Introduction to frustrated magnets

On the doping issue

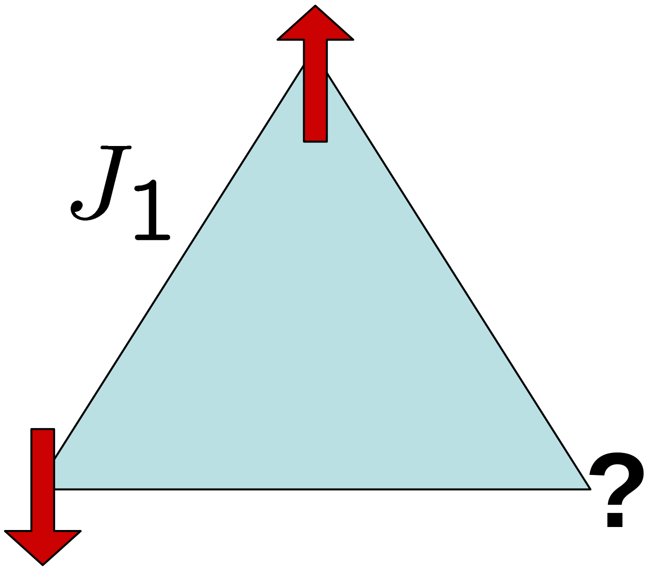
OUTLINE

- 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
- Effective models – Quantum dimer models
- Some doping issues – Impurities and mobiles holes in VBC & spin-liquid hosts

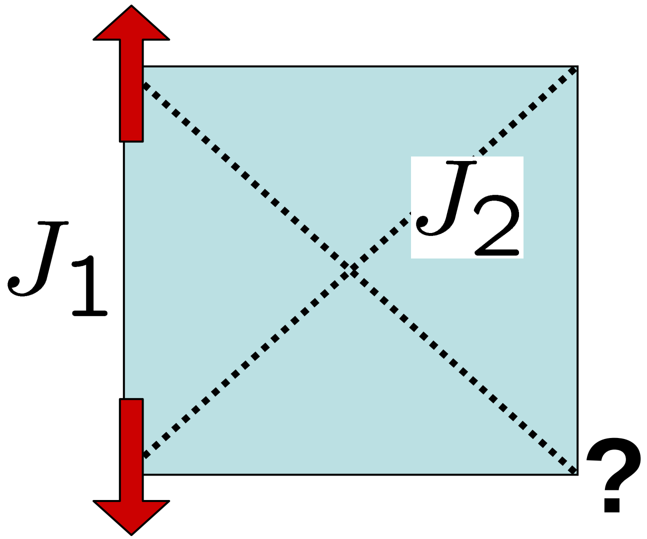
Recommended advanced reading on the subject

Review book “Frustrated Spin Systems”, Ed. H.T. Diep (World Scientific 2004)

The concept of frustration



Topological origin



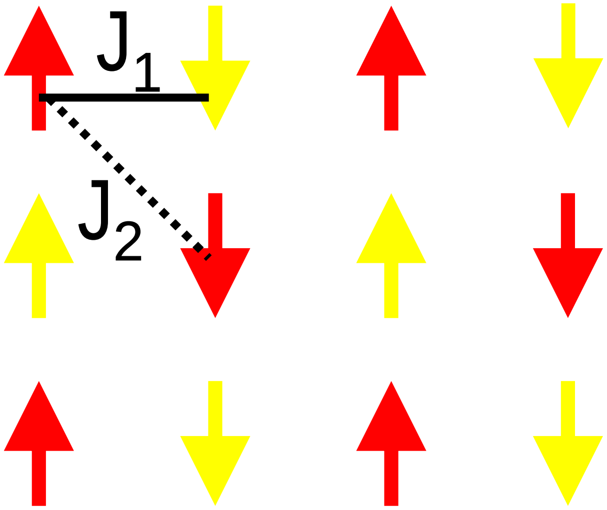
Extended range interaction

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

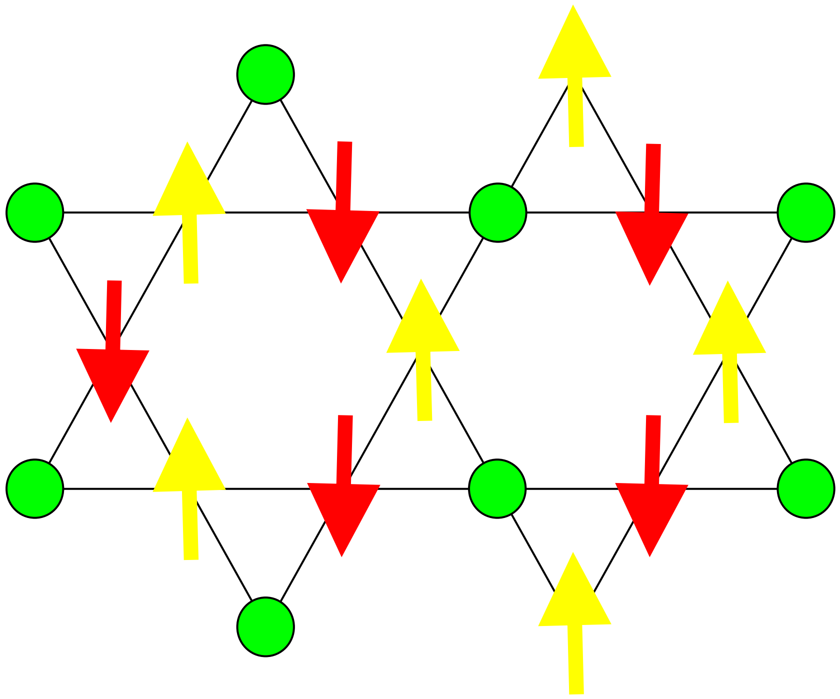
Defining frustration II

Frustration = infinite degeneracy of classical ground state

J_1-J_2 model (J_2>J_1/2)



Kagome lattice



Effect of quantum fluctuations?

Courtesy of Mila's family

Simple considerations for classical spins

$$E[\{\mathbf{S}_i\}] = \frac{1}{2}\sum_i \sum_r J(\mathbf{r})\mathbf{S}_i \cdot \mathbf{S}_{i+r}$$

with constraint $|\mathbf{S}_i| = 1$ on all sites

By Fourrier transform:

$$E = \frac{1}{2}\sum_k J(\mathbf{k})\mathbf{S}_k \cdot \mathbf{S}_{-k}$$

⇒ Minimize J(k)

Assume $J(\mathbf{k})$ minimized for $k = k_0$

$\Downarrow$

$\mathbf{S_k} = 0$ for all $\mathbf{k}$'s except $\mathbf{k} = \mathbf{k}_0$

$\Downarrow$

$$\mathbf{S}_i = \frac{1}{\sqrt{N}}(\mathbf{S}_{\mathbf{k}_0} e^{i\mathbf{k}_0.\mathbf{r}_i} + H.C.)$$

constraint $|\mathbf{S}_i| = 1$

$\Downarrow$

$$\mathbf{S}_i = (\cos(\mathbf{k}_0.\mathbf{r}_i), \sin(\mathbf{k}_0.\mathbf{r}_i), 0)$$

Spiral configuration (non-collinear – coplanar)

Classical J1-J2 model

$$J(\mathbf{k}) = 2J_1(\cos k_x + \cos k_y) + 4J_2 \cos k_x \cos k_y$$

Minimum of J(k)

* 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
$\Rightarrow$ highly degenerate

$$H = \text{cst} + \sum_{\text{plaquettes}} (\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2$$

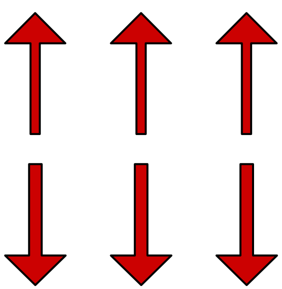
Quantum fluctuations

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

$$E = \text{cst} + \sum_{\mathbf{k}} (\alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} + \frac{1}{2}) \omega_{\mathbf{k}}$$

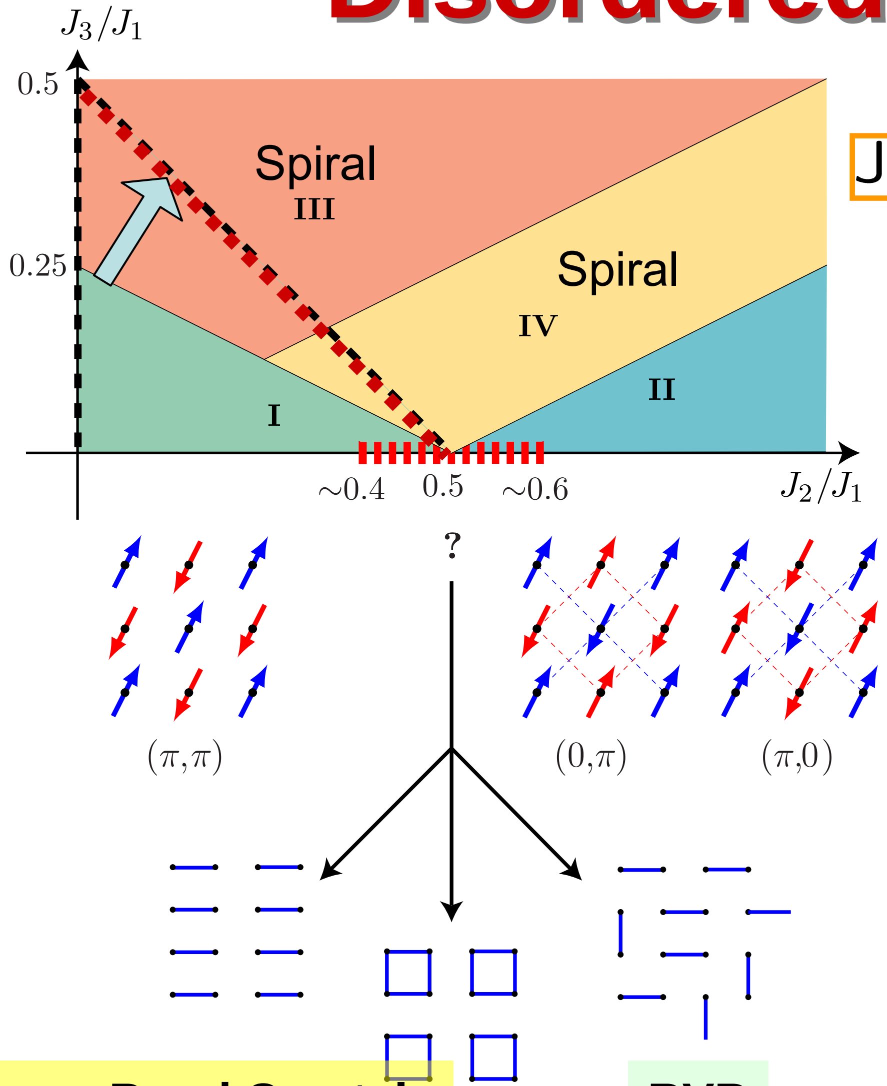
Point zero quantum fuctuations

For $J_2 > J_1/2$: collinear structures are selected



Order-by-disorder phenomenon (Villain)

Emergence of exotic Quantum Disordered Phases ?



Valence Bond Crystals

RVB

J_1-J_2-J_3 AF Heisenberg model

Classical phase diagram
A. Chubukov, PRB 90

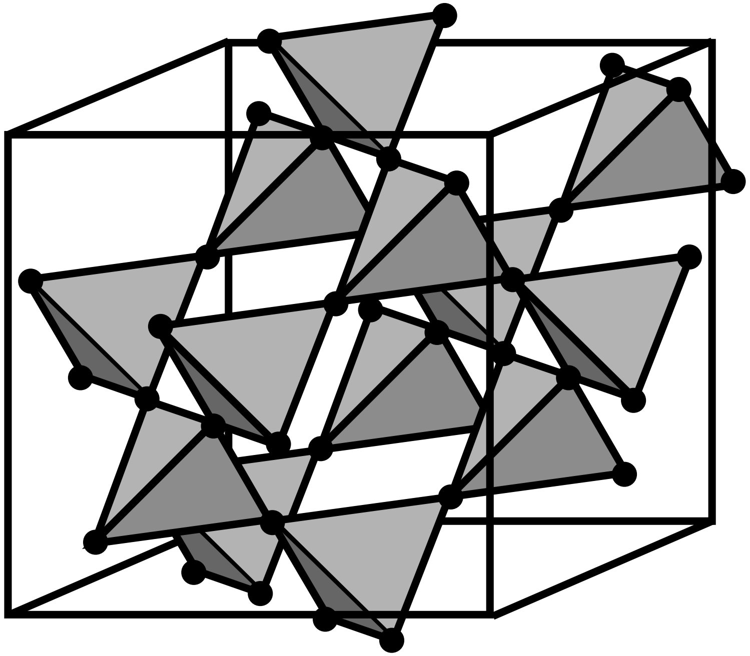
Quantum fluctuations

Simple frustrated lattices

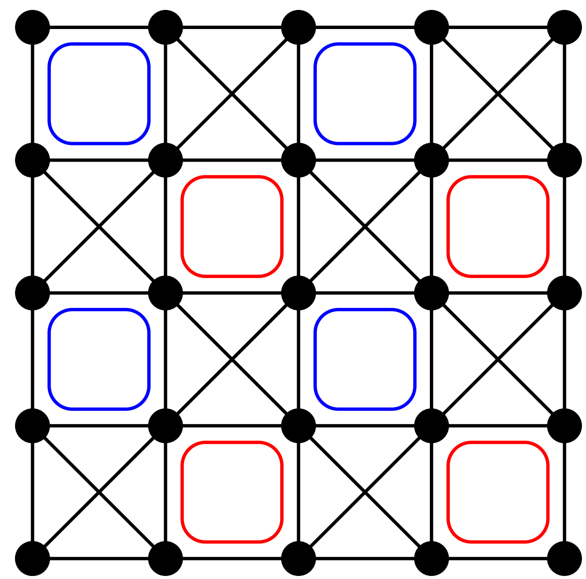
& related frustrated spin compounds

Lattices of corner-sharing units

Pyrochlore lattice



Checkerboard lattice

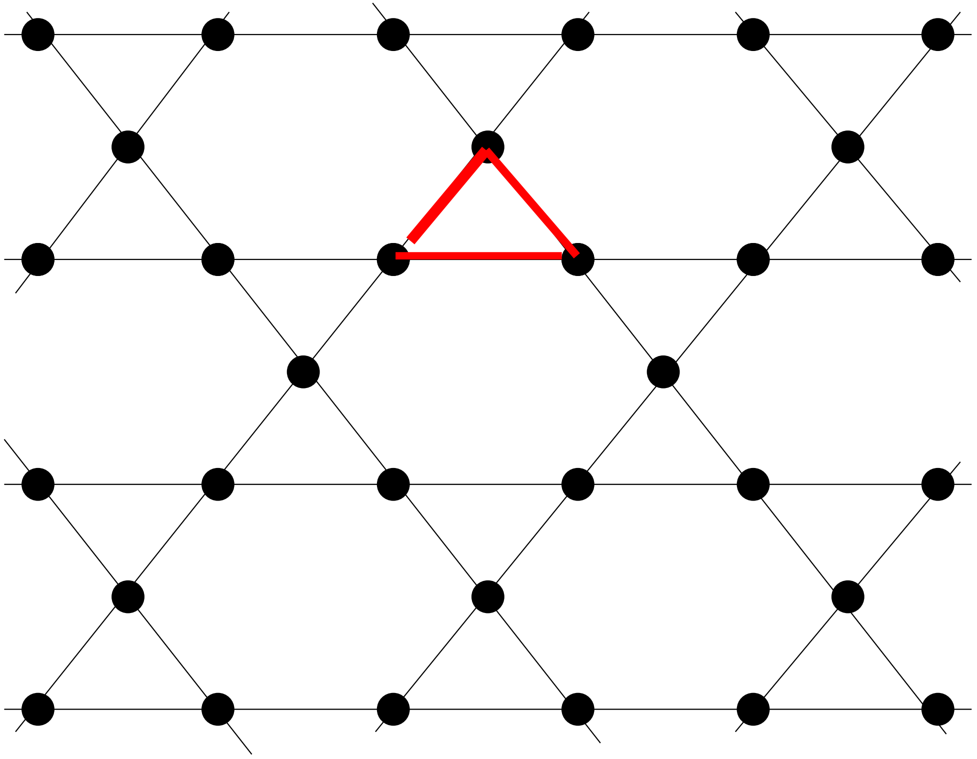


A lattice for theorists !

Corner-sharing tetraedras in 3D & 2D

The Kagome lattice

2D lattice of corner sharing triangles

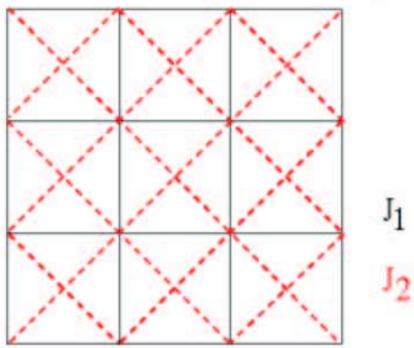


Very high degeneracy !!

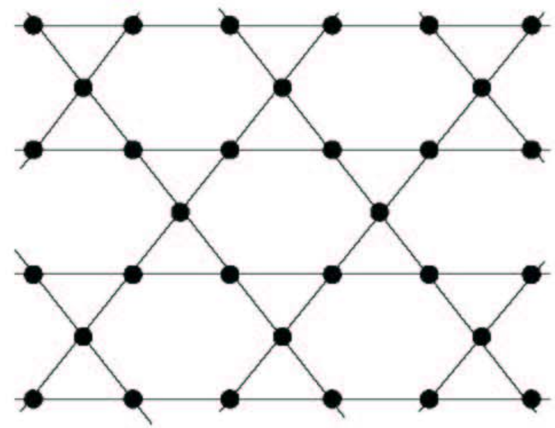
2D Frustrated magnets

Lattices with AF frustrating interactions

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



frustrated square lattice (S=1/2): Li_2VOSiO_4



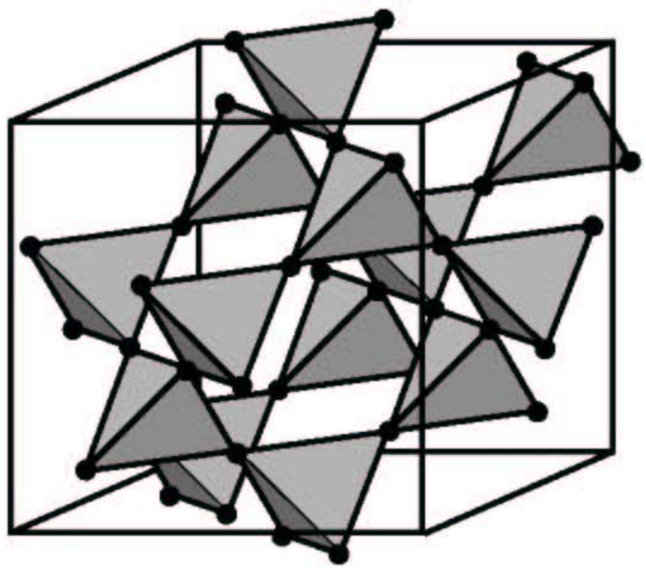
Kagome lattice like $SrCr_{9-x}Ga_{3+x}O_{19}$ (S=3/2)

Ramirez et al., PRL **64** ('90)

Broholm et al., PRL **65** ('90)

3D Frustrated magnets

pyrochlores and spinels



Transition metal oxides

- $ZnCr_2O_4$ spinel

- $A_2Ti_2O_7$ titanates

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

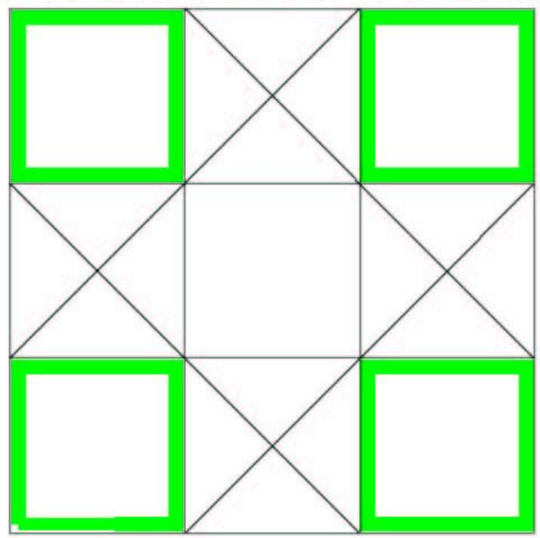
-no ordering down to low temperatures

Quantum disordered phases

& Quantum Critical Point (QCP) scenario

VBC vs SL

Checkerboard lattice

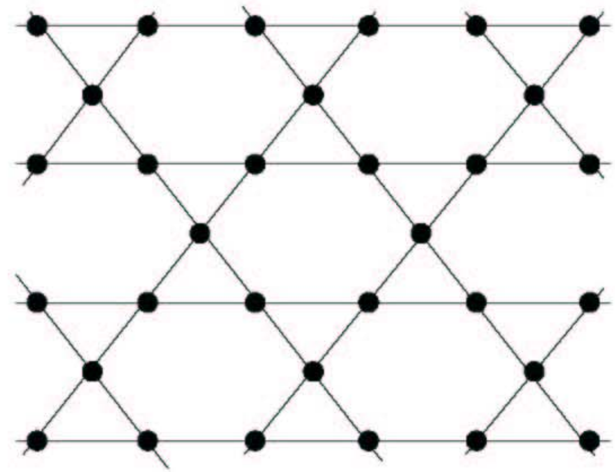


Valence bond crystal

- Finite gaps
- Spontaneous translation symm. breaking

(Fouet al.)

Kagome lattice

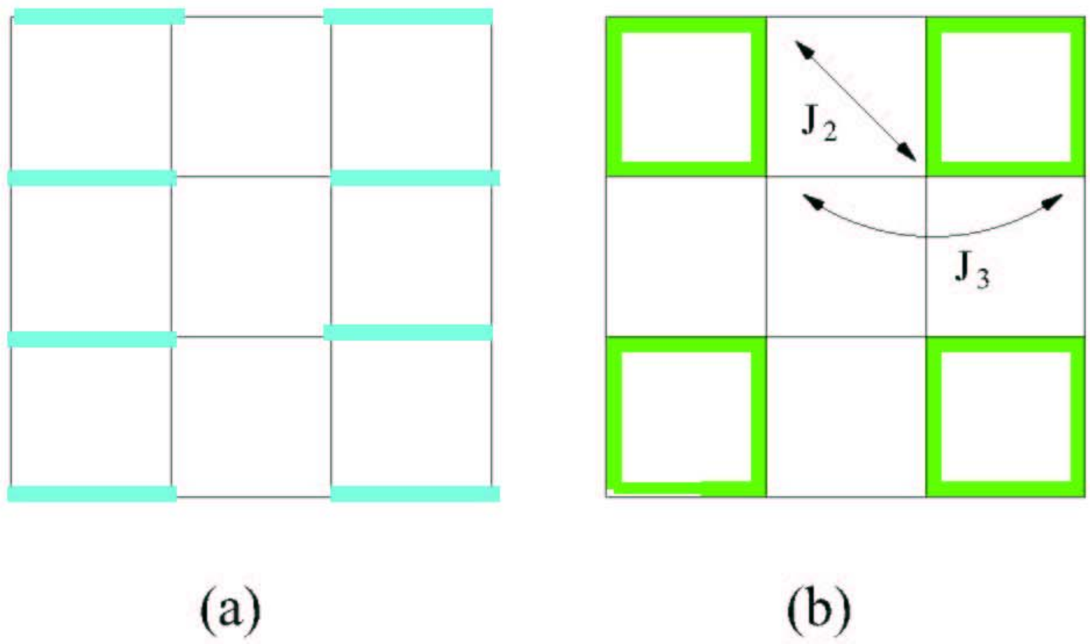


Spin liquid (SL)

- No symmetry breaking
- Large # of low energy singlets

(Mila et al.)

VBC candidates for the AF square lattice



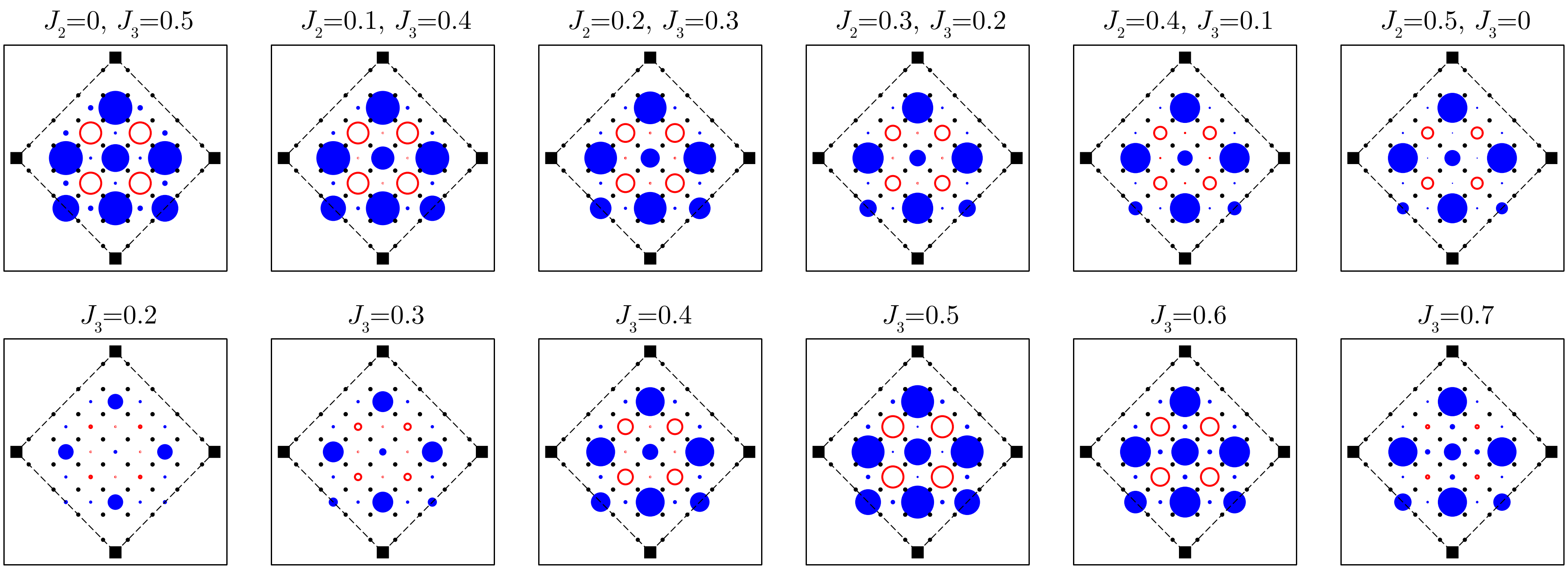
Next-nearest-neighbor J_2 and N.N.N.N J_3 stabilize 4-fold deg. plaquette VBC phase

Plaquette correlations in J1-J2-J3

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

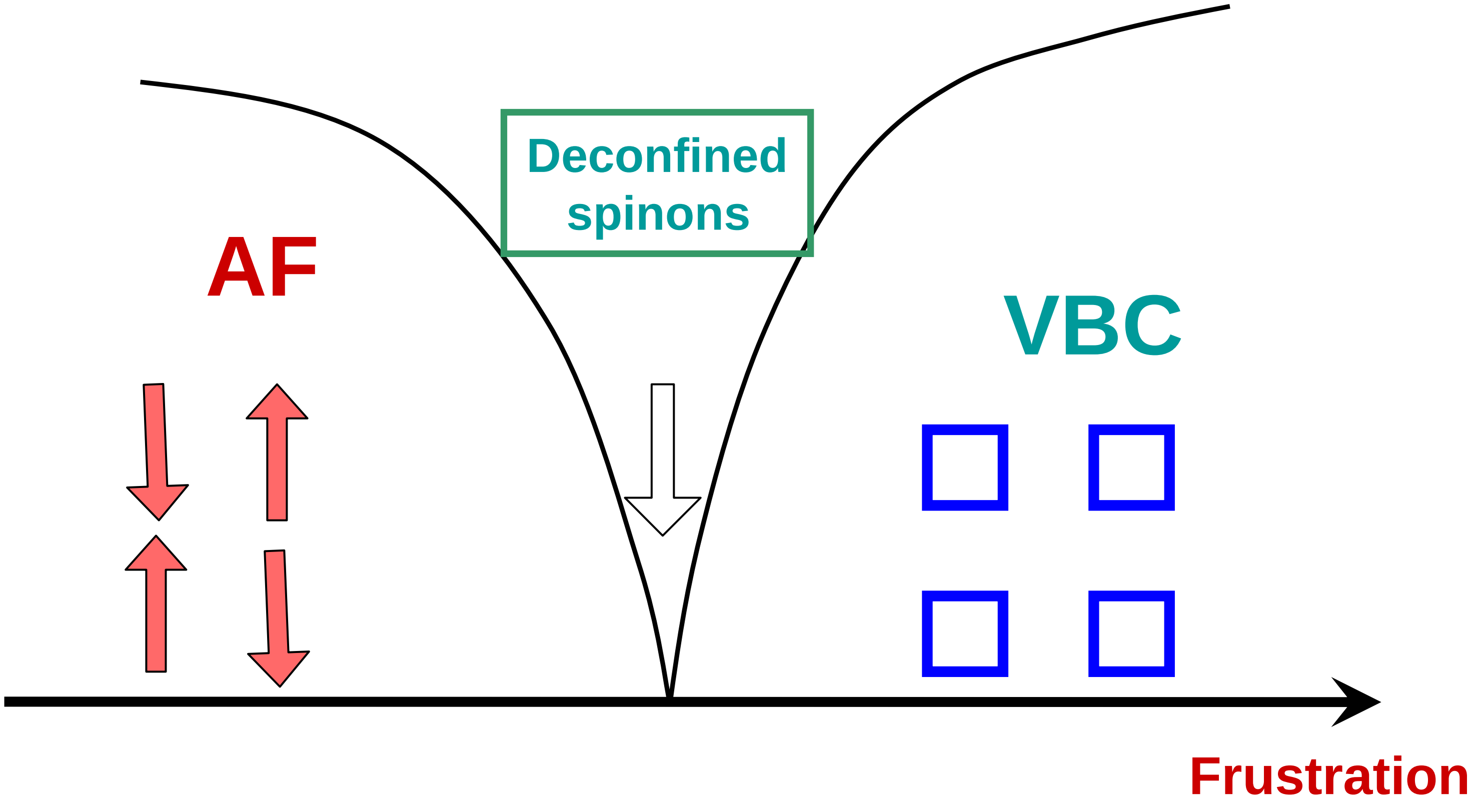
Plaquette operator $Q_{ijkl} = P_{ijkl} + P_{ijkl}^{-1}$

where P_{ijkl} cyclic permutation



Mambrini, Läuchli et al. 2006 (Exact diag. 32 sites cluster)

Deconfined Critical Point



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

Also investigated numerically by Sandvik et al.

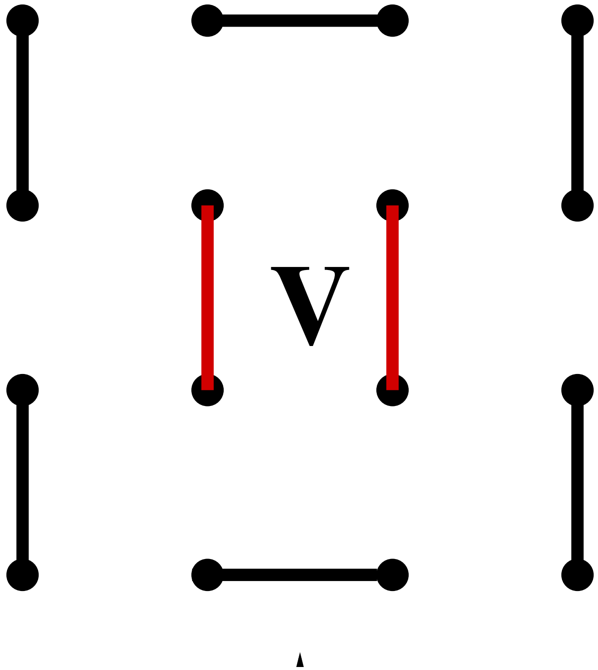
Effective models

Quantum dimer models

Motivations

- Construct models to focus on low energy dynamics in the **singlet** sector
- Ignore magnetic excitations: justified for **gapped** magnons or spinons
- Need for models **simpler than spin models** but can nevertheless exhibit both **dimer-liquid and VBC ground states**

Classical dimer model



A typical (hard-core) dimer covering of the square lattice

Dimer repulsion

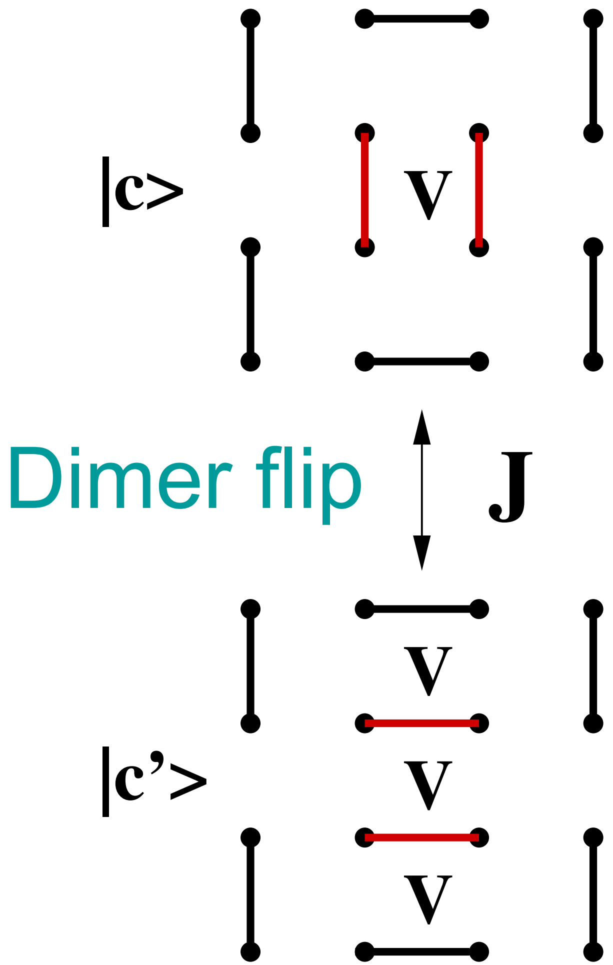
$$E_{\text{clas}} = V N_c = e_c$$

Number of “V” plaquette in configuration |c>

Adding quantum fluctuations:

The Quantum Dimer Model

Rokhsar & Kivelson, PRL 88



$$H_{\mathrm{QDM}} = \sum_c e_c |c\rangle\langle c| - J \sum_{c,c'} |c\rangle\langle c'|$$

Relation with SU(2) spin models

SU(2) Valence Bond ⇔ dimer covering

Orthogonal basis by construction

Sutherland, 1988:

$$|\langle a|b\rangle| = \sum_{\mathcal{L}} 2^{(1-L_{\mathcal{L}}/2)} = 2^{(n_{\mathcal{L}}-N/2)}$$

Length of the loops of overlap graph

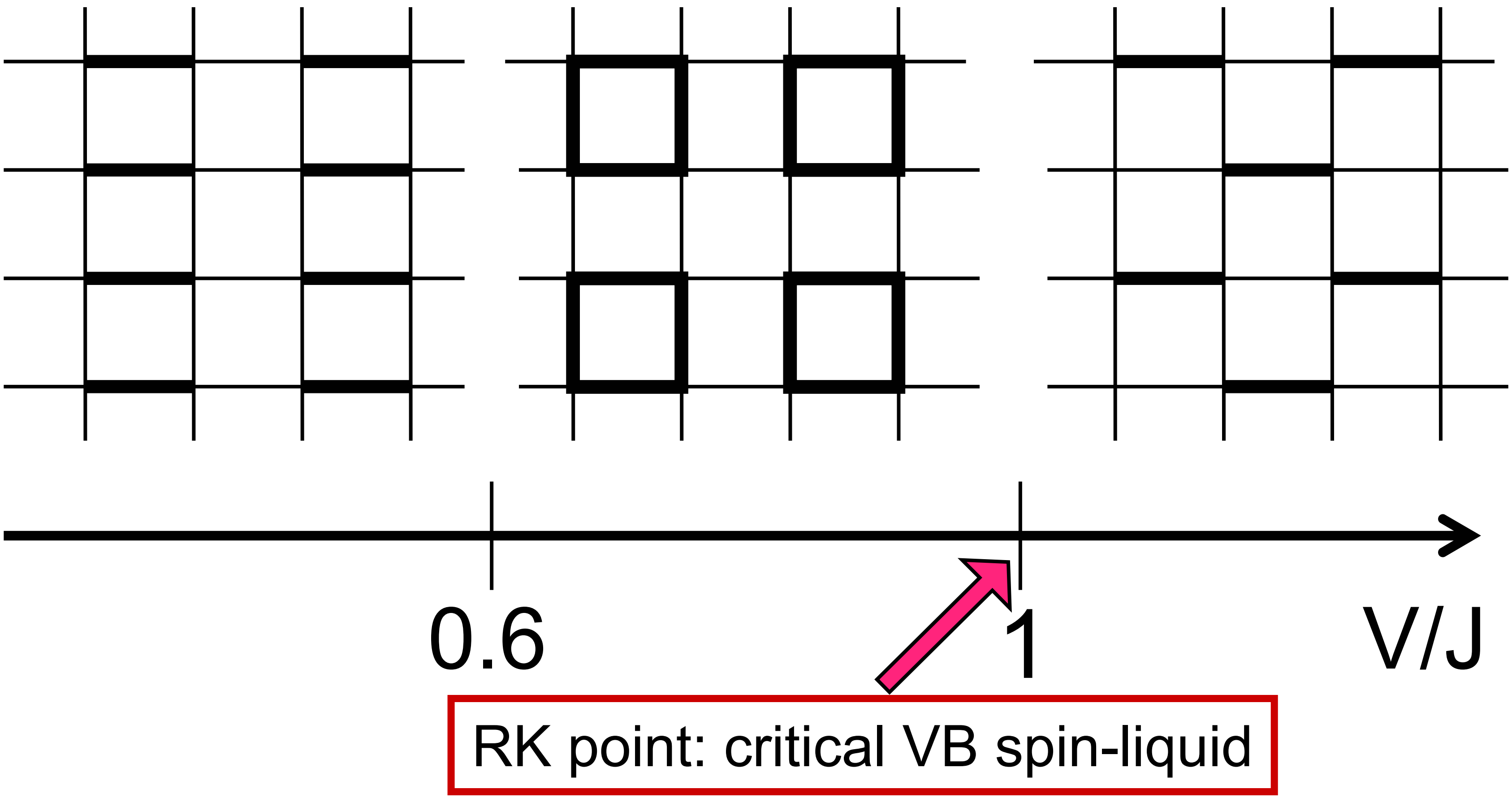
Small parameter : $(\frac{1}{\sqrt{2}})^{L_{\mathcal{L}}}$

RK, 1988: Expansion to order x^n

→ Hamiltonian with up to n-dimers terms

Phase diagram

No minus sign problem => QMC: Syljuasen, PRB 2006



Rokhsar-Kivelson point

For J=V: sum of projectors

$$H_{\mathrm{RK}} = \sum_{\mathrm{p}} |\Psi_p\rangle\langle\Psi_p|$$

$$|\Psi_p\rangle = |\,\|\,\|\,\rangle - |\,=\,\rangle$$

$$|\Phi_0\rangle = \frac{1}{Z}\sum_{\{c\}} |c\rangle$$

exact GS with energy E=0

$\Longleftrightarrow$ Infinite-T Classical DM

Quasi-long ranged (critical) dimer-dimer correlations

RVB liquid on the triangular lattice

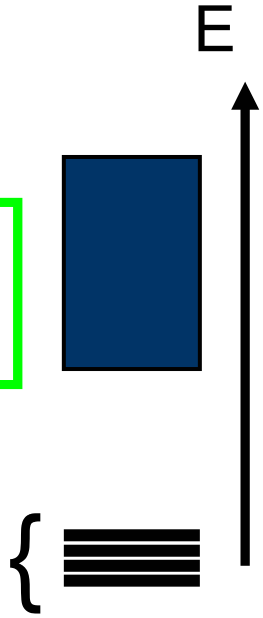
Moessner & Sondhi, PRL 2001

Dimer flips on all Rhombi (3 kinds) of the lattice

Again for V=J, mapping to classical problem (RK point)

Pfaffian calculation

Finite correlation length
Exponential decay of dimer-dimer correlations



Degeneracy from “topological order”
GS have different “winding numbers”

On doped frustrated magnets

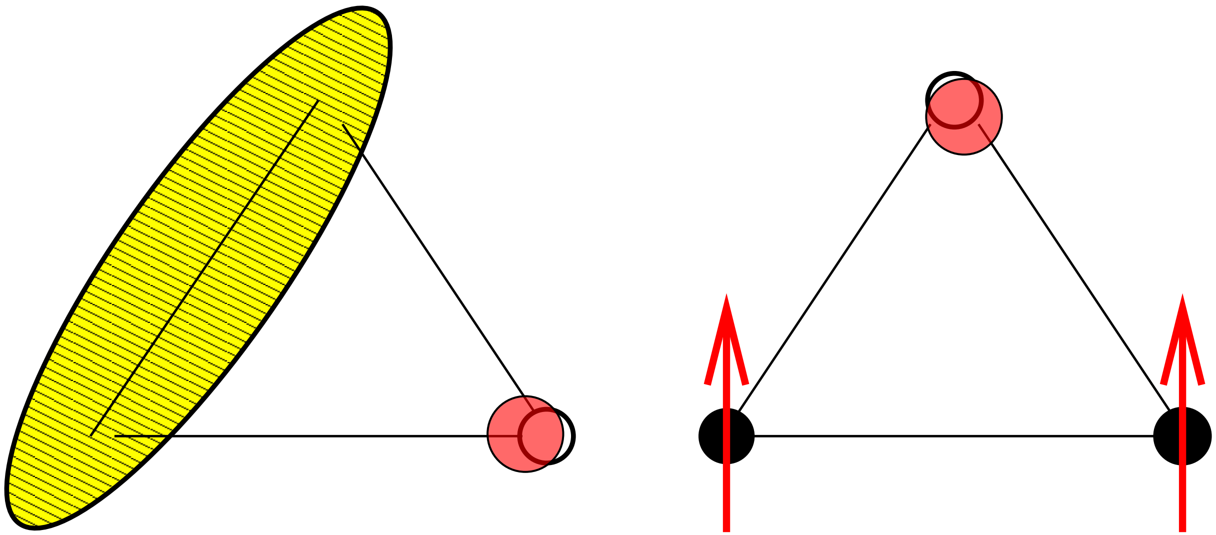
Itinerant frustrated systems

- spinel oxide $LiTi_2O_4$
  Sun et al., PRB **70**, 054519 (2004)
- 5d transition-metal pyrochlores as $Cd_2Re_20_7$ 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 !

Kinetic frustration

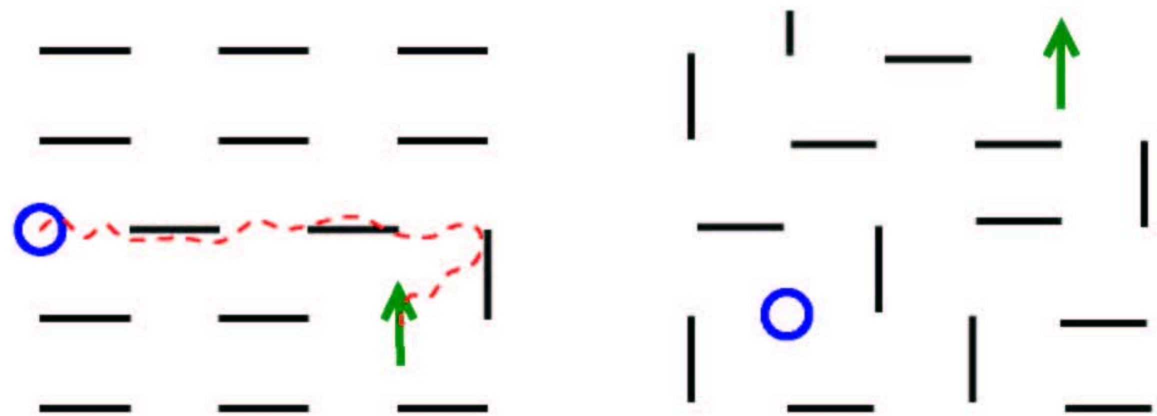
t-J model not particle-hole symmetric => sign of t matters !



	singlet	triplet
$t>0$:	$E=-2t$	$E=-t$
$t<0$:	$E=-\|t\|$	$E=-2\|t\|$

Confinement vs deconfinement

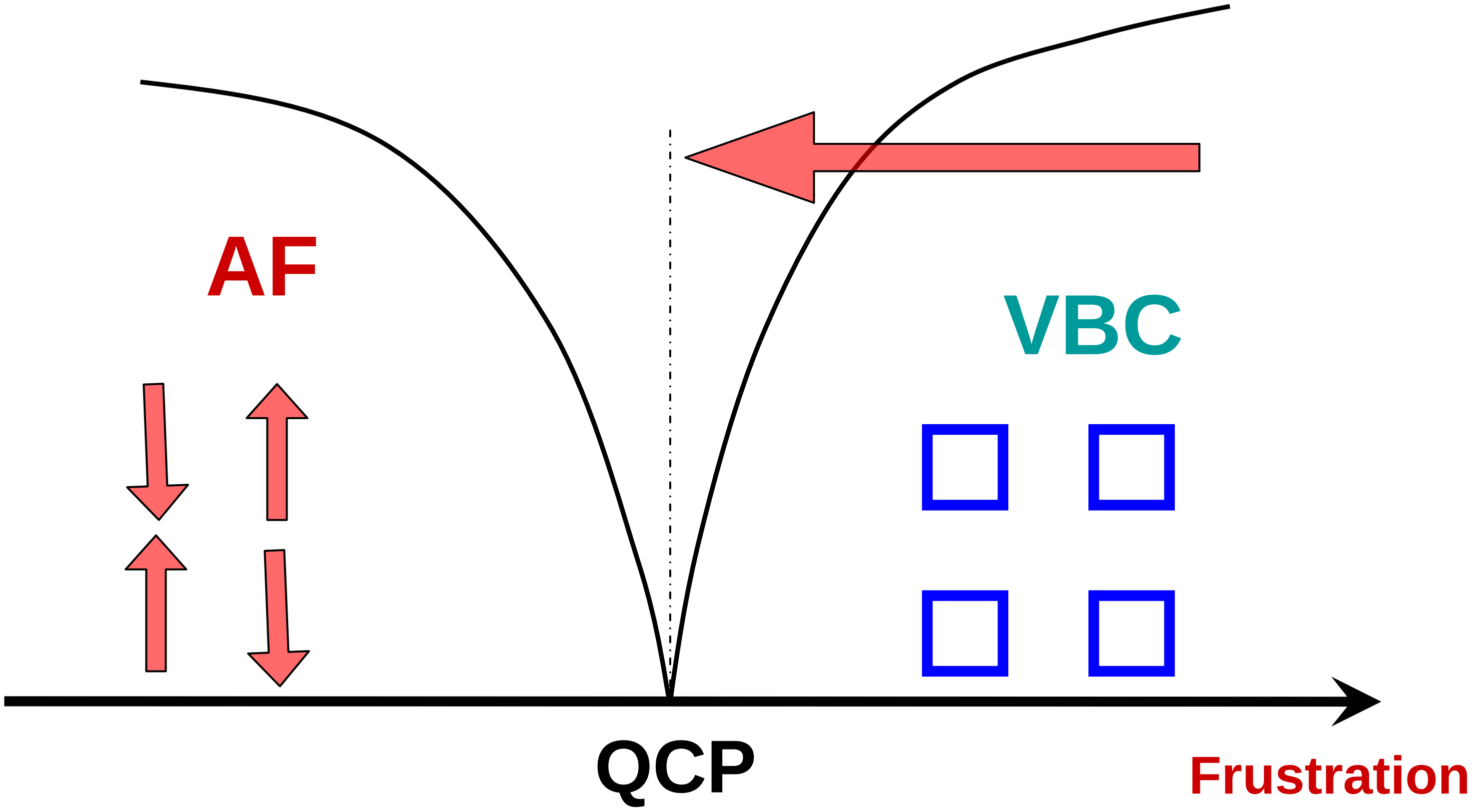
See Sachdev



(a) "string potential"

(b) "deconfined" spinon

Two emerging length scales



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

Senthil et al.

Injected hole acts like a probe: bare and dressed wavefunctions

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

Ground state of the Mott insulator

Remove a spin down at a given site O

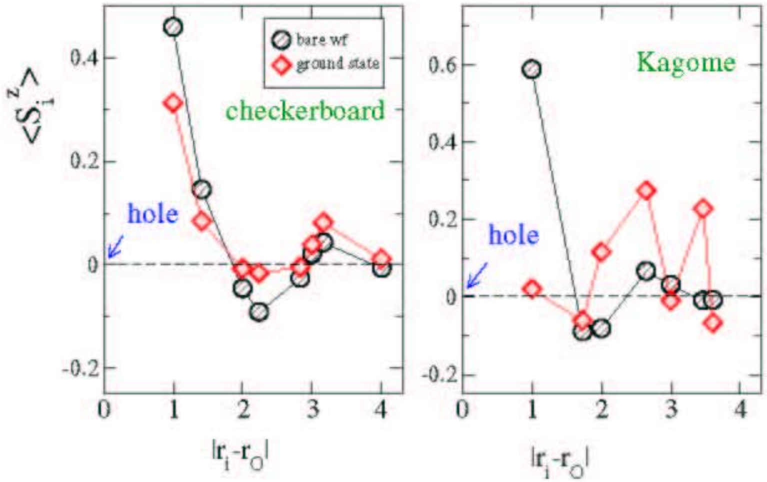
⇒ Leaves behind a spin up polarization at a typical distance ξ_{AF} from site O

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

$\langle S_i^z \rangle_{\mathsf{GS}}$ ⇒ Profile of spinon wavefunction

Spin density around a vacancy

$\langle S_i^z \rangle$ at distance $\mathbf{r} = \mathbf{r_i} - \mathbf{r_O}$ from defect



- $\langle S_i^z \rangle_{\mathrm{bare}} \rightarrow$ spin-spin correlation in host
- $\langle S_i^z \rangle_{\mathrm{gs}} \rightarrow$ "spinon" wavefunction

Kagomé: deconfined

Checkerboard: strongly confined

D.P. et al. PRB (2006)

Quasiparticle weight

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

$$Z_{\rm Kagome} = 0$$
$$Z_{\rm checkerboard} \simeq 1$$

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

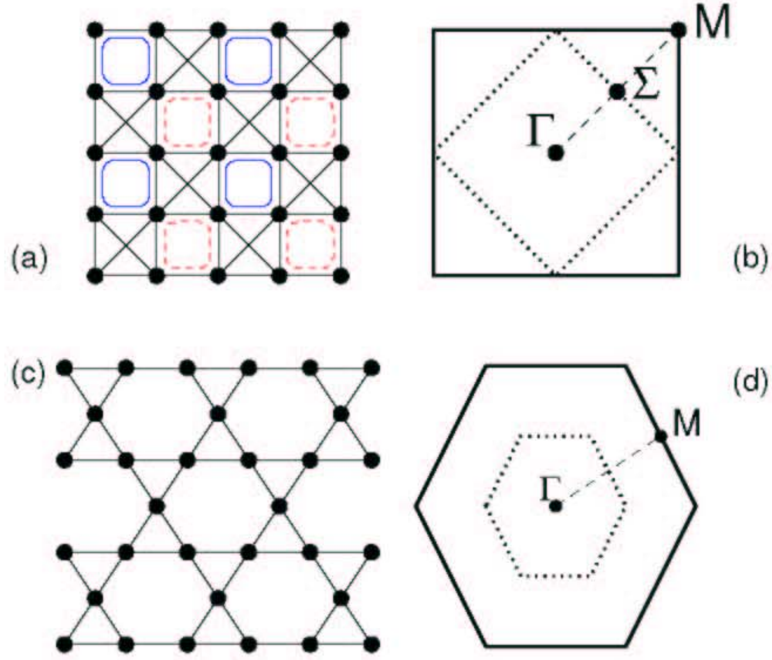
Single hole Green function

$$A(\mathbf{k},\omega) = \mathrm{Im}\{\langle\Phi_0|c^\dagger_{\mathbf{k}}\frac{1}{\omega+i\epsilon-H}c_{-\mathbf{k}}|\Phi_0\rangle\}$$

"Bare" wavefunction
(Bloch state)

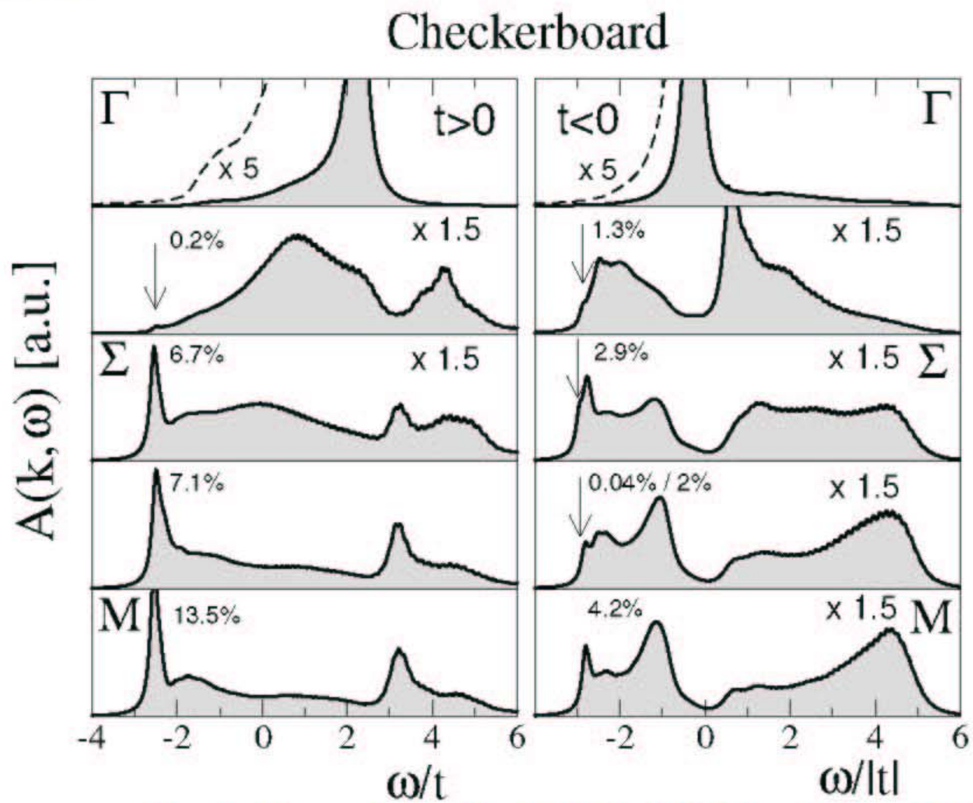
Use Lanczos continued-fraction method

Hole dynamics: t-J model



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

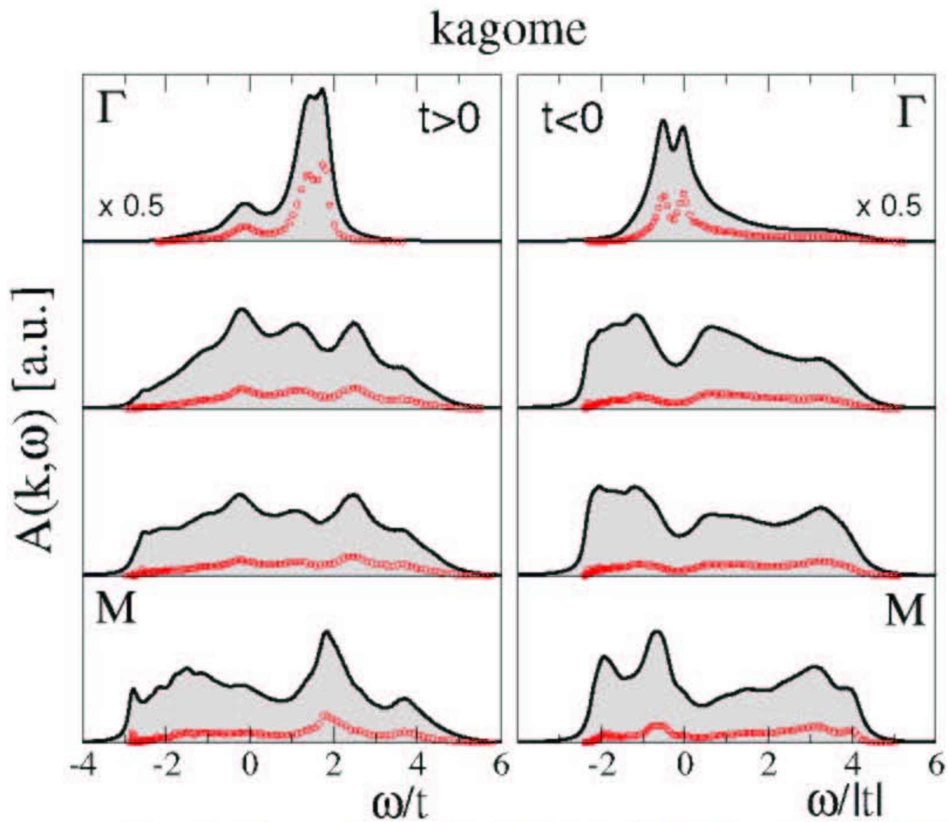
Hole dynamics in the VB Solid



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 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 effective QDM easier
- The doping issue might reserve many surprises but needs further investigations