Introduction to frustrated magnets

&
on the doping issue
OUTLINE

• Basic notions on frustration – Definition – Classical non-collinear configurations – Exemple of the J1-J2 model

• Some frustrated lattices & related materials – Quantum disordered phases (VBC & spin liquids) – Exotic QCP scenarios

• Some doping issues – Impurities and mobiles holes in VBC & spin-liquid hosts
Recommended advanced reading on the subject (reviews)

“Frustrated Spin Systems”,

“Introduction to Frustrated Magnetism”,
Eds. C. Lacroix, P. Mendels, F. Mila,
Springer Series in Solid-State Sciences 164
(Springer 2011)
The concept of frustration

Topological origin

Extended range interaction

For classical spins, one cannot minimize independently all bond (AF) interactions
Classical degeneracy

$J_1-J_2$ model ($J_2 > J_1/2$)
Simple considerations for classical spins

$$E[\{S_i\}] = \frac{1}{2} \sum_i \sum_r J(r) S_i \cdot S_{i+r}$$

with constraint $|S_i| = 1$ on all sites

By Fourrier transform:

$$E = \frac{1}{2} \sum_k J(k) S_k \cdot S_{-k}$$

Minimize $J(k)$
Assume $J(k)$ minimized for $k = k_0$

$S_k = 0$ for all k’s except $k = k_0$

$S_i = \frac{1}{\sqrt{N}}(S_{k_0} e^{ik_0 \cdot r_i} + H.C.)$

constraint $|S_i| = 1$

$S_i = (\cos (k_0 \cdot r_i), \sin (k_0 \cdot r_i), 0)$

Spiral configuration (non-collinear – coplanar)
Classical J1-J2 model

\[ J(k) = 2J_1(\cos k_x + \cos k_y) + 4J_2 \cos k_x \cos k_y \]

* For \( J_2/J_1 < 1/2 \): Néel order
* For \( J_2/J_1 > 1/2 \): \((k_x, k_y) = (\pi, 0)\) or \((0, \pi)\) 
  free angle between spins in A & B sublattices

* For \( J_2 = \frac{1}{2}J_1 \): \(k_x = \pi\) all \(k_y\) or vice versa
  \[ H = \text{cst} + \sum_{\text{plaquettes}}(S_1 + S_2 + S_3 + S_4)^2 \]
Quantum fluctuations

1/S expansion (using Holstein-Primakoff) transformation
=> bosons

\[ E = \text{cst} + \sum_k (\alpha_k^\dagger \alpha_k + \frac{1}{2}) \omega_k \]

Point zero quantum fluctuations

For \( J_2 > J_1/2 \): collinear structures are selected

Order-by-disorder phenomenon (Villain)
Emergence of exotic Quantum Disordered Phases?

$J_1$-$J_2$-$J_3$ AF Heisenberg model

Classical phase diagram
A. Chubukov, PRB 90

Quantum fluctuations

Valence Bond Crystals
RVB
Simple frustrated lattices

& related frustrated spin compounds
Lattices of corner-sharing units

Pyrochlore lattice

Checkerboard lattice

A lattice for theorists!

Corner-sharing tetraedras in 3D & 2D
2D lattice of corner-sharing triangles

\[ H = J \vec{S}_i \cdot \vec{S}_j = J \sum_{\text{triangles}} (\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 \]
Extensive classical degeneracy
2D Frustrated magnets

Lattices with **AF frustrating interactions**

**Melzi et al., PRB 85, 1318 (2000)**

- frustrated square lattice ($S=1/2$):
  - $\text{Li}_2\text{VOSiO}_4$

- Kagome lattice like $\text{SrCr}_{9-x}\text{Ga}_{3+x}\text{O}_{19}$ ($S=3/2$)

  **Ramirez et al., PRL 64 ('90)**
  **Broholm et al., PRL 65 ('90)**
3D Frustrated magnets

pyrochlores and spinels

Transition metal oxides
- ZnCr$_2$O$_4$ spinel
- A$_2$Ti$_2$O$_7$ titanates

Ramirez et al., PRL 89, 067202 (2002)

-no ordering down to low temperatures
Examples of Kagome Quantum S=1/2 Antiferromagnets

(cf. P. Mendels & Z. Hiroi work)
Quantum disordered phases

& Quantum Critical Point (QCP) scenario
**VBC vs SL**

**Checkerboard lattice**
- Finite gaps
- Spontaneous translation symm. breaking

(Fouet al.)

**Kagome lattice**
- No symmetry breaking
- Large $\#$ of low energy singlets

(Mila et al.)

*Exotic phenomena in doped frustrated quantum magnets – p.*
Low-energy spectrum
N=36 sites

Sindzingre & Lhuillier,
EPL 2009

Finite spin gap?
Jiang et al., PRL 2008

Exponential # of singlets
Lecheminant et al., PRB 97

S=0

S=1

S=2

S=3

Excitation gaps

$\Delta E(0)$ ED
$\Delta E(1)$ DMRG
$\Delta E(0)$ DMRG
Do Valence Bonds order?

Series expansion

Singh & Huse, PRB 2008

36-site unit cell

See also:

Marston & Zeng, JAP 1991

Nikolic & Senthil, PRB 2003

but dimer correlations should be small...

Exact diag.

Leung & Elser, PRB ‘93

\[ C_{(i,j)(k,l)} = \langle (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) \rangle - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2 \]

Competition between VBC and dimer liquids

(field theory: Sachdev 1991)
VBC candidates for the AF square lattice

Next-nearest-neighbor $J_2$ and N.N.N.N.N $J_3$ stabilize 4-fold deg. plaquette VBC phase
Plaquette correlations in J1-J2-J3

\[ C_{\text{plaquette}}(p, q) = \langle Q_p Q_q \rangle \]

Plaquette operator \( Q_{ijkl} = P_{ijkl} + P_{ijkl}^{-1} \)

where \( P_{ijkl} \) cyclic permutation

Mambrini, Läuchli et al. 2006 (Exact diag. 32 sites cluster)
Beyond Ginzburg-Landau paradigm of phase transitions!
Senthil, Sachdev, Fisher et al.

Also investigated numerically by Sandvik et al.
Doping frustrated magnets
Itinerant frustrated systems

- Spinel oxide LiTi$_2$O$_4$
  Sun et al., PRB 70, 054519 (2004)

- 5d transition-metal pyrochlores as Cd$_2$Re$_2$O$_7$
  or KO$_2$S$_2$O$_6$
  Hanawa et al., PRL 87, 187001 (2001)
  Hiroi et al., JPSJ 73, 1651 (2004)

- CoO triangular layer based compound

All superconducting with $T_c$ up to 13.7 K!
Confinement vs deconfinement

See Sachdev

Holon

(a) "string potential"
Checkerboard ??

(b) "deconfined" spinon
Kagome ??
Two emerging length scales

\[ \xi_{\text{conf}} \sim \xi_{\text{VBC}} \gg \xi_{\text{AF}} \]

Senthil et al.
Injected hole acts like a probe: bare and dressed wavefunctions

$|\Phi_{\text{bare}}\rangle = c_{O,\downarrow} |\Phi_0\rangle$

- Ground state of the Mott insulator

Remove a spin down at a given site $O$

Leaves behind a spin up polarization at a typical distance $\xi_{\text{AF}}$ from site $O$

$|\Phi_{\text{GS}}\rangle = \"one impurity-one spinon\"$ GS

Profile of spinon wavefunction
Spin density around a vacancy

\[ \langle S^z \rangle \text{ at distance } r = r_i - r_O \text{ from defect} \]

- \( \langle S^z \rangle_{\text{bare}} \rightarrow \text{spin-spin correlation in host} \)
- \( \langle S^z \rangle_{\text{gs}} \rightarrow \text{“spinon” wavefunction} \)

Kagomé: deconfined
Checkerboard: strongly confined

DP et al. PRB (2006)
Quasiparticle weight

Overlap (squared) $Z = |\langle \Phi_{gs} | \Phi_{bare} \rangle|^2$

zero or finite?

\[ Z_{\text{Kagome}} = 0 \]
\[ Z_{\text{checkerboard}} \approx 1 \]

Dynamic hole (finite $t$) $\rightarrow Z_k$

\[ A(k, \omega) = Z_k \delta(\omega - \omega_k) + A_{inc} \]
Single hole Green function

\[ A(k, \omega) = \text{Im} \left\{ \langle \Phi_0 | c_{k \uparrow}^\dagger \frac{1}{\omega + i\epsilon - H} c_{-k \downarrow} | \Phi_0 \rangle \right\} \]

Use Lanczos continued-fraction method

“Bare” wavefunction (Bloch state)
Hole dynamics: t-J model

\[ H = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P} \left( c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.} \right) \mathcal{P} + J \sum_{\langle i,j \rangle} S_i \cdot S_j - \frac{1}{4} n_i n_j \]
Hole dynamics in the VB Solid

Small quasi-particle peaks: holon-spinon boundstate

Single hole doped in a spin liquid

Incoherent spectrum
Weights distributed on many poles even at low energies

Summary / Conclusions

- **Frustration + quantum fluctuations** lead to exotic disordered GS (VBC, SL, …)
- Possible realization of exotic physics (deconfined spinons, Deconfined Critical Points, etc…)
- Variety of **fascinating materials** (insulators) to look for such behaviors (pyrochlores, Kagome, etc…)
- Microscopic models are hard to simulate (Exact diagonalisations) but can construct effective models...
- The doping issue might reserve many surprises but needs further investigations