



**The Abdus Salam
International Centre for Theoretical Physics**



1855-11

**School and Workshop on Highly Frustrated Magnets and Strongly
Correlated Systems: From Non-Perturbative Approaches to
Experiments**

30 July - 17 August, 2007

Mobile holes in frustrated quantum magnets

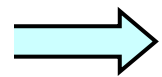
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Université Paul Sabatier, Toulouse, France

Mobile holes in frustrated quantum magnets

An Introduction

To be covered in the book chapter:

Covered in this Lecture

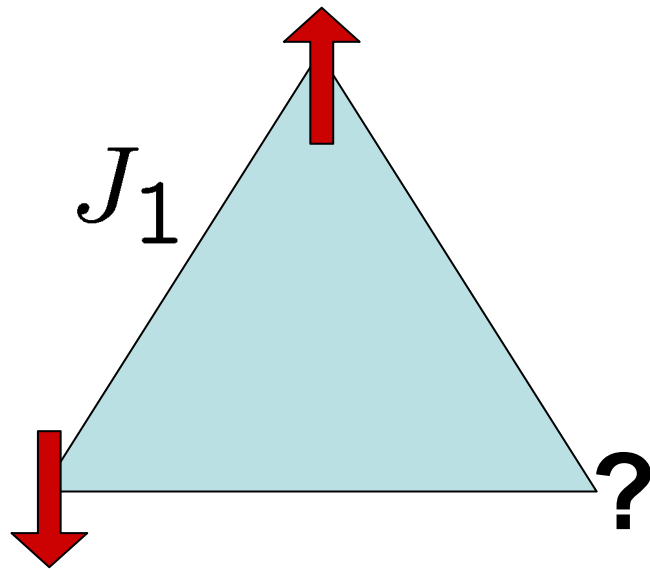


- Mobile holes in frustrated quantum magnets
- Ordering phenomena at commensurate fermion densities on frustrated geometries
- Doping Quantum Dimer Models

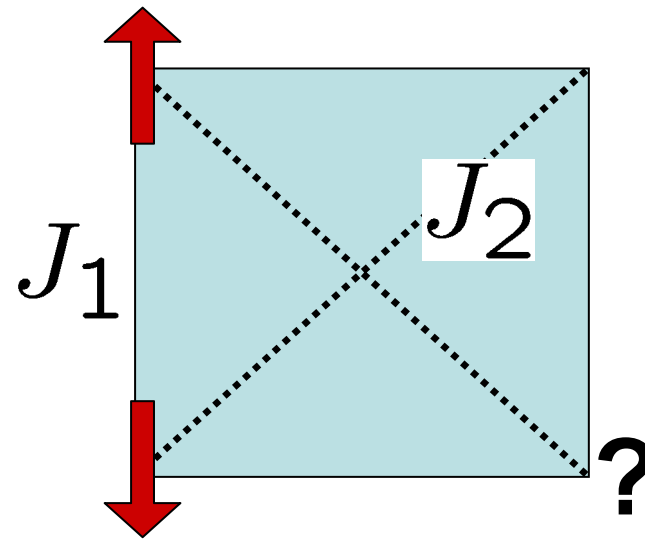
OUTLINE

- Basic notions on frustration
 - Some frustrated lattices
 - Quantum disordered phases (VBC & spin liquids)
- Some doping issues – Impurities and mobile holes in VBC & spin-liquid hosts

The concept of frustration



Topological origin



Extended range interaction

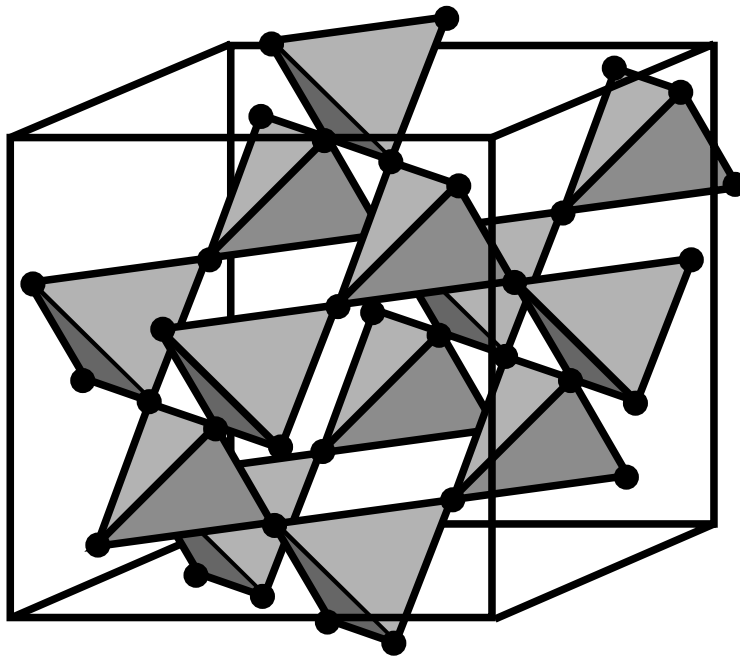
For classical spins, one cannot minimize independently all bond (AF) interactions

Simple frustrated lattices

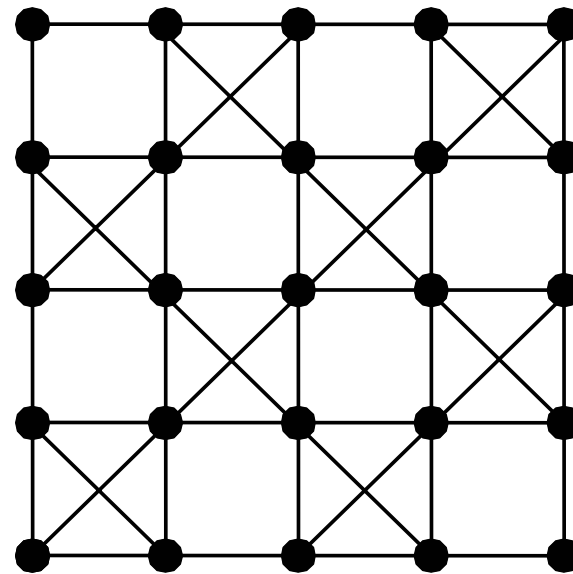
Reminder from previous lectures

Lattices of corner-sharing units

Pyrochlore lattice



Checkerboard lattice

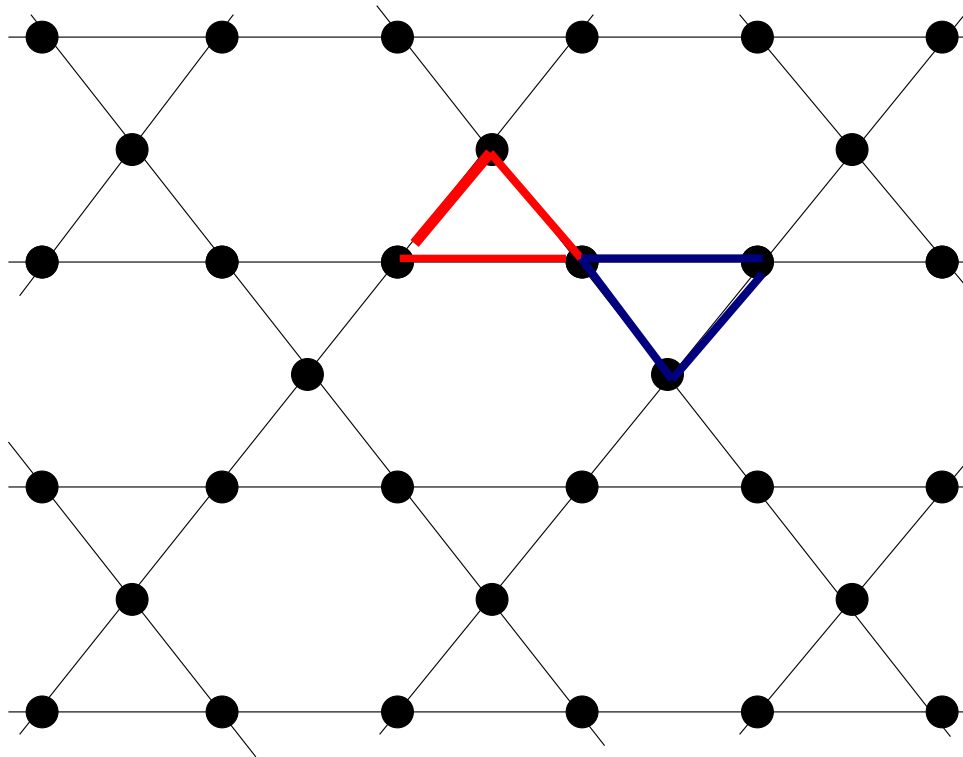


A lattice for theorists !

Corner-sharing tetraedras in 3D & 2D

The Kagome lattice

2D lattice of corner sharing triangles



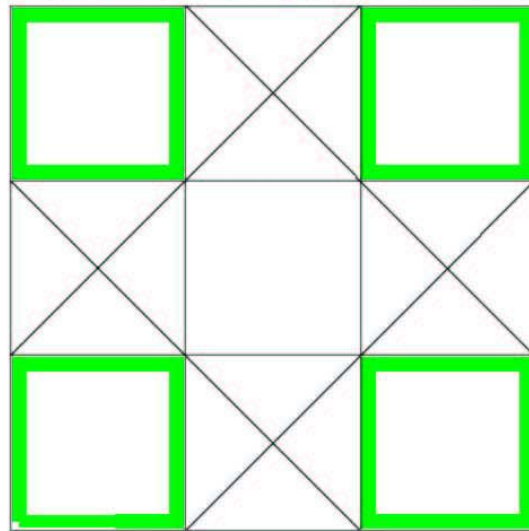
Very high classical degeneracy !!

Quantum disordered phases

& Quantum Critical Point (QCP) scenario

VBC vs SL

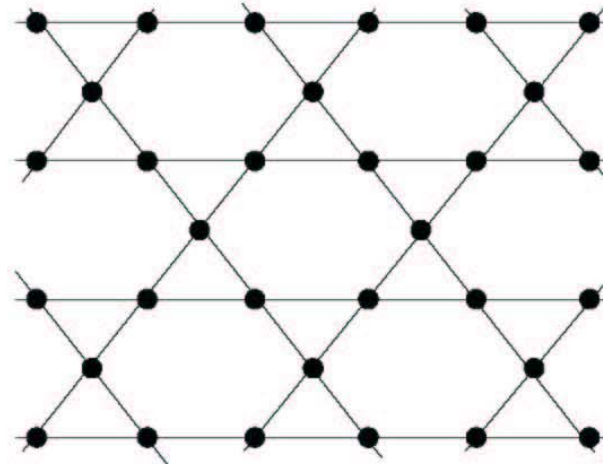
Checkerboard lattice



Valence bond crystal

- Finite gaps
- Spontaneous translation symm. breaking
(Fouet et al.)

Kagome lattice



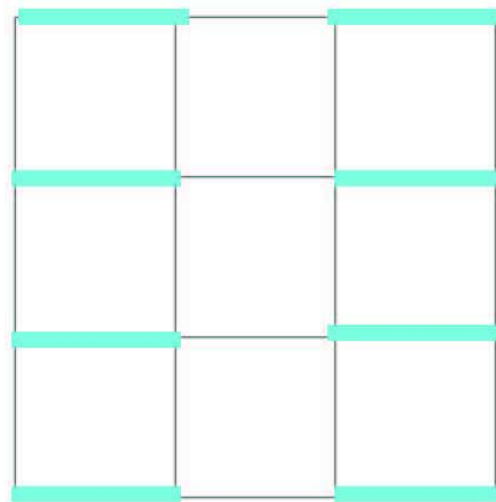
Spin liquid (SL)

- No symmetry breaking
- Large # of low energy singlets

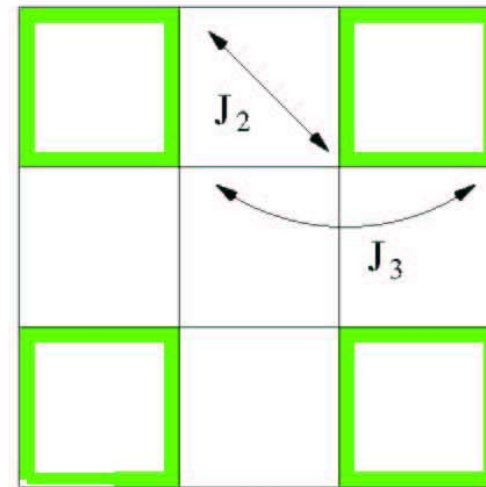
Exotic phenomena in doped frustrated quantum magnets – p.

(Mila et al.)

VBC candidates for the AF square lattice



(a)



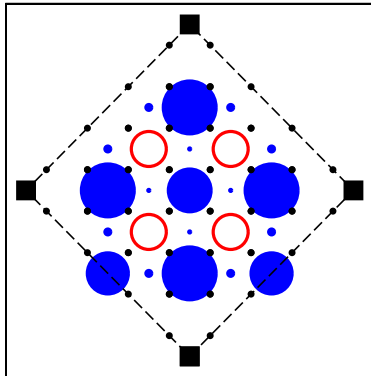
(b)

Next-nearest-neighbor J_2 and N.N.N.N J_3 stabilize 4-fold deg. plaquette VBC phase

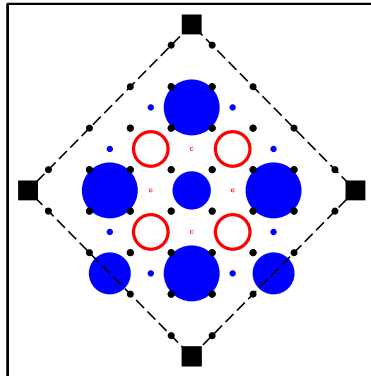
Plaquette correlations in J1-J2-J3

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

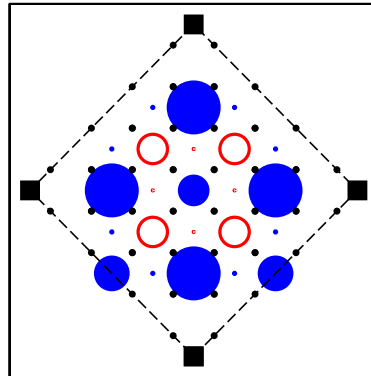
$J_2=0, J_3=0.5$



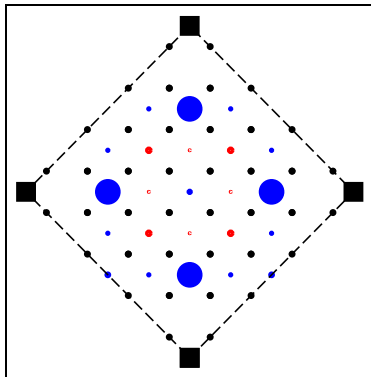
$J_2=0.1, J_3=0.4$



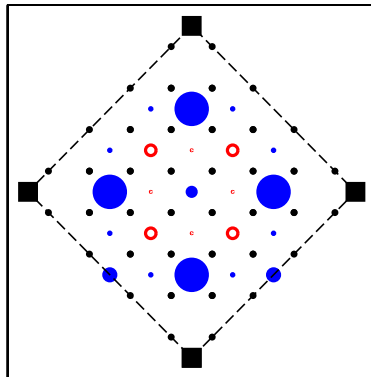
$J_2=0.2, J_3=0.3$



$J_3=0.2$



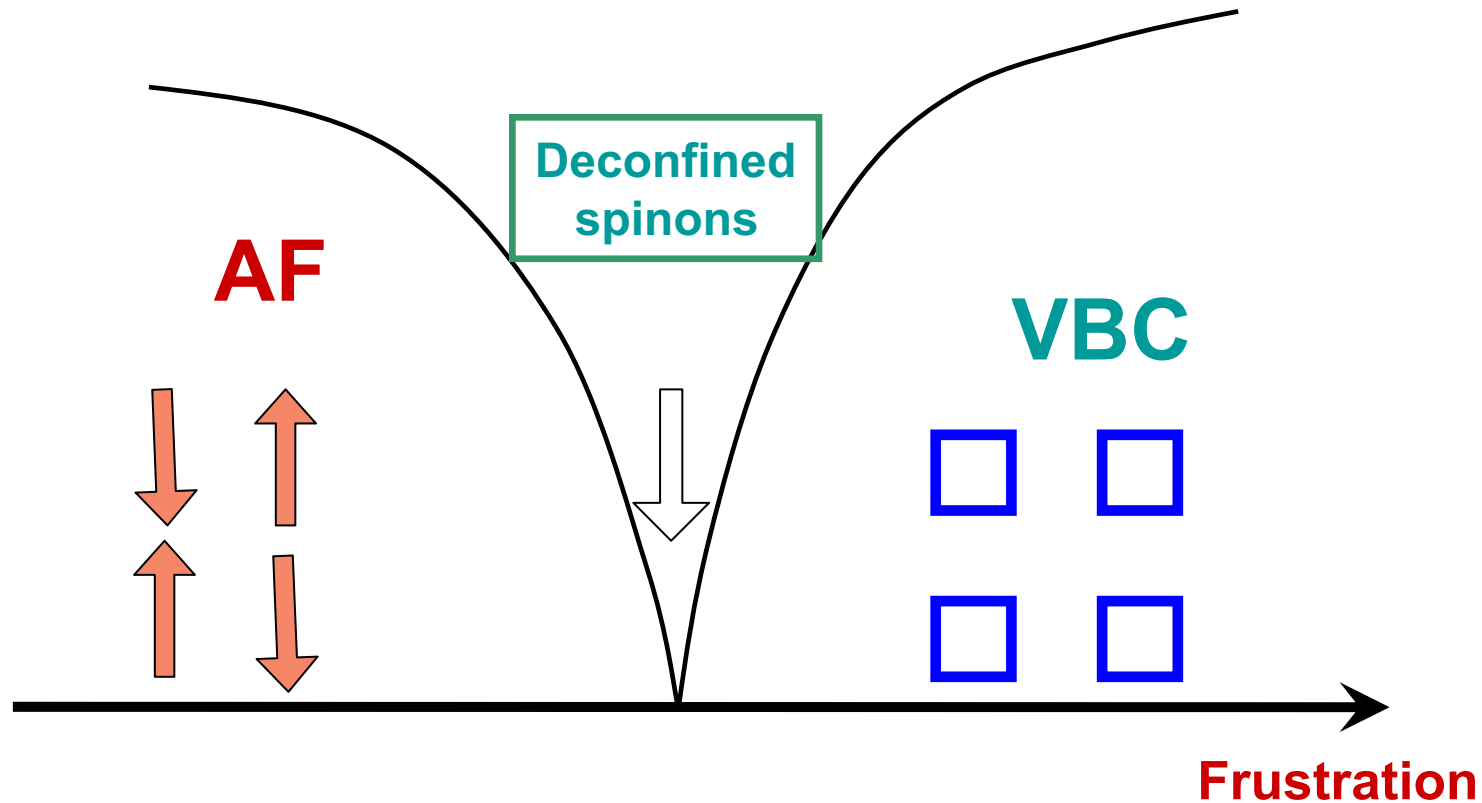
$J_3=0.3$



Plaquette operator $Q_{ijkl} = P_{ijkl} + P_{ijkl}^{-1}$
 where P_{ijkl} cyclic permutation

Mambrini et al., PRB **74**, 144422 (2006)
 (Exact diag. 32 sites cluster)

Deconfined Critical Point



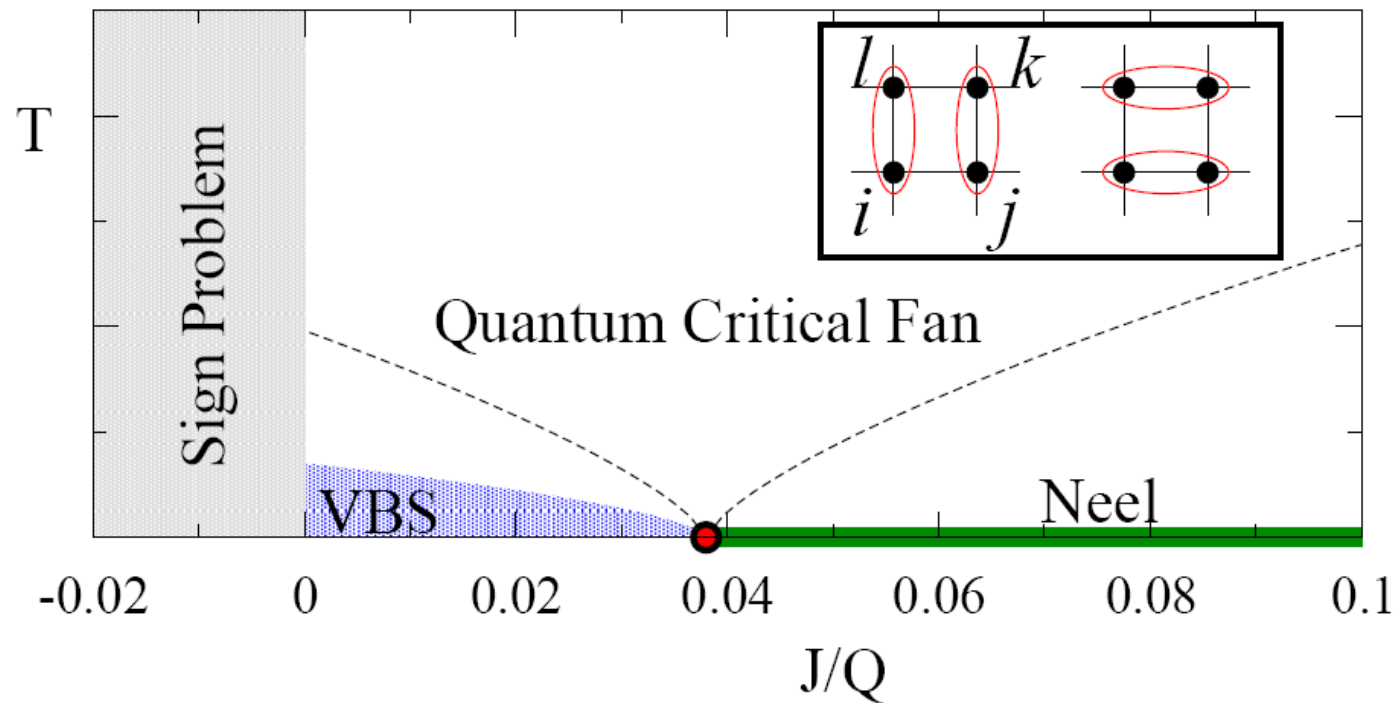
Beyond **Ginzburg-Landau** paradigm of phase transitions !
Senthil, Sachdev, Fisher et al.

Other proposal ...

Sandvik, Phys. Rev. Lett. **98**, 227202 (2007)

Melko & Kaul, arXiv:0707.2961

$$H_{JQ} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - 1/4)(\mathbf{S}_k \cdot \mathbf{S}_l - 1/4)$$



SSE-QMC

Doping frustrated magnets

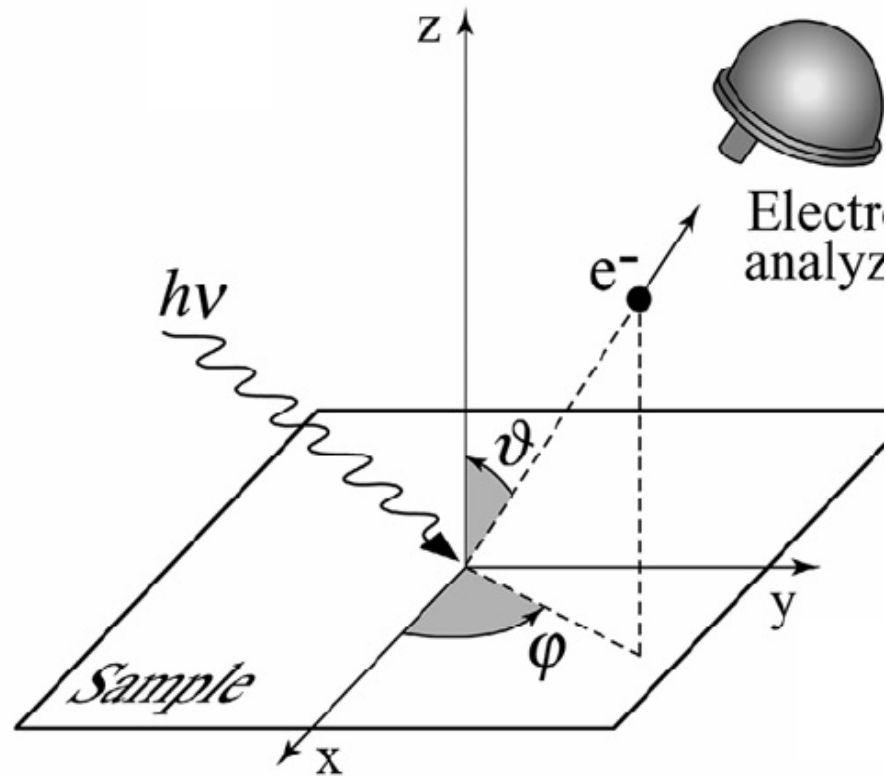


Itinerant frustrated systems

- spinel oxide LiTi_2O_4
Sun et al., PRB 70, 054519 (2004)
- 5d transition-metal pyrochlores as $\text{Cd}_2\text{Re}_2\text{O}_7$
or KOs_2O_6
Hanawa et al., PRL 87, 187001 (2001)
Hiroi et al., JPSJ 73, 1651 (2004)
- CoO triangular layer based compound
Takada et al., Nature 422, 53 (2003)

All superconducting with T_c up to 13.7 K !

Injecting a hole by ARPES



Andrea Damascelli

Physica Scripta. Vol. T109, 61–74, 2004

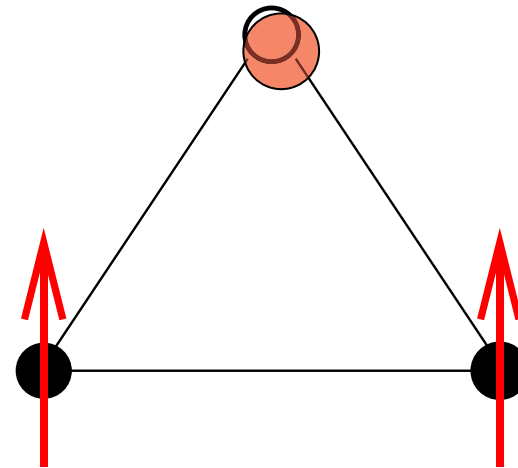
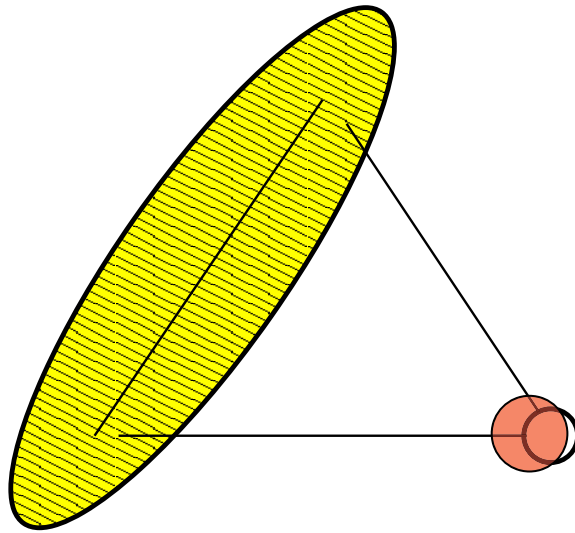
Photoemission geometry

$$A(\mathbf{k}, \omega) = A^+(\mathbf{k}, \omega) + A^-(\mathbf{k}, \omega) = -(1/\pi) \text{Im } G(\mathbf{k}, \omega)$$

Kinetic frustration

t-J model not particle-hole symmetric => sign of t matters !

J=0



singlet

triplet

t > 0 :

$$E = -2t$$

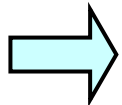
$$E = -t$$

t < 0 :

$$E = -|t|$$

$$E = -2|t|$$

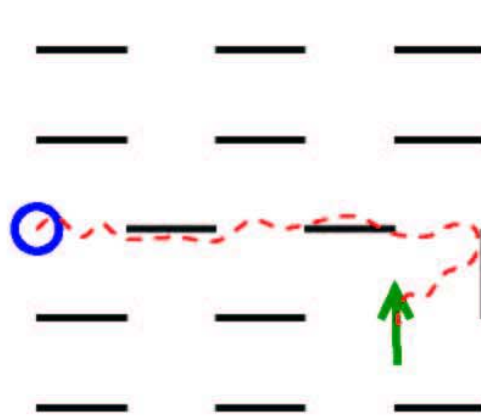
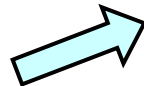
Nagaoka



Confinement vs deconfinement

See **Sachdev**

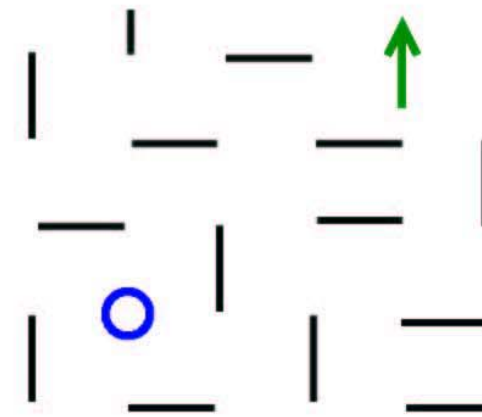
Holon



(a)

"string potential"

Checkerboard ??

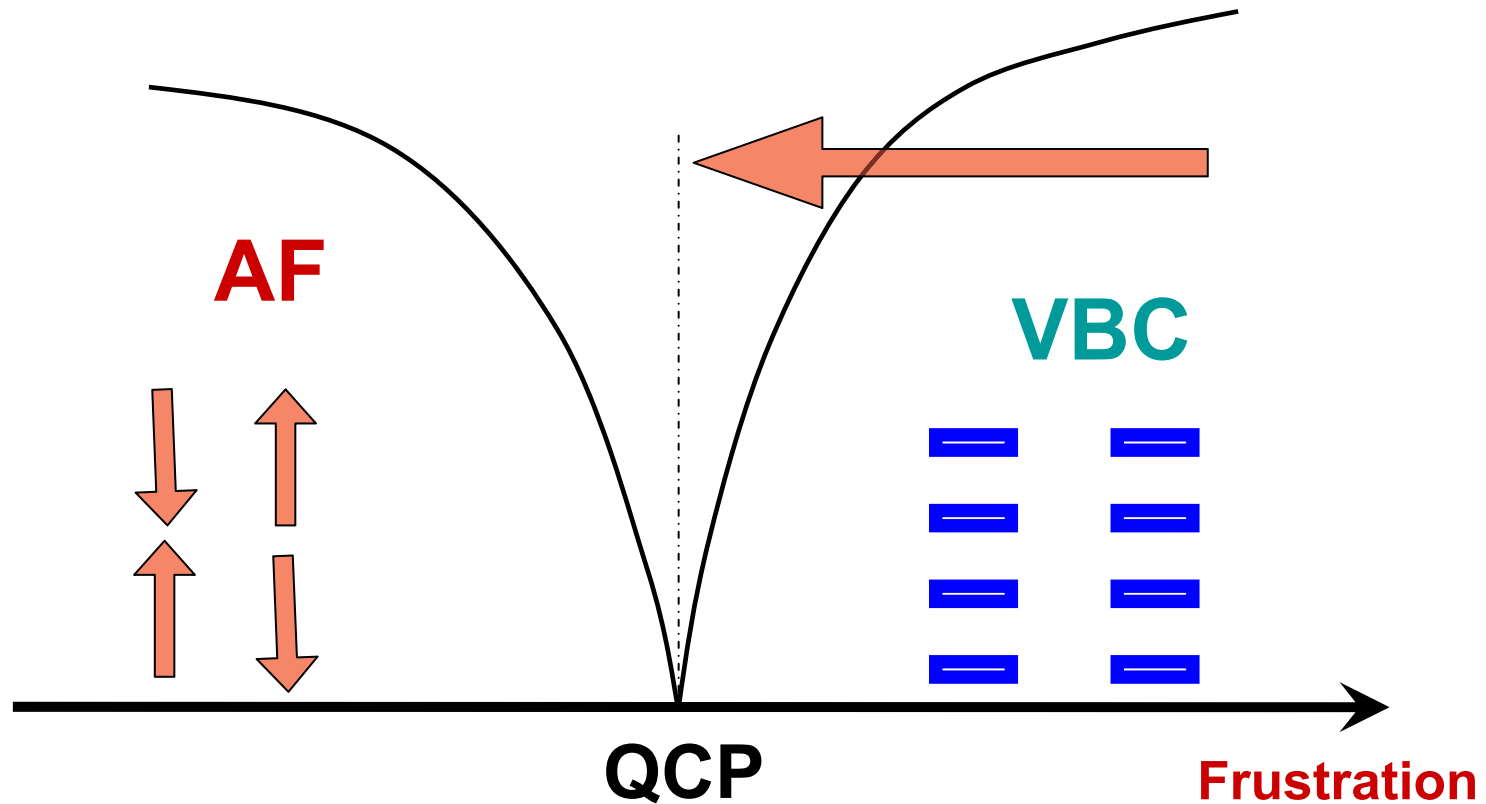


(b)

"deconfined" spinon

Kagome ??

Two emerging length scales



$$\xi_{\text{conf}} \sim \xi_{\text{VBC}} \gg \xi_{\text{AF}}$$

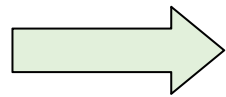
Injected hole acts like a probe: bare and dressed wavefunctions

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



Ground state of the Mott insulator

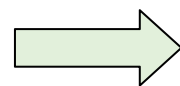
Remove a spin down at a given site O



Leaves behind a spin up polarization
at a typical distance ξ_{AF} from site O

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

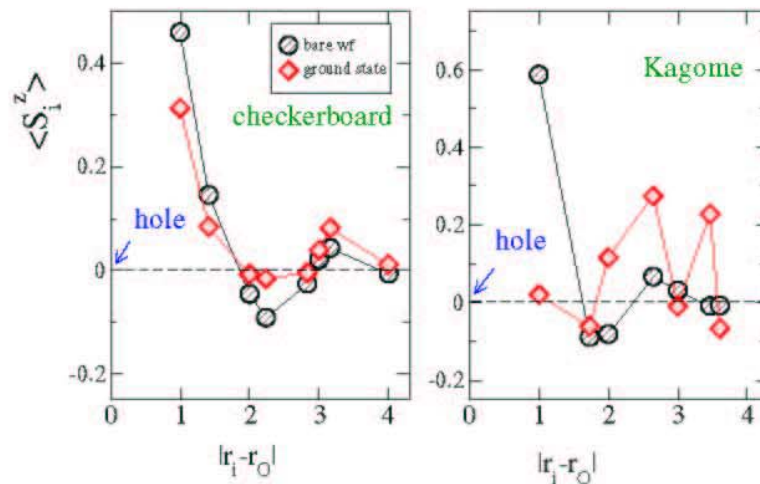
$$\langle S_i^z \rangle_{GS}$$



Profile of spinon wavefunction

Spin density around a vacancy

$\langle S_i^z \rangle$ at distance $r = r_i - r_0$ from defect



■ $\langle S_i^z \rangle_{\text{bare}} \rightarrow$ spin-spin correlation in host

■ $\langle S_i^z \rangle_{\text{gs}} \rightarrow$ “spinon” wavefunction

Kagomé: deconfined

Checkerboard: strongly confined



Quasiparticle weight

Overlap (squared) $Z = |\langle \Phi_{\text{gs}} | \Phi_{\text{bare}} \rangle|^2$
zero or finite ?

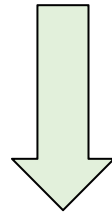
$$Z_{\text{Kagome}} = 0$$

$$Z_{\text{checkerboard}} \simeq 1$$

Dynamic hole (finite t) $\longrightarrow Z_{\mathbf{k}}$
 $A(\mathbf{k}, \omega) = Z_{\mathbf{k}} \delta(\omega - \omega_{\mathbf{k}}) + A_{\text{inc}} ??$

Single hole Green function

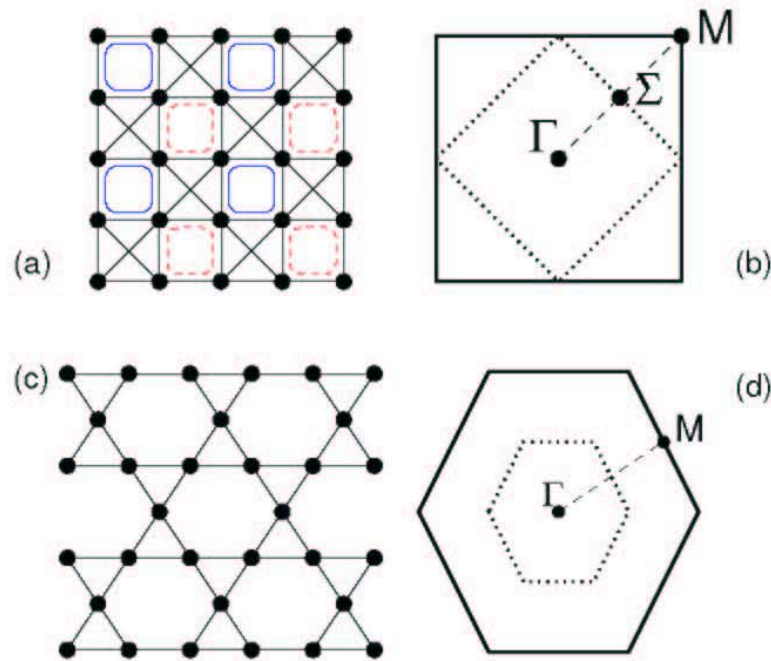
$$A(\mathbf{k}, \omega) = \text{Im} \left\{ \langle \Phi_0 | c_{\mathbf{k}\uparrow}^\dagger \frac{1}{\omega + i\epsilon - H} c_{-\mathbf{k}\downarrow} | \Phi_0 \rangle \right\}$$



“Bare” wavefunction
(Bloch state)

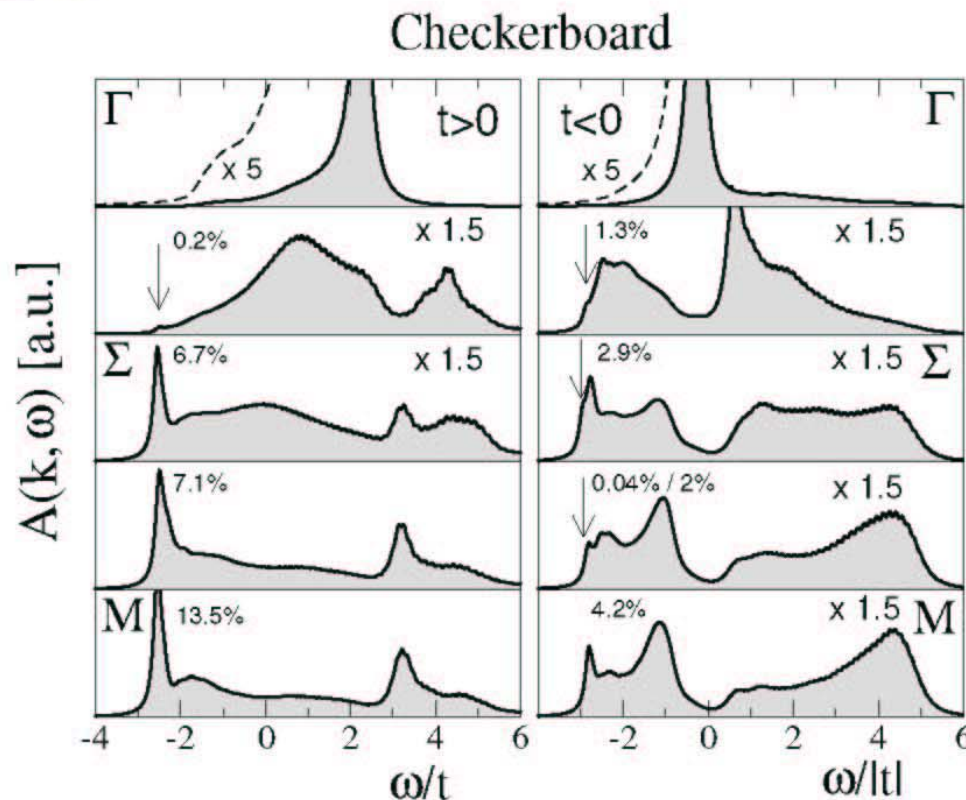
Use Lanczos continued-fraction method

Hole dynamics: t-J model



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

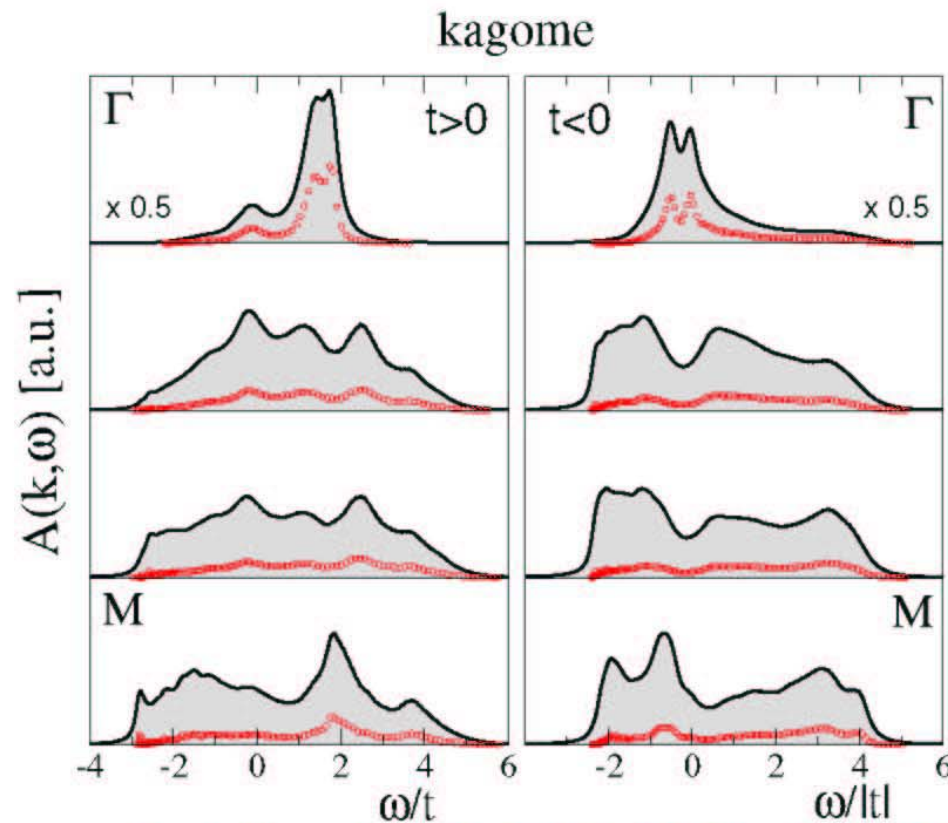
Hole dynamics in the VB Solid



Small
quasi-particle
peaks:
holon-spinon
boundstate

A. Läuchli & DP, PRL **92**, 236404 (2004)

Single hole doped in a spin liquid



Incoherent
spectrum

Weights
distributed on
many poles
even at low
energies

A. Läuchli & DP, PRL **92**, 236404 (2004)

Summary / Conclusions

- Frustration + quantum fluctuations lead to exotic disordered GS (VBC, SL, ...)
- Possible realization of exotic physics (Deconfined Critical Points, etc...)
- The doping issue might reserve many surprises but needs further investigations