_1 - J_2 - J_3 - J_3' interactions



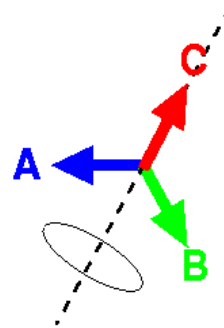
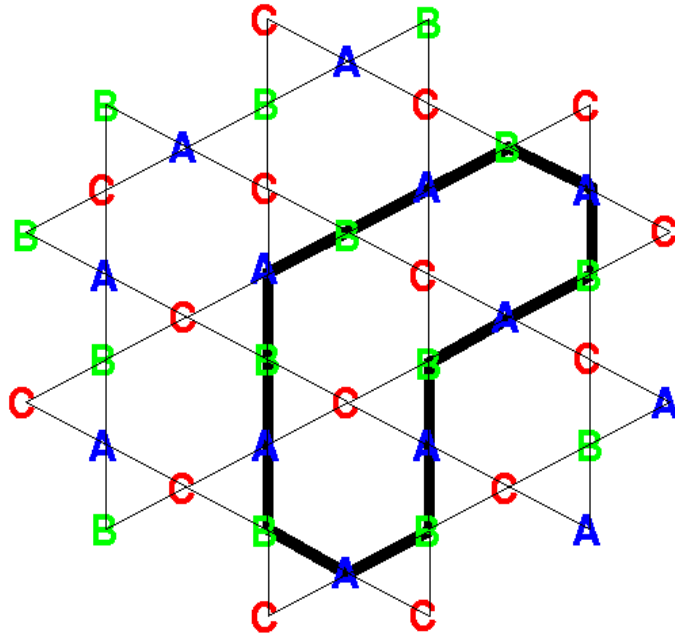
(d) $J_1 = -1$, $J_3' = 0.2$

Messio, Lhuillier & GM
[arXiv:1101.1212](https://arxiv.org/abs/1101.1212)

Classical $O(3)$ model on the kagome lattice & zero modes

- Planar ground-state $\leftrightarrow$ three-coloring of the lattice. “A B C”

→ exponential number of planar ground-states



A and B can rotate freely about the C axis.

→ non-planar ground-states

→ **Local zero mode**

- ☐ Physics when $T \rightarrow 0$? Not completely settled !

Spontaneous selection of a plane. Long range magnetic order in the plane ?

Shender, Holdsworth & Chalker, [1992](#). Huse & Rutenberg [1992](#). M. Zhitomirsky [2008](#). C. Henley [2008](#).

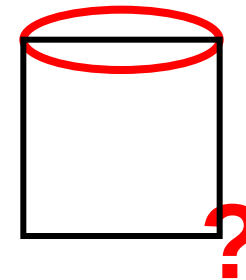
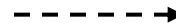
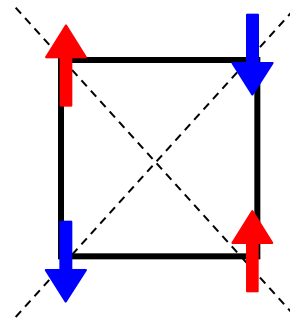
Quantum spin systems

Heisenberg antiferromagnets & quantum frustration

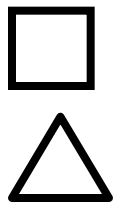
$$H = \sum_{\langle ij \rangle} \vec{s}_i \cdot \vec{s}_j$$

$$\frac{1}{\sqrt{2}} \left| \begin{array}{c} \text{red up} \text{---} \text{blue down} \end{array} \right\rangle - \left| \begin{array}{c} \text{blue down} \text{---} \text{red up} \end{array} \right\rangle$$

Singlet $S_{\text{tot}}=0$



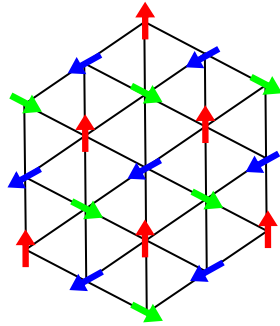
Quantum AF
are (almost) always
“frustrated” according to
the (classical) definition !



- **Sign problem** in quantum Monte Carlo
 Square (bipartite) → easy to simulate numerically
 Triangular (non-bipartite) → very hard to simulate (almost impossible in QMC)
- Other methods: exact diagonalizations (small number of spins ≤ 42)
 DMRG, and tensor networks methods ?

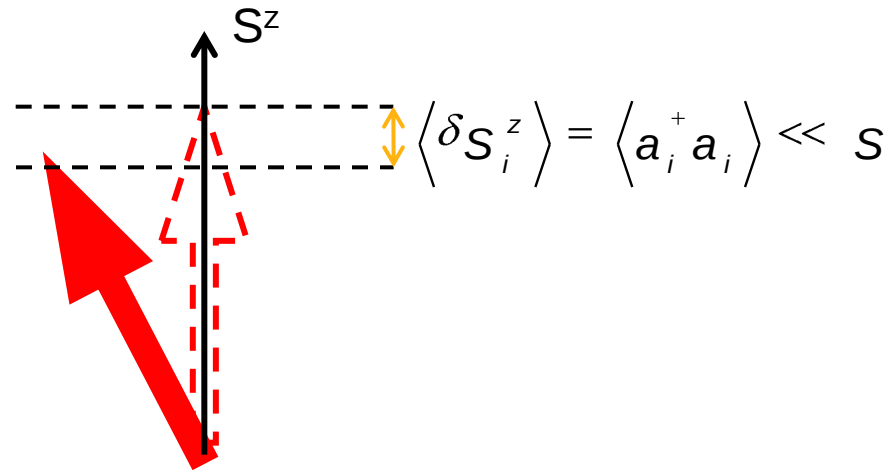
Spin wave theory & magnetic (Néel) long range order

- Start from the **classical ground-state**

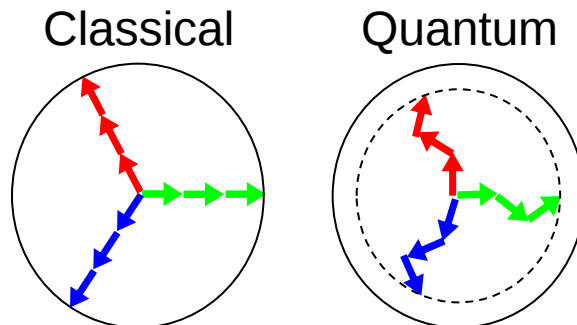


$$H = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

- Assume **small deviations**
(should be ok for large enough S)

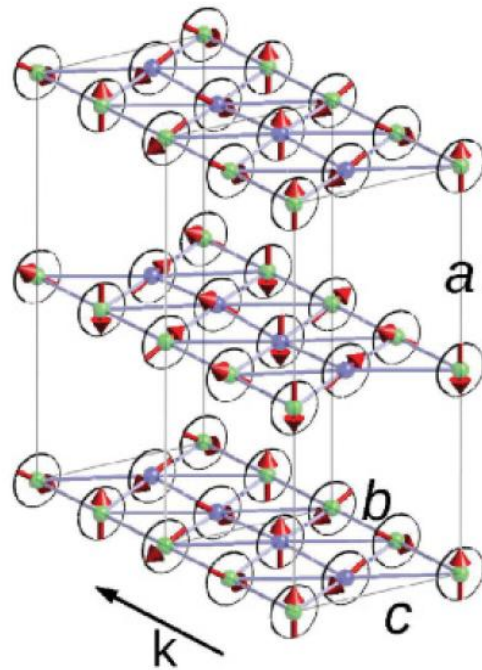


- Treat these deviations as (coupled) **quantum harmonic oscillators**
- Ground-state $\approx$ classical ground-state + zero-point fluctuations**

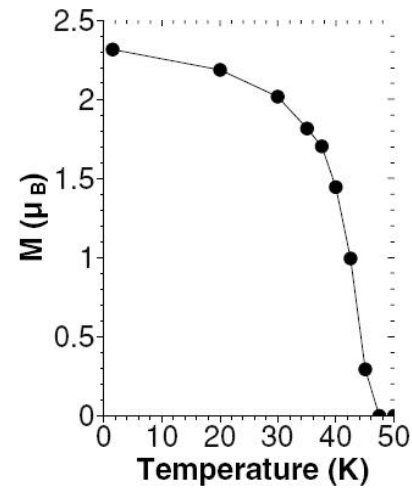


Example of the triangular AF Heisenberg model
Linear spin-wave calculation: Jolicoeur & Le Guillou, [1989](#)
Exact diagonalization numerics for $S=1/2$:
Huse & Elser [1988](#), Bernu, Lhuillier & Pierre, [1992](#).

Triangular quantum AF: an example



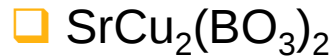
α - CaCr_2O_4



Chapon *et al.*, Phys. Rev. B [2011](#)

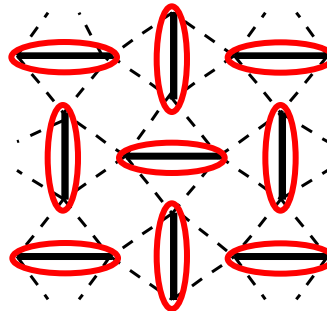
Do quantum antiferromagnets
always order at low temperature ?
No !

“Spin gap” materials

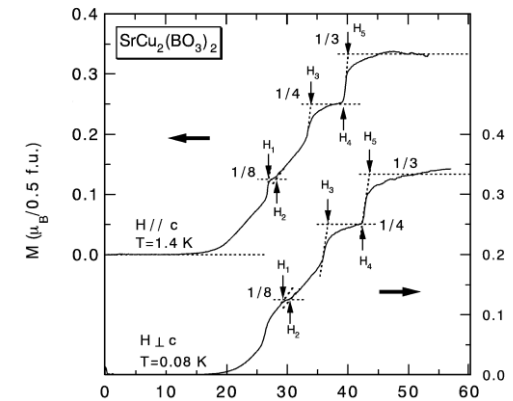


$$J_{\text{—}} \approx 100 \text{ K}$$

$$J'_{\text{---}} \approx 68 \text{ K}$$



Kageyama *et al.* (1999)



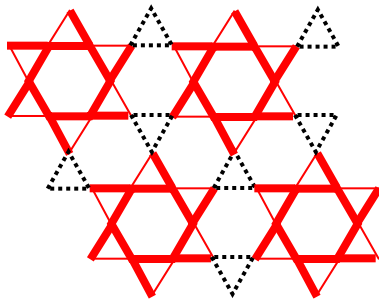
Magnetization plateaux
Onizuka *et al.* 2000

□ Ground-state is (almost) a product of uncorrelated singlets

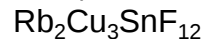
Shastry-Sutherland (1981)

$$\text{Singlet} = \frac{1}{\sqrt{2}} \left(\left| \uparrow\downarrow \right\rangle - \left| \downarrow\uparrow \right\rangle \right) \quad S=0 \text{ singlet}$$

□ Example with a bigger unit cell



example with 12 sites/cell:



Morita *et al.*, 2008; Ono *et al.*, 2009;

Yang & Kim, 2009

□ Theoretical picture: **weakly coupled** units. Possible description of the wave-function in perturbation theory.

Related phase: “valence bond crystals” with spontaneous lattice symmetry breaking.

So far:

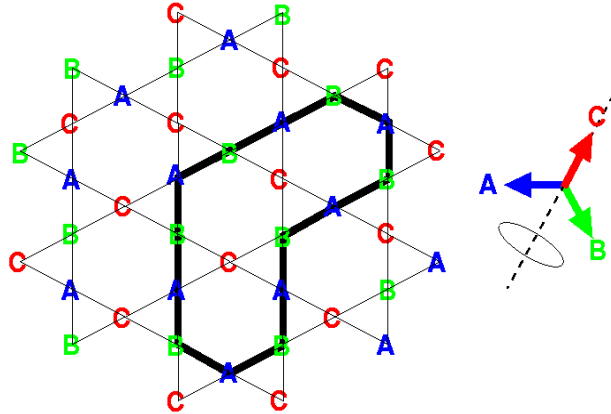
- 1) magnetic long-range order or
- 2) “weakly-coupled-singlets” ground-states

... is that all ?

No !

Spin-1/2 kagome Heisenberg model

- Many soft modes



→ Break-down of the spin wave theory (at least the most naïve one) because of the divergent zero-point motion of the harmonic oscillators.

- Nature of the ground-state ?

1989 (Elser) → 2011: **we still do not know !**

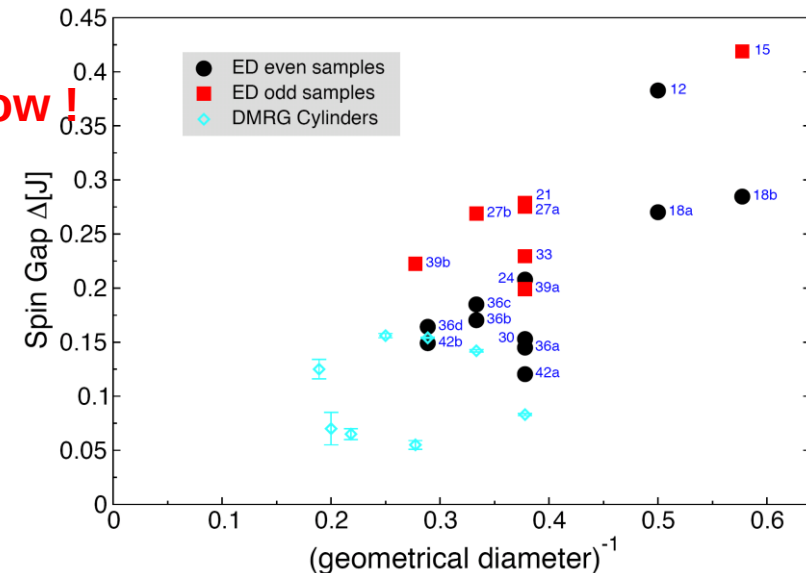
Numerics: no magnetic LRO at $T=0$.
and probably no order at all.

Diagonalization 42 spins

Lauchli *et al.*, [arXiv:1103.1159](https://arxiv.org/abs/1103.1159)

DMRG: Yan *et al.*, [arXiv:1011.6114](https://arxiv.org/abs/1011.6114)

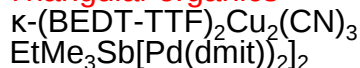
- What about experiments ?



Some spin liquid candidates (no long range order detected down to $T \ll J$)



□ Triangular organics



Proximity to the Mott transition $\rightarrow$ charge fluctuations $\rightarrow$ ring exchange interactions ?

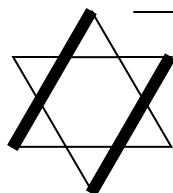
Spinon Fermi surface or other gapless QSL ?

Quantum critical point in EtMe $_3$ Sb[Pd(dmit)) $_2$] $_2$?

Shimizu *et al.* [2003](#)

Itou *et al.* [2008](#)

Motrunich [2005](#); Lee & Lee [2005](#); Kyung & Tremblay [2006](#); Tocchio *et al.* [2009](#)



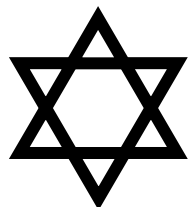
□ Volborthite Cu $_3$ V $_2$ O $_7$ (OH) $_2$ +2H $_2$ O

low impurity concentration

but possible magnetic order (freezing?) at very low-T ($T/J \sim 1/100$).

distorted kagome lattice (and maybe not kagome at all: Jason *et al.* [2010](#))

Hiroi *et al.* 2001; Bert *et al.*, [2005](#); Yoshida *et al.*, [2009](#).



□ Herbertsmithite ZnCu $_3$ (OH) $_6$ Cl $_2$

undistorted kagome lattice, looks critical ?

but many missing spins in the kagome planes (Cu $\rightarrow$ Zn) $\otimes$.

Helton *et al.* [2007](#), Mendels *et al.* [2007](#), Bert *et al.* [2007](#), Ofer *et al.* [2007](#), Imai *et al.* [2007](#), Olariu *et al.* [2008](#)

□ Vesignieite BaCu $_3$ V $_2$ O $_8$ (OH) $_2$.

almost undistorted kagome lattice, no antisite disorder (but some mag. Impurities $\sim 7\%$).

Okamoto *et al.* [2009](#)

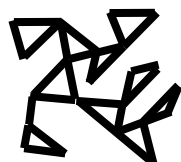


□ He 3 films (Nuclear magnetism)

Ring exchange interactions (but not precisely known).

Experiment are very difficult (J $\sim$ mK).

Ikegami *et al.* [2000](#), Masutomi *et al.* [2004](#)



□ "Hyper kagome" Na $_4$ Ir $_3$ O $_8$ (3d)

Gapless QSL ? Lawler *et al.* [2008](#); Zhou *et al.* [2008](#) (spinon Fermi surface ?)

some anisotropies ? Chen & Balents [2008](#)

Okamoto *et al.* [2007](#)

ALL SEEM GAPLESS !

Why are theoreticians so excited about systems which are just “disordered” ?

Lieb-Schultz-Mattis-Hastings theorem

The absence of order (=spontaneously broken symmetry) is a very interesting situation if the spin is half-odd integer spin per unit cell (=Mott insulator) !

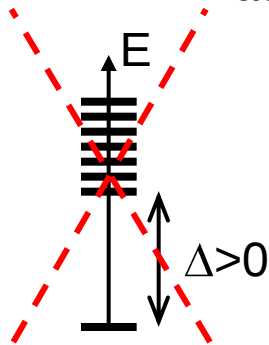
Lieb-Schultz-Mattis Theorem for spin chains ($d=1$), [1961](#)

Recent proof valid in any dimension ($d>1$) :

□ Hastings [2004](#)

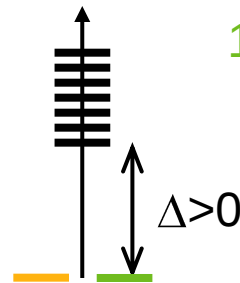
See also Affleck [1988](#); Bonesteel [1989](#); Oshikawa [2000](#)

□ Nachtergaele & Sims, Com. Math. Phys. 276, 437 ([2007](#)).



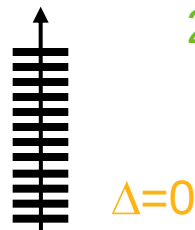
Conditions:

- half-odd-integer spin in the unit cell
- short-range interactions
- Global $U(1)$ symmetry: $[S^z_{\text{tot}}, H]=0$
- dimensions $L_1 \ L_2 \ \dots \ L_D$ with $L_2 \ \dots \ L_D = \text{odd}$
- periodic bound. conditions in direction 1
- thermodynamic limit



1) Ground-state degeneracy

- a- “Conventional” broken symmetry
- b- Topological degeneracy



2) Gapless spectrum

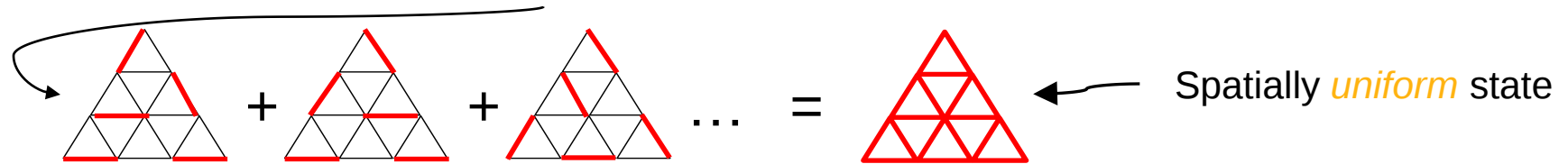
- a- Continuous broken sym. (Néel order)
- b- Critical phase (or crit. point)

spin liquids
with **fractional**
excitations
($s=1/2$ spinons)

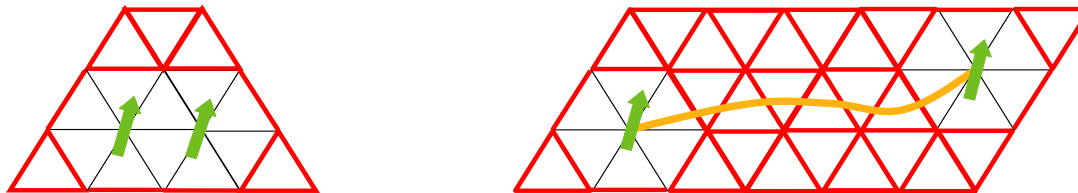
Gapped quantum spin liquids & short-range RVB picture

- P. W. Anderson's idea (1973) : (short-ranged) **resonating valence-bond** (RVB)

Linear superposition of many (exponential) low-energy short-range valence-bond configurations

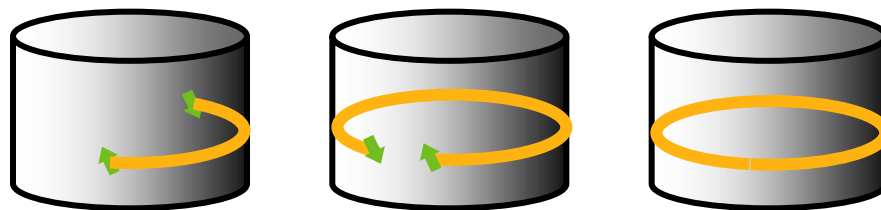


- Magnetic excitations ? Spinon with spin $S=1/2$



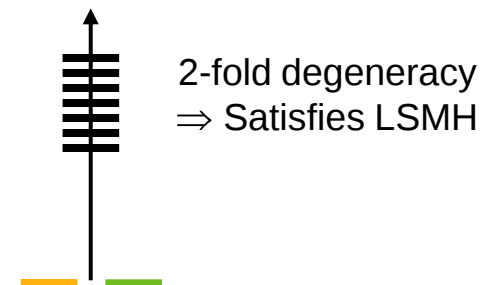
Solvable models realizing this idea
on the kagome lattice:
GM, Pasquier & Serban [2002](#)
Seidel [2009](#)

- Topological degeneracy & spinon fractionalization



adiabatic process → New ground-state

Topological degeneracy
(X. G. Wen 1991) ↔
fractionalization
See also Oshikawa & Senthil [2006](#)



A starting point to describe QSL: large-N (mean-field) limit

Review: Lee, Nagaosa & Wen, [Rev. Mod. Phys. 78, 17 \(2006\)](#)

- Express the spin operators using *fermions*

$$S^z = \frac{1}{2} (c_{\uparrow}^{\dagger} c_{\uparrow} - c_{\downarrow}^{\dagger} c_{\downarrow}) \quad c_{\uparrow}^{\dagger} \text{ (or } c_{\downarrow}^{\dagger}) \text{ changes } S^z \text{ by } +\frac{1}{2} \text{ (} -\frac{1}{2} \text{)}$$

$$S^{+} = c_{\uparrow}^{\dagger} c_{\downarrow} \quad S^{-} = c_{\downarrow}^{\dagger} c_{\uparrow} \quad \text{creates a "spinon"}$$

$$c_{\uparrow}^{\dagger} c_{\uparrow} + c_{\downarrow}^{\dagger} c_{\downarrow} = 1$$

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} (c_{i\mu}^{\dagger} c_{i\nu} c_{j\rho}^{\dagger} c_{j\sigma})$$

- Mean-field decoupling → quadratic Hamiltonian (solvable)
+ self consistency conditions

$$H_{MF} = \sum_{\langle ij \rangle} \chi_{ij} (c_{i\downarrow}^{\dagger} c_{j\downarrow} + c_{i\uparrow}^{\dagger} c_{j\uparrow}) + \eta_{ij} (c_{i\uparrow}^{\dagger} c_{j\downarrow} - c_{i\downarrow}^{\dagger} c_{j\uparrow}) + H.c$$

Spinon "hopping"
Spinon "pairing"

- Beyond mean-field ?

Fluctuations ? Spinon confinement ? Stability of gapless phases ?

Summary

- ❑ Rich collective phenomena can emerge in frustrated models
- ❑ Gapless spin liquids have recently been observed
- ❑ A lot remains to be understood on the theoretical side

Some references :

Introduction to frustrated magnetism

C. Lacroix, Ph. Mendels & F. Mila (Eds), Springer 2011



“[Quantum spin liquids and fractionalization](#)” GM (in the book above)

“Quantum Spin Liquids”, GM, [arXiv:0809.2257](#) (Les Houches lecture notes)