Kapellasite : un liquide de spin sur kagome avec des interactions en compétition

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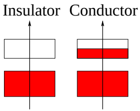
LPTMC, Université Paris VI

21 novembre 2013

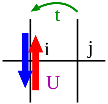
Heisenberg spin models



Band theory → the Mott insulators are conducting !...

The Hubbard model integrates interactions between electrons:

$$H_{Hub} = t \sum_{\langle ij \rangle, \sigma = \pm 1/2} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \underbrace{n_{i\uparrow}}_{c^{\dagger}_{i\uparrow} c_{i\uparrow}} n_{i\downarrow}.$$



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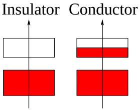

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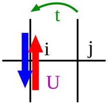
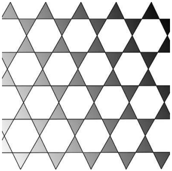
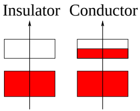


To 2^{nd} order in perturbation theory in $\frac{t}{U}$:

$$H = \frac{4t^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad \text{(Heisenberg model).}$$



Heisenberg spin models



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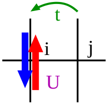
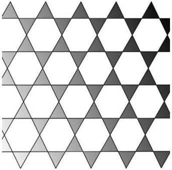


To 2^{nd} order in perturbation theory in $\frac{t}{U}$:

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \qquad \text{(Heisenberg model).}$$



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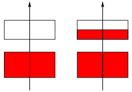

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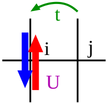

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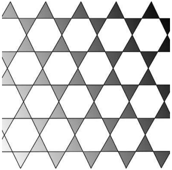
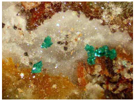


Frustration ⇒ spin liquids

Perfect $S = 1/2$ kagome compounds

Herbertsmithite (see F. Bert's talk)
Zn-paratacamite $Cu_3Zn(OH)_6Cl_2$



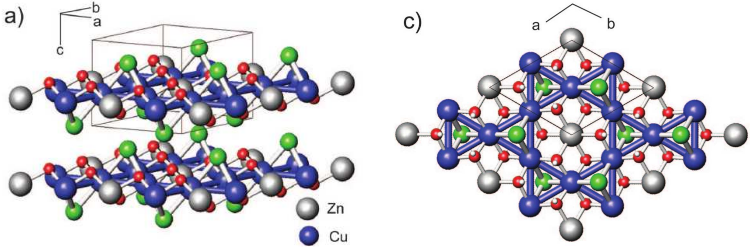
Kapellasite
Polymorph of Herbertsmithite,

R. H. Colman et al, Chem. Mater. 20 6897 (2008)

Important J_d interaction

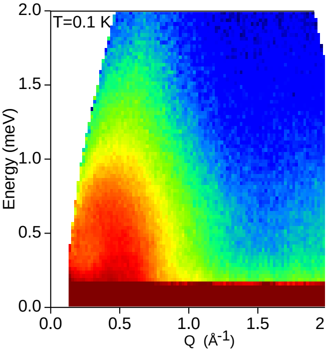
O. Janson et al, PRL 101 106403 (2008)

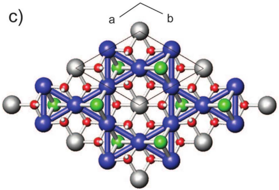
2D behaviour



Experiments on kapellasite

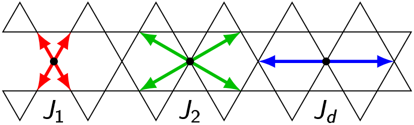
- NMR $\rightarrow$ $(Cu_{0.73}Zn_{0.27})_3(Zn_{0.88}Cu_{0.12})(OH)_6Cl_2$,
- Magnetic susceptibility and μ SR $\rightarrow$ gapless spin liquid state,
- Inelastic neutron scattering:





- No Bragg peak
  $\rightarrow$ no long range order.
- No gap
- Intensity around $0.5A^{-1}$

High temperature series analysis

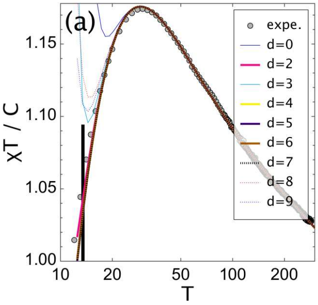


Analysis of

- the magnetic susceptibility,
- the low temperature specific heat data

Results for kapellasite :

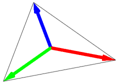
- $J_1 = -12K$ (F),
- $J_2 = -4K$ (F)
- $J_d = 15.6K$ (AF)

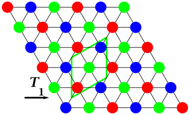


B. Bernu, C. Lhuillier, E. Kermarrec, F. Bert, P. Mendels, R. H. Colman, A. S. Wills, PRB 87 155107 (2013)

What is a regular state ?

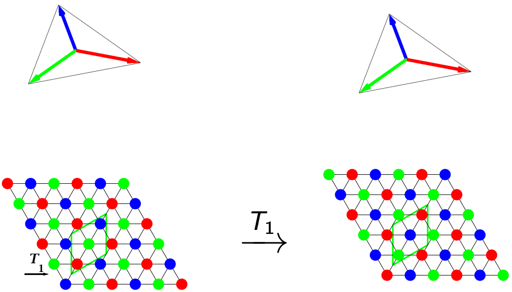
Example:





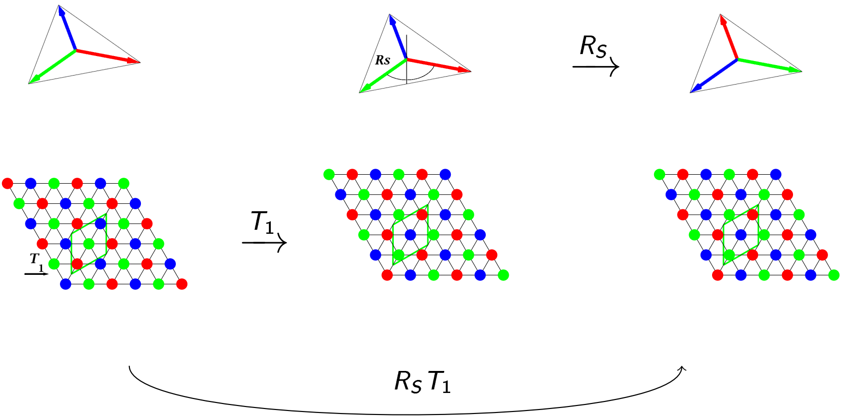
What is a regular state ?

Example: This state is not invariant by the translation T_1,



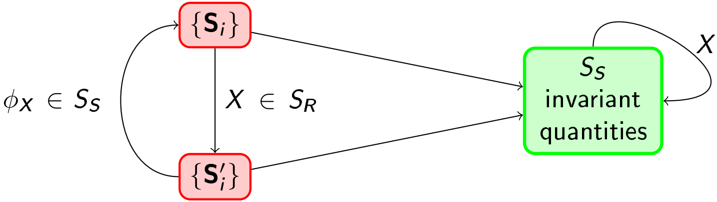
What is a regular state ?

Example: This state is not invariant by the translation T_1, but it is by T_1 followed by a global spin rotation R_S.



What is a regular state ?

We know the lattice and its symmetries S_R, the spin space and its symmetries S_S.



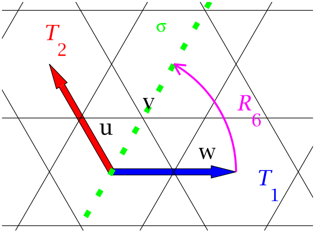
Definition:
A classical state is *regular* for the lattice symmetry X if there is a global spin transformation ϕ_X such that the state is unchanged by $\phi_X X$.

LM, Lhuillier and Misguich, PRB 83, 184401 (2011)

How to find the regular states ?

The research consists in two steps.

Example of the kagome lattice with Heisenberg spins



How to find the regular states ?

The research consists in two steps.
(1) Find the ϕ_X from S_S respecting the algebraic structure of S_R,

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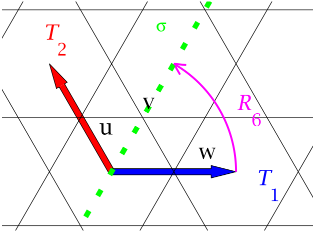


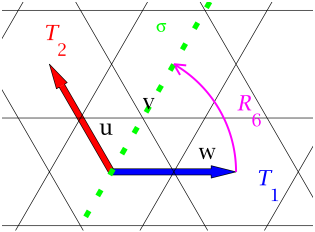
(1) Algebraic constraints on ϕ_X from $O(3)$:

$$\phi_{T_1}\phi_{T_2} = \phi_{T_2}\phi_{T_1} \qquad \phi_{T_1}\phi_{R_6}\phi_{T_2} = \phi_{R_6}$$
$$\phi_{R_6}\phi_\sigma\phi_{R_6} = \phi_\sigma \qquad \phi_{T_1}\phi_\sigma = \phi_\sigma\phi_{T_2}$$
$$\phi_{R_6}^6 = I \qquad \phi_\sigma^2 = I$$
$$\phi_{R_6}\phi_{T_1}\phi_{T_2} = \phi_{T_2}\phi_{R_6}.$$

How to find the regular states ?

The research consists in two steps.
(1) Find the ϕ_X from S_S respecting the algebraic structure of S_R,
(2) For each set of ϕ_X, find the compatible states.

Example of the kagome lattice with Heisenberg spins



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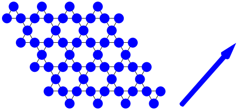
$$\phi_{R_6}^6 = I \qquad \phi_\sigma^2 = I$$
$$\phi_{R_6}\phi_{T_1}\phi_{T_2} = \phi_{T_2}\phi_{R_6}.$$

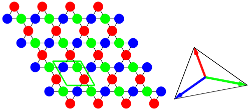
(2) Constraints on the spin state :

$$\phi_\sigma \mathbf{S}_v = \mathbf{S}_v, \qquad \phi_{T_1}\phi_{T_2}\phi_R^3 \mathbf{S}_v = \mathbf{S}_v.$$

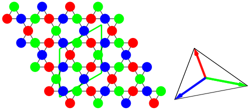
Regular states on the kagome lattice



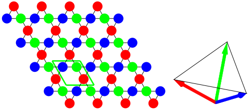
Ferromagnetic state



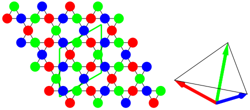
$\mathbf{q} = \mathbf{0}$ state



$\sqrt{3} \times \sqrt{3}$ state



$\mathbf{q} = \mathbf{0}$ umbrella state



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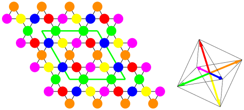
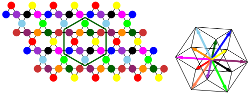
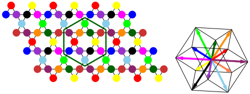


Octahedral state

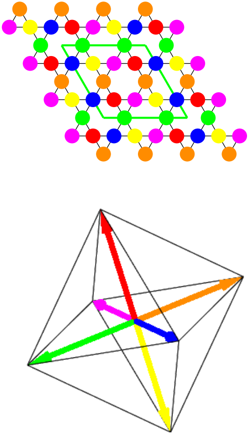


Cuboc1 state



Cuboc2 state

Regular chiral states on the kagome lattice



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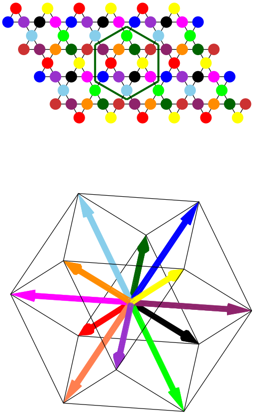

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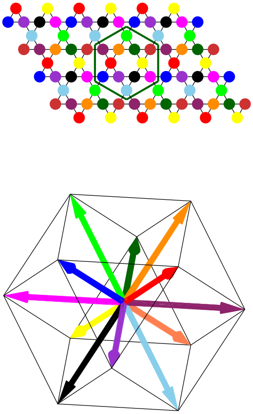
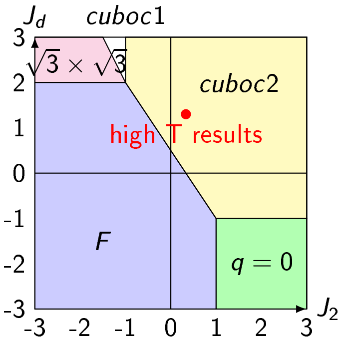
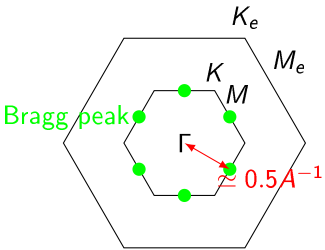


Cuboc2 state

Classical phase diagram for $J_1 = -1$





The low T phase in kapellasite is a spin liquid with short range correlations similar to the cuboc2 state → chiral spin liquid

How to theoretically describe this phase ?

Theoretical description

In spin liquids, excitations are fractional quasiparticles: spinons ($S = 1/2$).

- bosonic description $\rightarrow$ Néel phases and gapped spin liquids,
- fermionic descrition $\rightarrow$ gapped and non gapped spin liquids. (work in progress with Samuel Bieri).

In both cases, all spin liquid phases can be listed using the projective symmetry group approach (Wen, 2002), and fluxes can be calculated and used to identify similar phases obtained through different approaches.

Taking into account chiral spin liquids is something new and leads to still unexplored phases !

Thanks to

For the synthesis

R. H. Colman (University College London),
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For the measurements

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P. Mendels (LPS, Orsay),
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A. D. Hillier (ISIS, STFC, UK),
A. Amato (LMU, PSI, Switzerland),

For the theory

B. Bernu (LPTMC, Paris),
C. Lhuillier (LPTMC, Paris),
S. Bieri (LPTMC, Paris),

The Schwinger boson mean-field theory (SBMFT)

On each site j, bosons with spin $1/2 \uparrow$ ($\downarrow$) are created by $a_j^\dagger$ ($b_j^\dagger$).

$$2S_j^z = a_j^\dagger a_j - b_j^\dagger b_j, \qquad S_j^+ = a_j^\dagger b_j, \qquad n_j = 2S$$

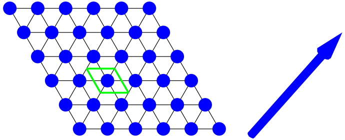
$$\widehat{A}_{ij} = \frac{1}{2}(a_i b_j - b_i a_j) = \text{rotationally invariant bond operator}$$

$$\widehat{A}_{ij}^\dagger \widehat{A}_{ij} \to MF \to \langle \widehat{A}_{ij}^\dagger \rangle \widehat{A}_{ij} + \langle \widehat{A}_{ij} \rangle \widehat{A}_{ij}^\dagger - |\langle \widehat{A}_{ij} \rangle|^2$$

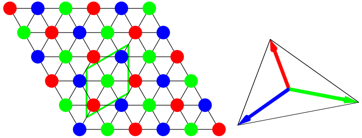
Average number of bosons adjusted to be κ (real) :

$$a_i^\dagger a_i + b_i^\dagger b_i = 2S \to \langle a_i^\dagger a_i + b_i^\dagger b_i \rangle = \kappa.$$

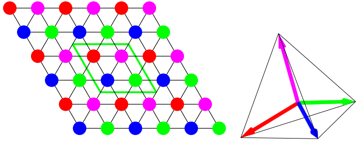
Regular states on the triangular lattice



Ferromagnetic state



$\mathbf{q} = \mathbf{0}$ state



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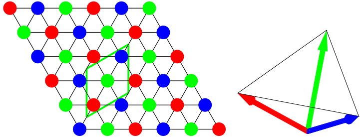
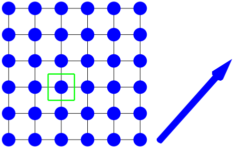
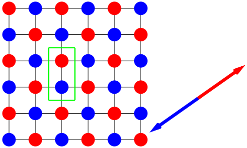


Cuboc1 state

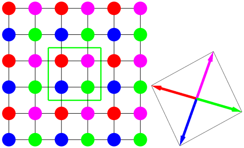
Regular states on the square lattice



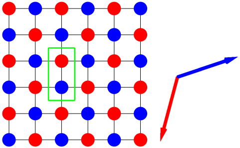
Ferromagnetic state.



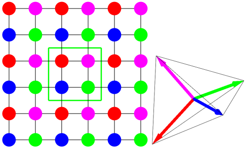
(π, π) Néel state.



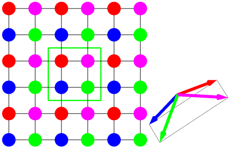
Orthogonal state.



V states.



AF umbrellas



F umbrellas