Some exotic phenomena in undoped and doped quantum frustrated antiferromagnets

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Strongly correlated systems

- **Magnetism,**
- **Superconductivity.**

Closely related problems

- Superconductors are **Doped Mott insultors**
- Underlying magnetism drives the **effective interaction** between charge carriers

General goals

- Understand the **insulating phase**
- Look for **general mechanisms** away from half-filling

Mott insulators $\rightsquigarrow$ Localized spins. Heisenberg model

$$\mathcal{H} = \sum_{(i,j)} J_{ij} \vec{S}_i.\vec{S}_j$$

Classical case

$\vec{S}$: vector

Neel state

$\ldots \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \ldots$

Quantum case

$\vec{S}$: quantum spin

Fluctuations:

$$\vec{S}_i.\vec{S}_j = S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$$

Relevance of quantum fluctuation ? / AF order ?

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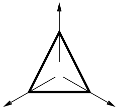
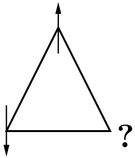
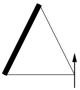
FRUSTRATION

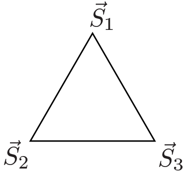


Global compromise &
Ground state degeneracy





Ground state ?
Degeneracy ?
Density of states ?



$$\vec{S}_1.\vec{S}_2 + \vec{S}_2.\vec{S}_3 + \vec{S}_3.\vec{S}_1 = (1/2)\{(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 - \vec{S}_1^2 - \vec{S}_2^2 - \vec{S}_3^2\}$$

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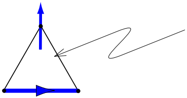
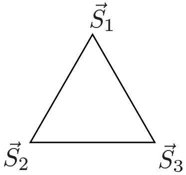
Quantum case $(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 = (1/2)_{\mathrm{R}}\ (1/2)_{\mathrm{L}}\ (3/2)$

$$\vec{S}_1.(\vec{S}_2 + \vec{S}_3) \longrightarrow 0$$
$$\vec{S}_2.\vec{S}_3 \longrightarrow -3/4$$



$$\frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$$



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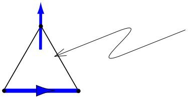

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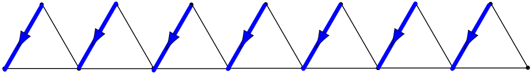
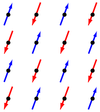


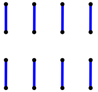
Frustration **Corner sharing geometry**



Semi-classical systems Néel order

Irrelevant quantum fluctuations $\Delta_{S=0,S=1} = 0$

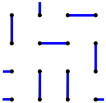
SU(2) and spatial symetries broken



Valence bond crystal $\langle S_0.S_r \rangle \sim \exp(-r/\xi)$

« dimer crystal », « plaquette crystal » $\Delta_{S=0,S=1} \neq 0$

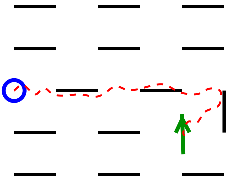
SU(2) restored but spatial symetries broken



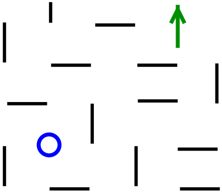
Spin liquids No order

SU(2) and spatial symetries restored

- Type I : $\Delta_{S=0,S=1} \neq 0$ et $\Delta_{S=0,S=0} \neq 0$
- Type II : $\Delta_{S=0,S=1} \neq 0$ et $\Delta_{S=0,S=0} = 0$ (kagomé)



“String potential”



“Deconfined” spinon

$\xi_{\text{conf}} > \xi_{\text{AF}}$

DCP scenario, two emerging lenghts

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

Undopped Frustrated antiferromagnets

- Exotic disordered states,
- Emergence of short range valence bond states,

Doping frustrated AF

- Mechanism for holon-spinon confinement/deconfinement,
- Monitoring of quantum phase transitions,

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Rest of the talk

- Use of short range valence bond states,
- Two examples of doped/undoped frustrated AF with static hole(s) :
  1. $J_1 - J_2 - J_3$ model on the square lattice (VBC),
  2. Kagomé antiferromagnet (SL).

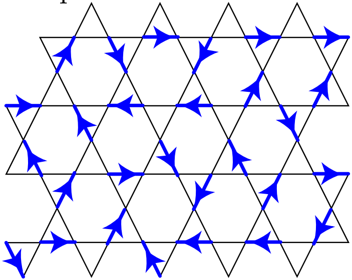
2d Frustrated Antiferromagnets

- no approximation
- everything can be computed

$\rightsquigarrow$ Exact Diagonalizations

- small systems
- finite size effects

Low energy singlets
RVB phases



$\rightsquigarrow$ RVB method

$\mathcal{N}_{\text{coverings}} \sim k\alpha^N$
$\alpha \simeq 1.26$ (kagome)
$\alpha \simeq 1.34$ (square)
$\alpha \simeq 1.53$ (triangular)
$\mathcal{N}_{S=0} \sim N^{-3/2} 2^N$

Significant reduction of the Hilbert Space Size

RVB state are non-orthogonal

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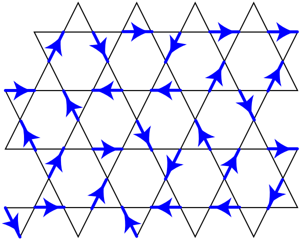
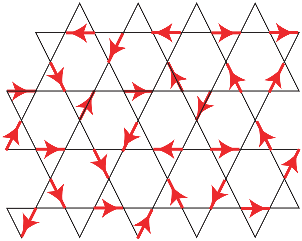
$\langle\varphi|$



RVB state are non-orthogonal

$\langle \varphi | \psi \rangle$



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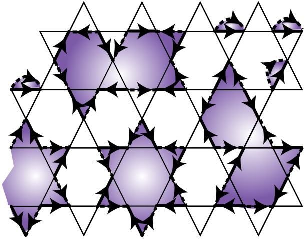
$$\langle\varphi|\psi\rangle = \qquad 2^{n_l(\mathcal{G})-N/2}$$



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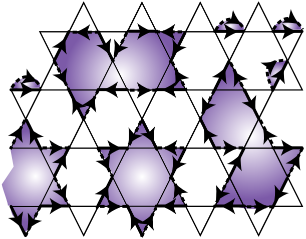

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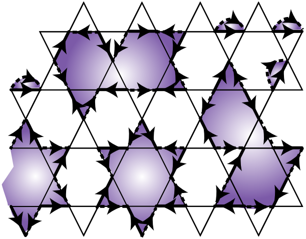
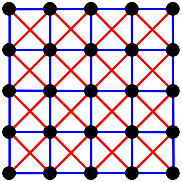
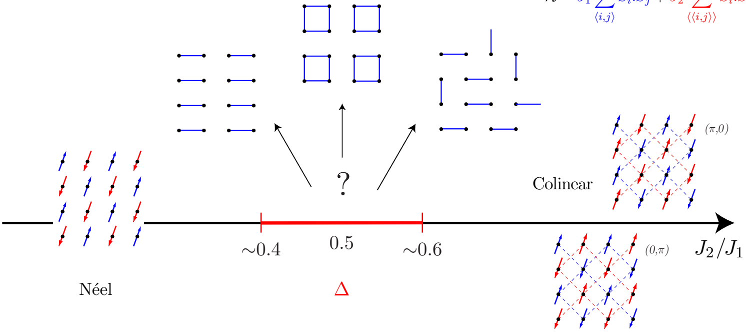


- Generalized eigenvalue problem, $\det(\mathcal{H} - E\mathcal{O}) = 0$
- $\mathcal{O}_{\varphi,\psi} = \langle\varphi|\psi\rangle$ and $\mathcal{H}_{\varphi,\psi} = \langle\varphi|\mathcal{H}|\psi\rangle$
- Non sparse matrices, No iterative methods (e.g. Lanczos)



$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i.\vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i.\vec{S}_j$$



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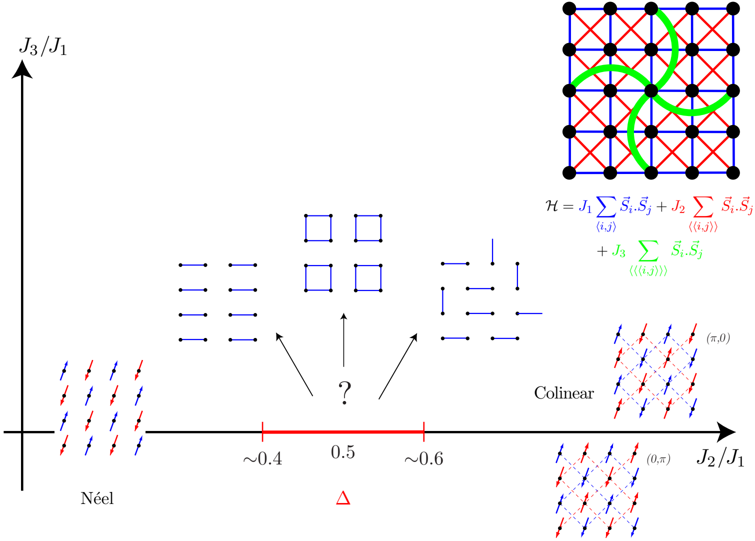

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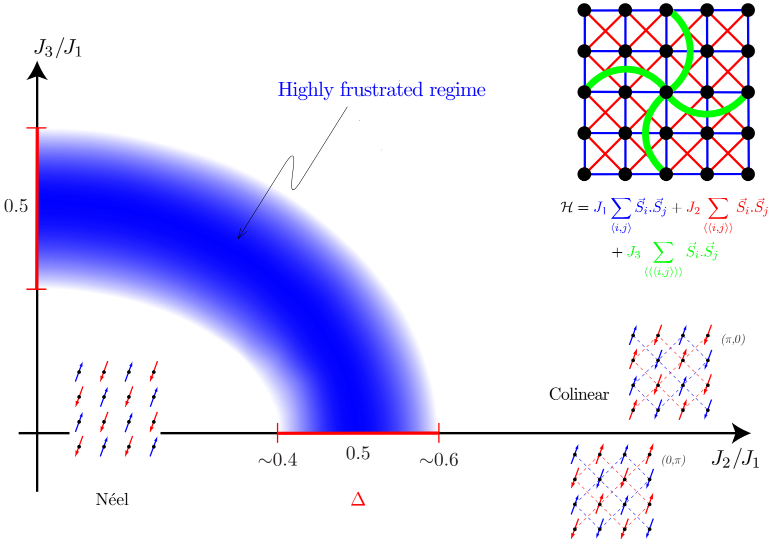

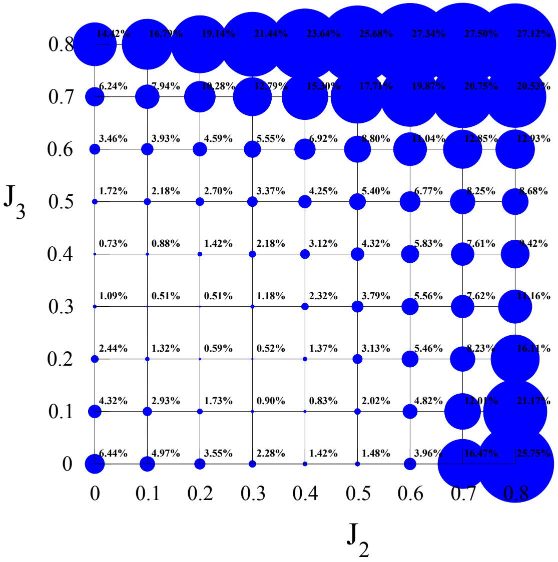

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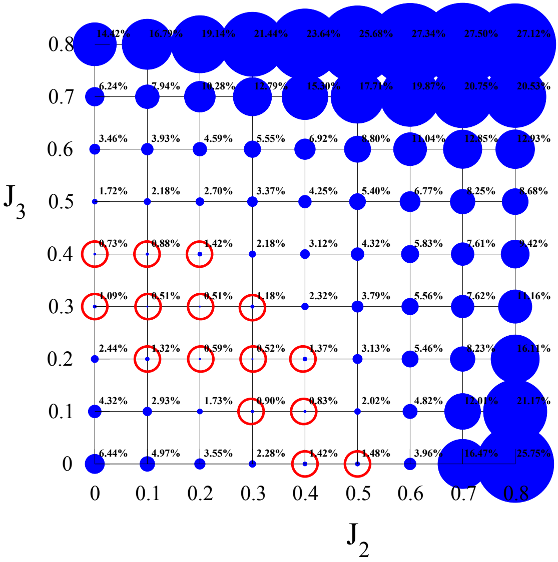
$$(E_0^{\rm RVB} - E_0)/E_0$$



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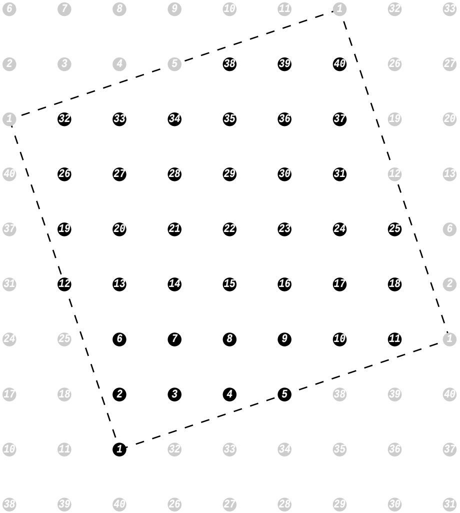
Only 182 states / $\sim 10^6$



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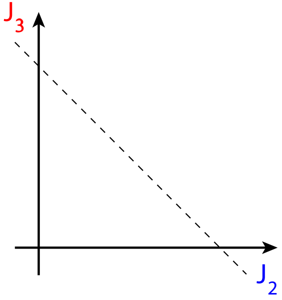

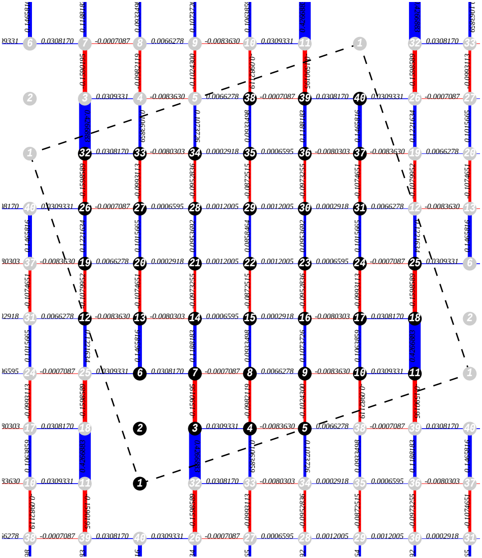

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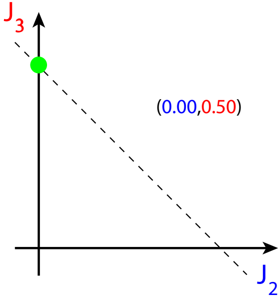

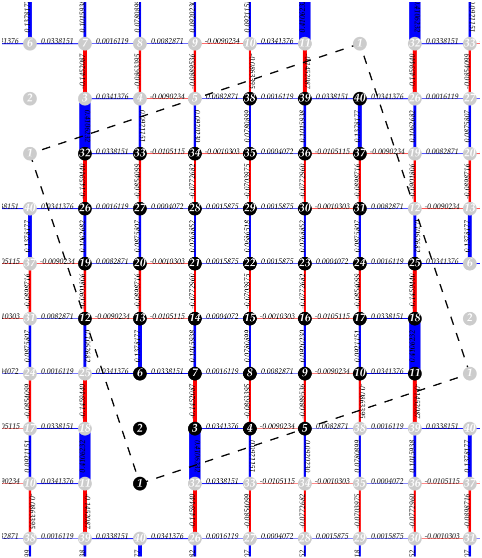

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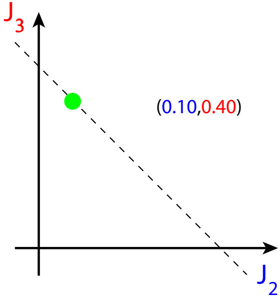

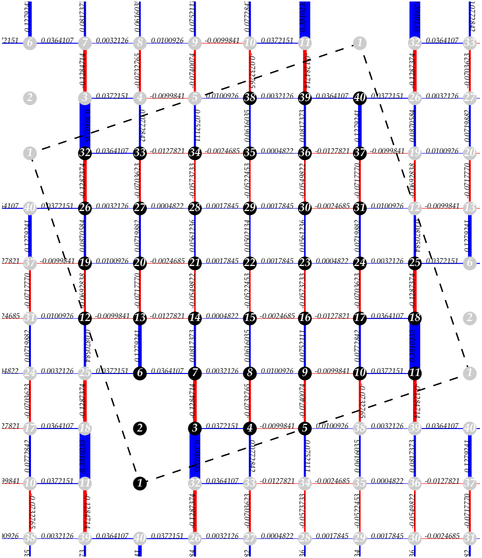

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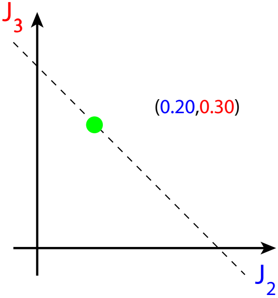

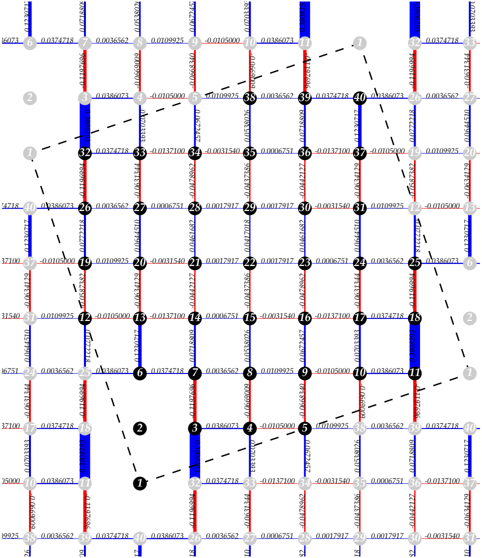

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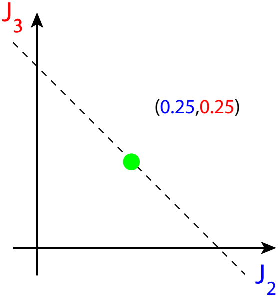

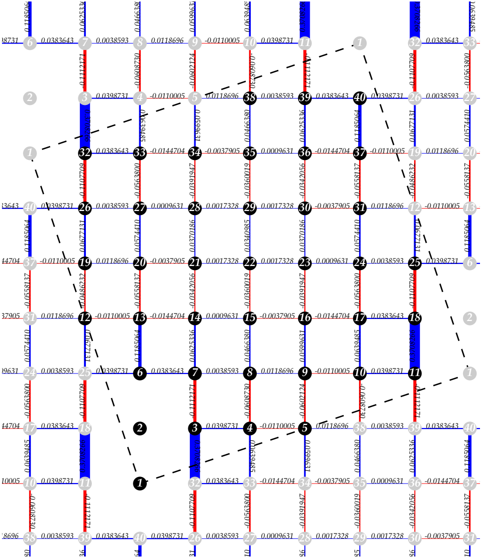

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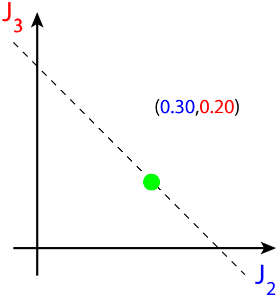

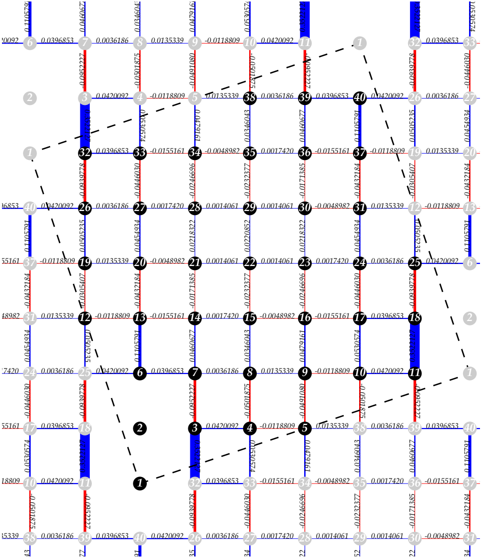

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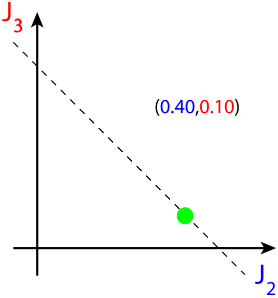

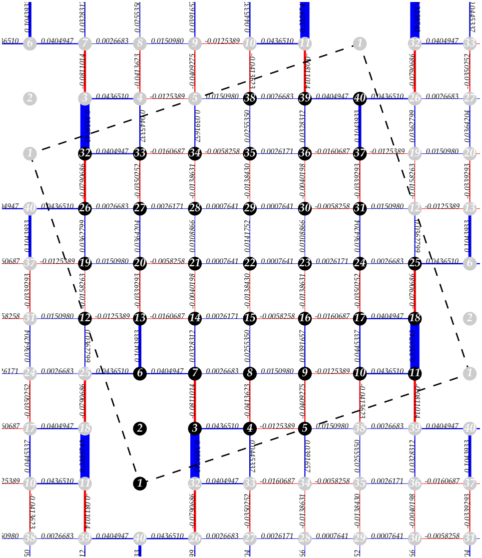

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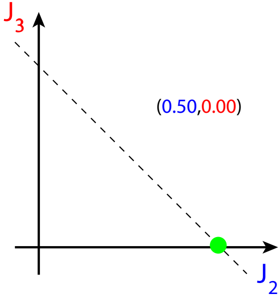

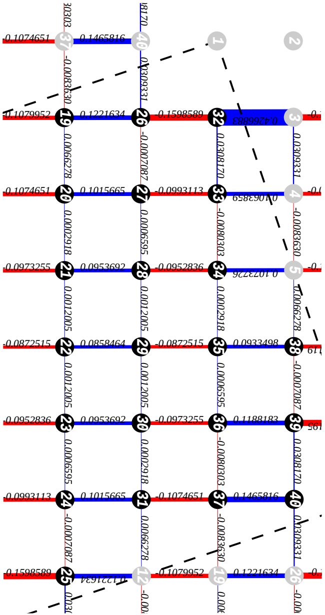

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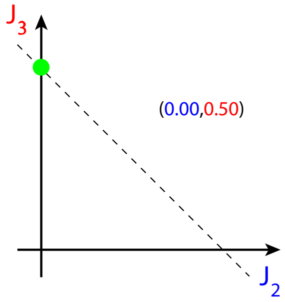

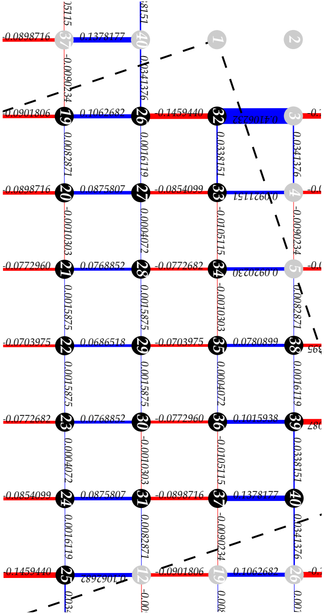

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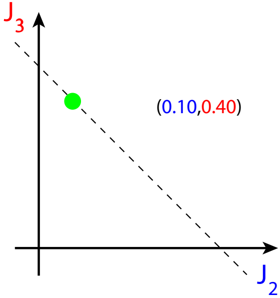

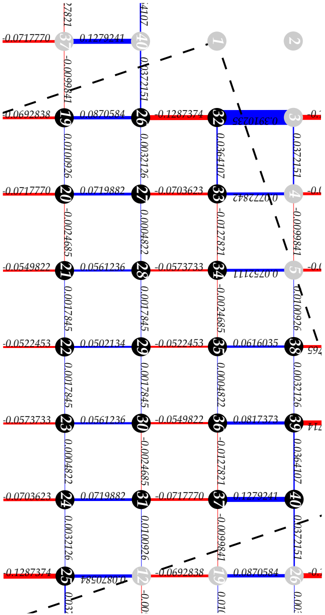

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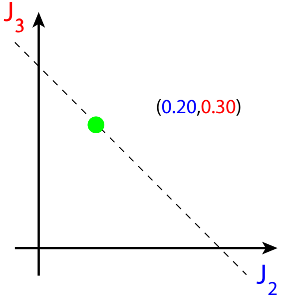

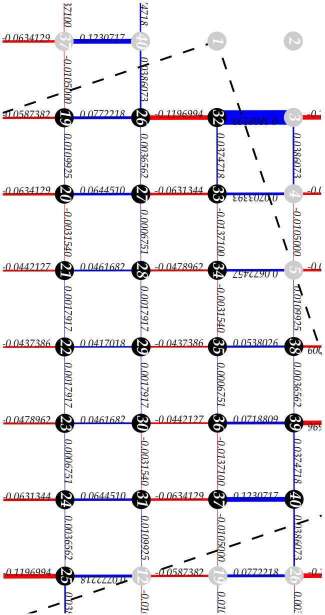

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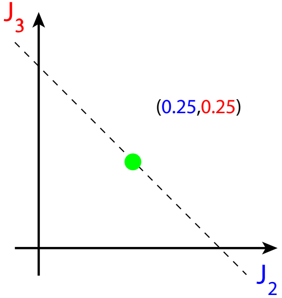

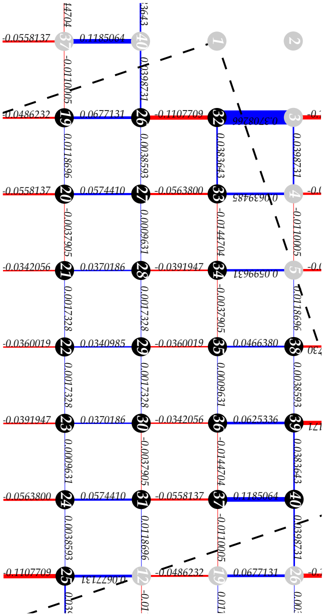

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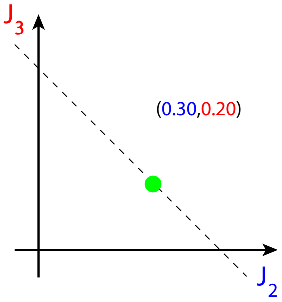
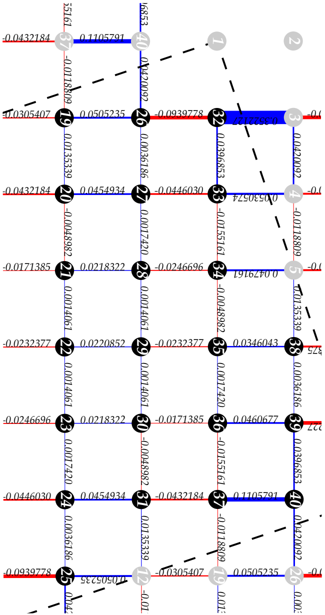
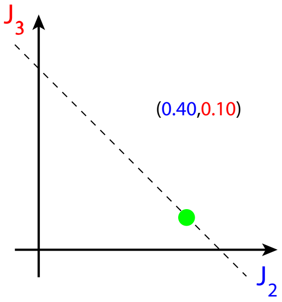
$$\langle(\vec{S}_1.\vec{S}_2)(\vec{S}_i.\vec{S}_j)\rangle - \langle\vec{S}_1.\vec{S}_2\rangle^2$$

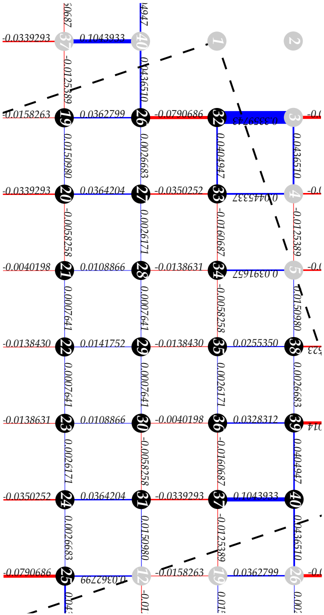




$$N = 40$$

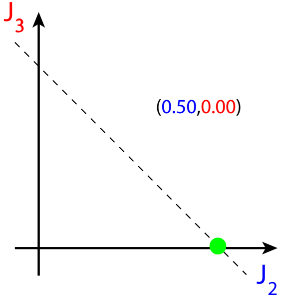
$$\langle(\vec{S}_1.\vec{S}_2)(\vec{S}_i.\vec{S}_j)\rangle - \langle\vec{S}_1.\vec{S}_2\rangle^2$$

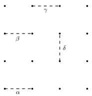


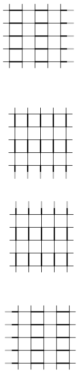


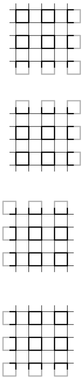
$$N = 40$$

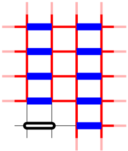
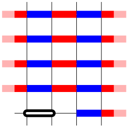
$$\langle(\vec{S}_1.\vec{S}_2)(\vec{S}_i.\vec{S}_j)\rangle - \langle\vec{S}_1.\vec{S}_2\rangle^2$$

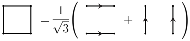






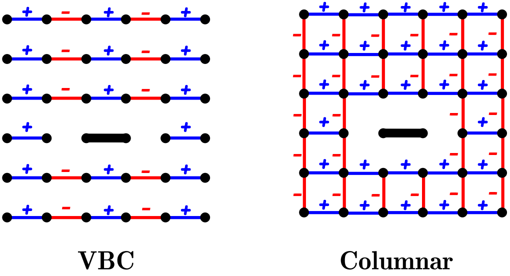


	Columnar state	**Plaquette state**
$\langle(\mathbf{S}.\mathbf{S})_\alpha(\mathbf{S}.\mathbf{S})_\beta\rangle - \langle(\mathbf{S}.\mathbf{S})_\alpha\rangle^2$ Normalized (α,β)	27/256 **1**	1/16 **1**
$\langle(\mathbf{S}.\mathbf{S})_\alpha(\mathbf{S}.\mathbf{S})_\gamma\rangle - \langle(\mathbf{S}.\mathbf{S})_\alpha\rangle^2$ Normalized (α,γ)	-9/256 **-1/3**	-1/16 **-1**
$\langle(\mathbf{S}.\mathbf{S})_\alpha(\mathbf{S}.\mathbf{S})_\delta\rangle - \langle(\mathbf{S}.\mathbf{S})_\alpha\rangle^2$ Normalized (α,δ)	-9/256 **-1/3**	0 **0**
Correlations snapshot		



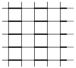
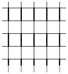
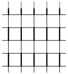
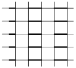
Suceptibilities

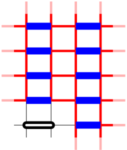
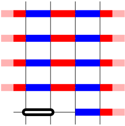
$$\frac{\chi}{N} = \frac{1}{N}\sum_{(i,j)} \epsilon_{i,j}(\langle(\vec{S}_1.\vec{S}_2)(\vec{S}_i.\vec{S}_j)\rangle - \langle\vec{S}_1.\vec{S}_2\rangle^2)$$



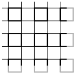
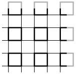
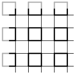
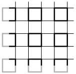
χ_{VBC} diverges in both columnar and plaquette phases

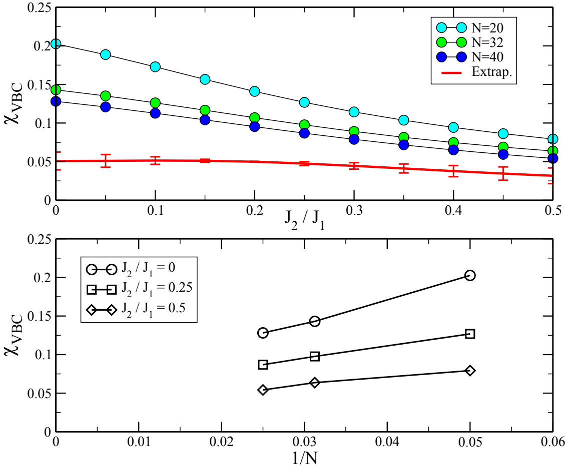
χ_{Col} only diverges in the columnar phase

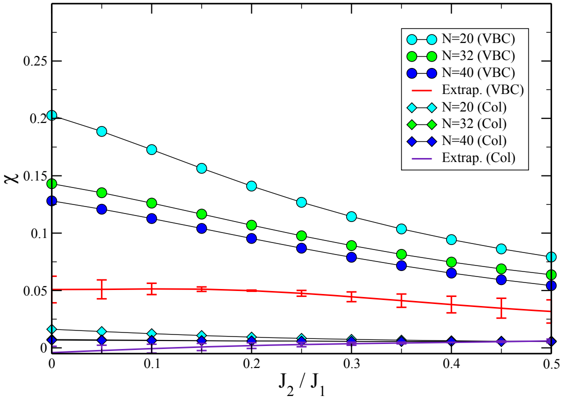





	Columnar state	Plaquette state
$\langle(\mathbf{S.S})_\alpha(\mathbf{S.S})_\beta\rangle - \langle(\mathbf{S.S})_\alpha\rangle^2$ Normalized (α,β)	27/256 **1**	1/16 **1**
$\langle(\mathbf{S.S})_\alpha(\mathbf{S.S})_\gamma\rangle - \langle(\mathbf{S.S})_\alpha\rangle^2$ Normalized (α,γ)	-9/256 **-1/3**	-1/16 **-1**
$\langle(\mathbf{S.S})_\alpha(\mathbf{S.S})_\delta\rangle - \langle(\mathbf{S.S})_\alpha\rangle^2$ Normalized (α,δ)	-9/256 **-1/3**	0 **0**
Correlations snapshot		

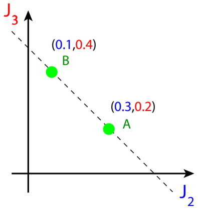
$\chi_{\mathrm{VBC}}/\mathrm{bond}$	**9/128~0.070**	**1/16~0.063**
$\chi_{\mathrm{Col}}/\mathrm{bond}$	**9/256~0.035**	**0**

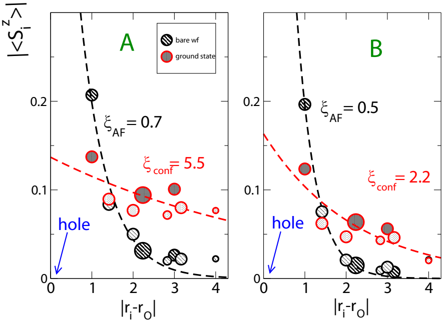






N=20
N=32
N=40
Extrap.
χ_{VBC}
J_2 / J_1
0
0.05
0.1
0.15
0.2
0.25
0.3
0.4
0.5
$J_2 / J_1 = 0$
$J_2 / J_1 = 0.25$
$J_2 / J_1 = 0.5$
χ_{VBC}
1/N
0.01
0.02
0.03
0.04
0.05
0.06


N=20 (VBC)
N=32 (VBC)
N=40 (VBC)
Extrap. (VBC)
N=20 (Col)
N=32 (Col)
N=40 (Col)
Extrap. (Col)
χ
0.25
0.2
0.15
0.1
0.05
0
0
0.1
0.2
0.3
0.4
0.5
J2 / J1

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



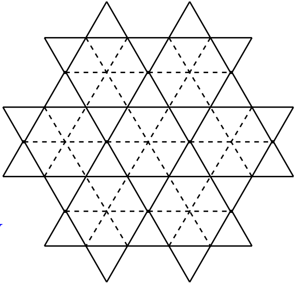


$\xi_{\rm conf} \gg \xi_{\rm AF}$

D.Poilblanc, A.Laeuchli, M.M & F. Mila, PRB (2006) *kagomé*

$z = 4$

Macroscopic degeneracy



Triangular

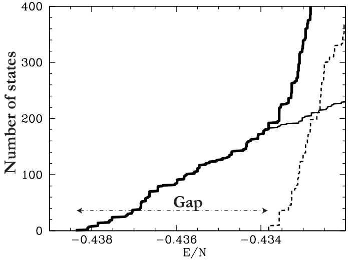
$z = 6$

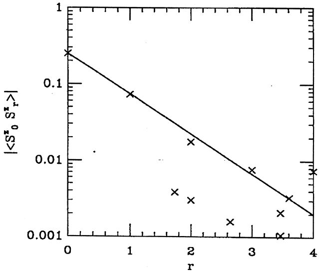
Ground state determined up to global rotations

$$\vec{S}_1.\vec{S}_2 + \vec{S}_2.\vec{S}_3 + \vec{S}_3.\vec{S}_1 = (1/2)\{(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 - \vec{S}_1^2 - \vec{S}_2^2 - \vec{S}_3^2\}$$

$$\mathcal{E} = J \sum_{\langle i,j \rangle} \vec{S}_i.\vec{S}_j \propto \sum_t (\vec{S}_t)^2$$

Ground state : $\vec{S}_t = \vec{0} \quad \forall t$





Spectrum structure

C. Waldtmann et al., Eur. Phys. J. B **2**, 501, (1998).

$\rightsquigarrow$ *Exponential number of low lying signglets*

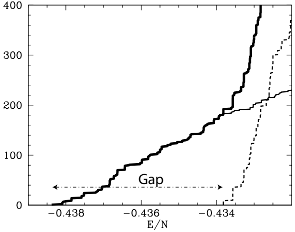
$$\mathcal{N}_{singlets} \sim 1,15^N$$

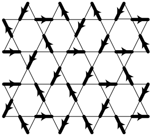
Spin-Spin correlations

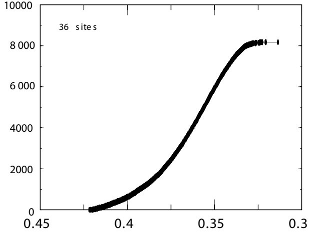
P. Leung and V. Elser, Phys. Rev. B **47**, 5459, (1993).

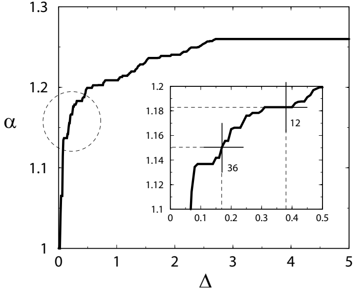
$\rightsquigarrow$ *No long range order*

$$|\vec{S}_0.\vec{S}_r| \sim \exp(-r/\xi)$$

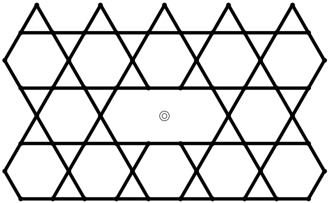


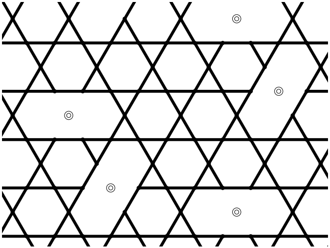






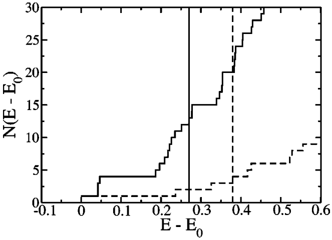
$$\mathcal{N}_N(\Delta) = A(\Delta)\alpha(\Delta)^N$$

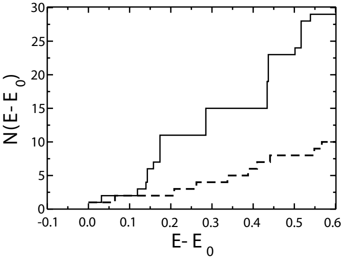




Techniques :

- **ED**
  27 sites with 1 hole
  24 sites with 2 holes
- **SRRVB**
  39 sites with 1 hole
  36 sites with 2 holes

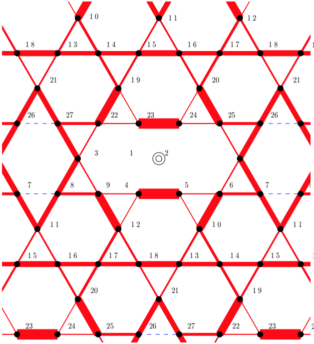


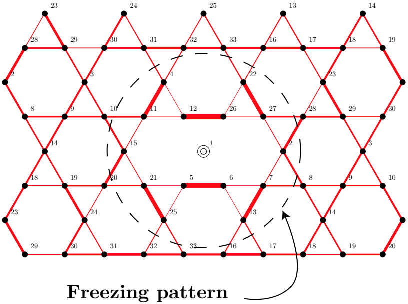


No free spin degrees of freedom localised around impurities

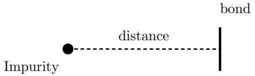
Dimer ordering ?

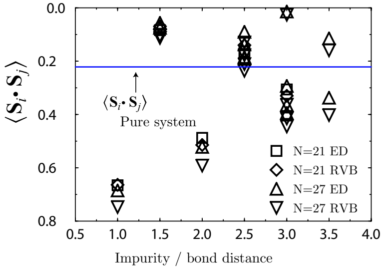
Dimer freezing

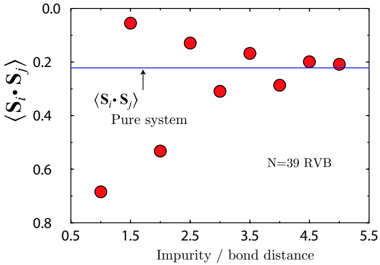




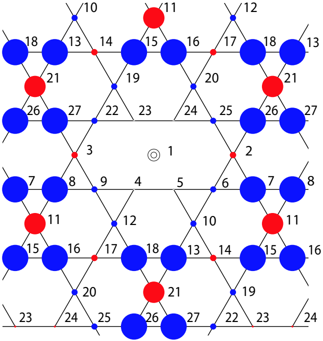
Hole-dimer correlations

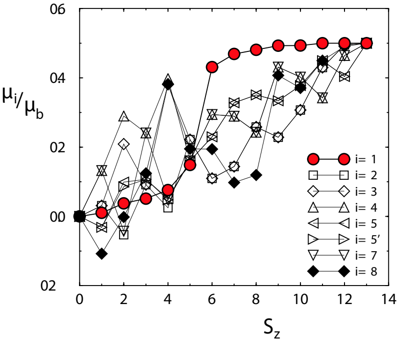






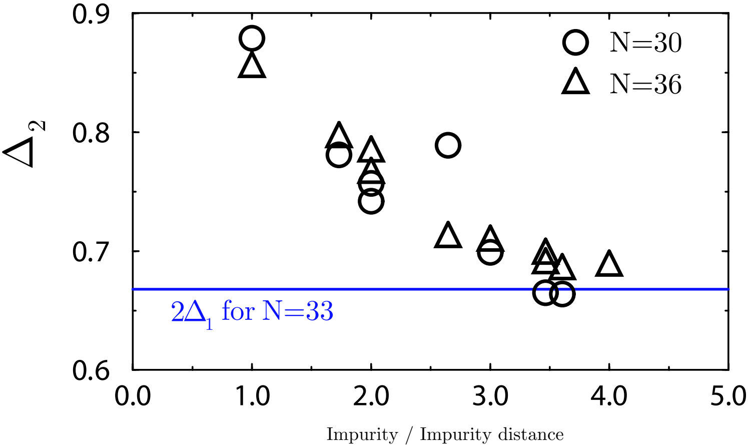
Magnetization profile around impurities



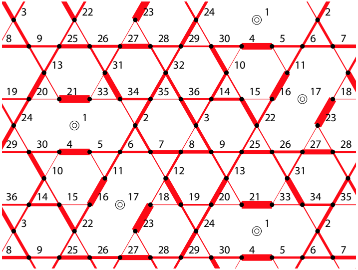


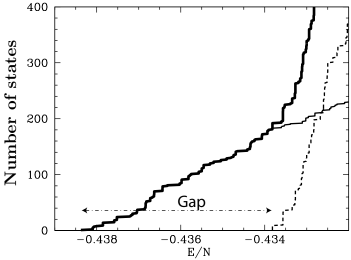
Deconfinement of magnetization away from the impurity

Effective interaction between impurities



Large distance interaction





Conclusion

- Emergence of SRRVB states in higlhy frustrated insulators,
- Natural framework to compute on these systems,
- Exotic phases : VBC to spin liquid,
- Non trivial properties when doped.

S. Capponi	A. Läuchli	B. Normand
S. Dommange	Cl. Lhuillier	K. Penc
P. Fazekas	F. Mila	D. Poilblanc
J.B. Fouet	G. Misguich	P. Sindzingre