Simulations
of
Quantum Dimer Models

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A wide range of applications

- Disordered frustrated quantum magnets
- Correlated fermions on frustrated lattices (Mott)
- XXZ (frustrated) magnets under magnetic field
- Ultra-cold atom systems
- Josephson junction arrays
- Spin orbital models
- Quantum computing

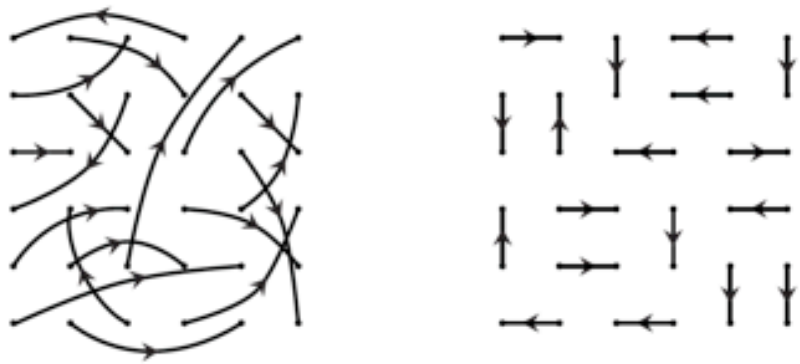
OUTLINE

- Quantum dimer models for frustrated magnets
  - From short-range valence-bond basis to “dimer” basis ...
  - Rokhsar-Kivelson expansion
  - Green function’s QMC for QDM’s: a new phase

- Doped quantum dimer models
  - Spinon doping: still a (non-frustrated) “bosonic” problem
  - Holon doping: minus sign problem !

SU(2)-dimer basis

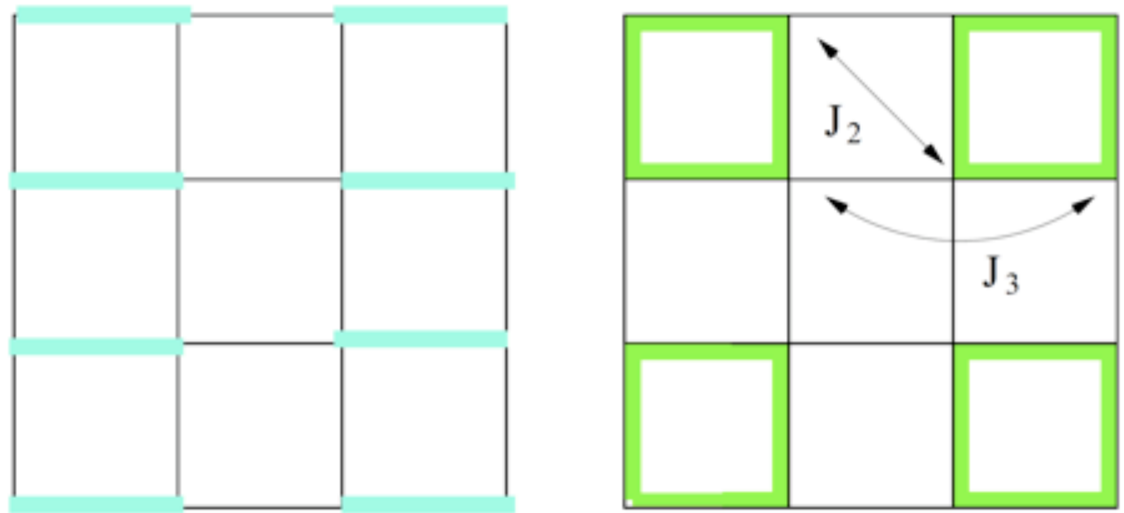
Long Range Valence Bond basis vs Short Range VB basis



(a) (b)

- Singlet subspace spanned by LR VB basis
- SR VB $\rightarrow$ small fraction of full S=0 subspace: $\propto 1.3^N$
- NN Valence bond basis relevant for Quantum Disordered phases

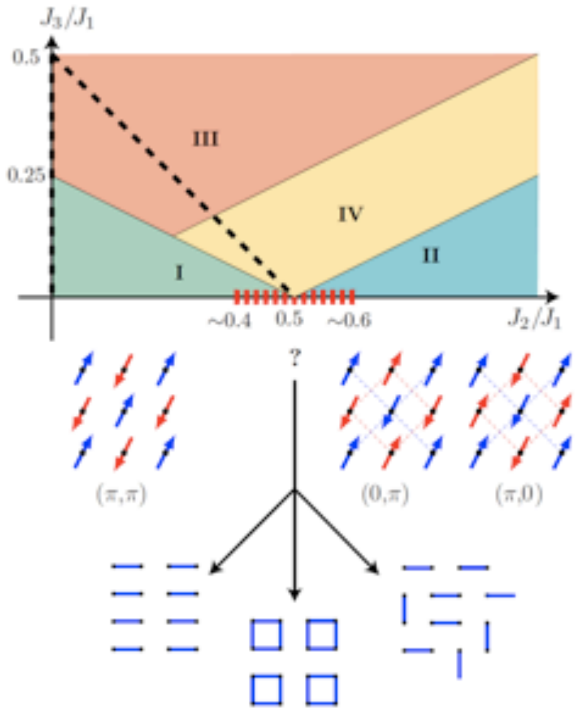
VBC candidates for the AF square lattice



(a) (b)

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

J_1-J_2-J_3 AF Heisenberg model



- Classical phase diagram (Chubukov et al., PRB 90)
  $\rightarrow$ collinear vs spiral
- Quantum case:
  AF $\rightarrow$ VBC transition ?
  deconfined critical point (Senthil et al.) ?

Quantum disordered phases between magnetic phases

SL vs VBC order ?

How to deal with overlaps ?

SU(2) Valence Bond ⇔ dimer covering

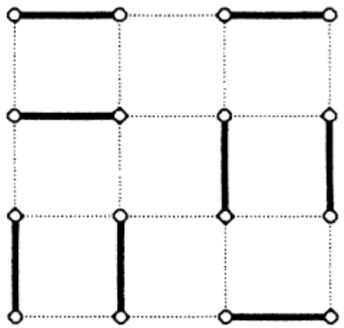
Orthogonal basis by construction

- Sutherland, 1988:

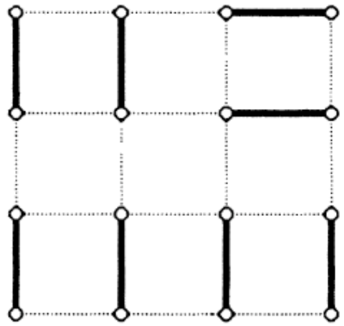
$$|\langle a|b\rangle| = \prod_{\mathcal{L}} 2^{(1-L_{\mathcal{L}}/2)}$$

Length of the loops of overlap graph

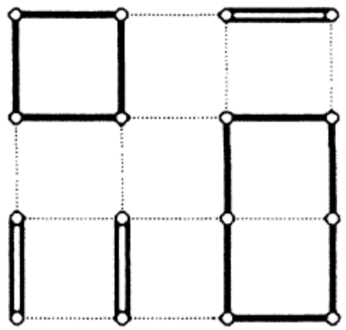
"Loop formula" also for matrix elements
of S=1/2 Heisenberg hamiltonian



(a)

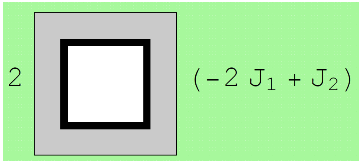


(b)



Systematic "loop" expansion

Mambrini, Ralko et al.
(unpublished)



Order 2

....

Order 4

Order 6 & 8 !!

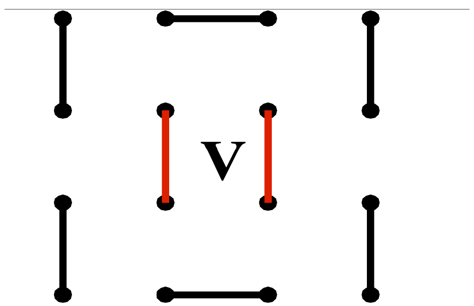
....

Effective model

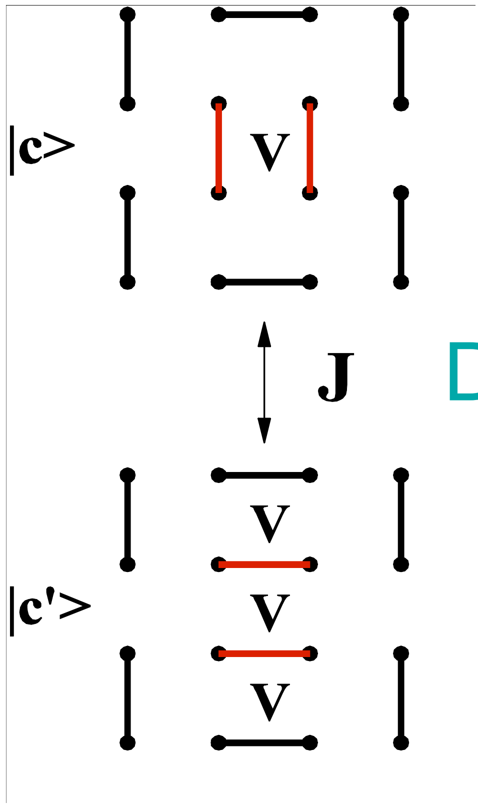
Keep only plaquette terms ⇨ *Quantum Dimer Model*

Rokhsar & Kivelson, PRL 88

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



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

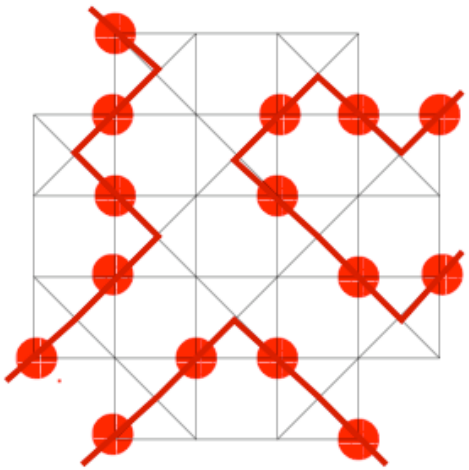


Dimer flip

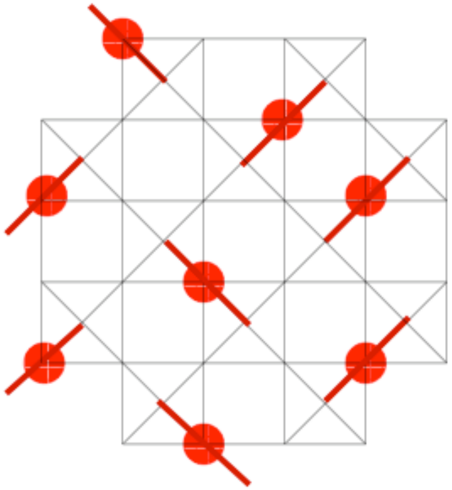
$$H_{\text{QDM}} = \sum_c e_c |c\rangle\langle c| - J \sum_{c,c'} |c\rangle\langle c'|$$

QDM can also describe (hardcore) fermions/bosons on frustrated lattices at **fractional filling**

n=1/2



n=1/4



U=∞ and V >> t
extended-Hubbard model

insulator !

"Ice rule" constraint:
Exactly 2 or 1 particles/tetraedra

Quantum Loop or Quantum Dimer model

Pollman, Fulde et al.

DP, K. Penc & N. Shannon, PRB 75, 220503® (2007)
DP, PRB 76, 115104 (2007)
F. Trousselet, DP & R. Moessner, ArXiv 2008.

Belong to the class of **constrained models**

Hilbert space cannot be written
as tensor product of HS of sub-systems !

Emerging global conservation laws

⇒ Interesting **topological** properties

Rokhsar-Kivelson point

For J=V: sum of projectors

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

$$|\Psi_{c,c'}\rangle = \frac{1}{\sqrt{2}}(|c\rangle - |c'\rangle)$$

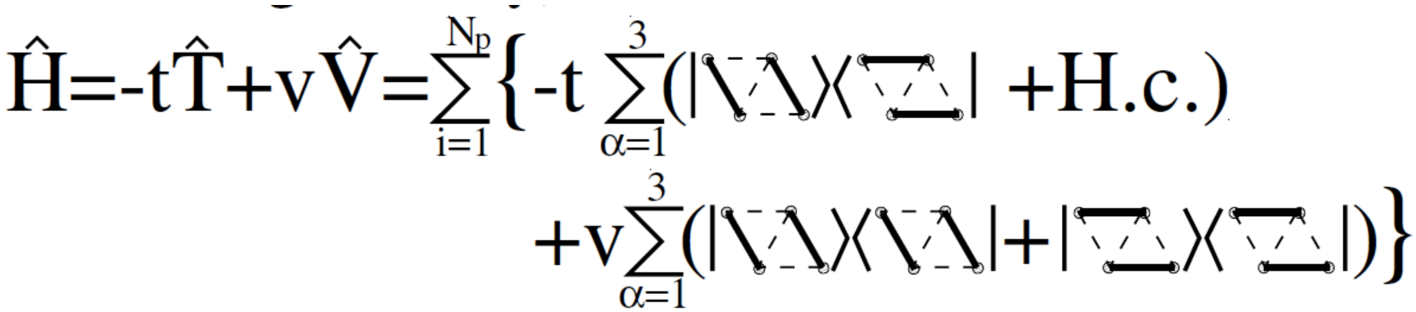
$$|\Phi_0\rangle = \frac{1}{Z}\sum_{\{c\}} |c\rangle$$

exact GS with energy E=0

$\Longleftrightarrow$ Infinite-T Classical DM

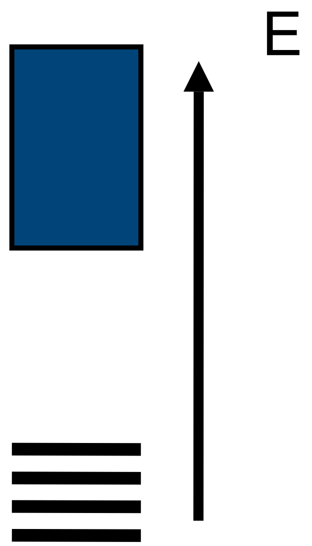
Short-range RVB liquid on the triangular lattice

Moessner & Sondhi, PRL 2001

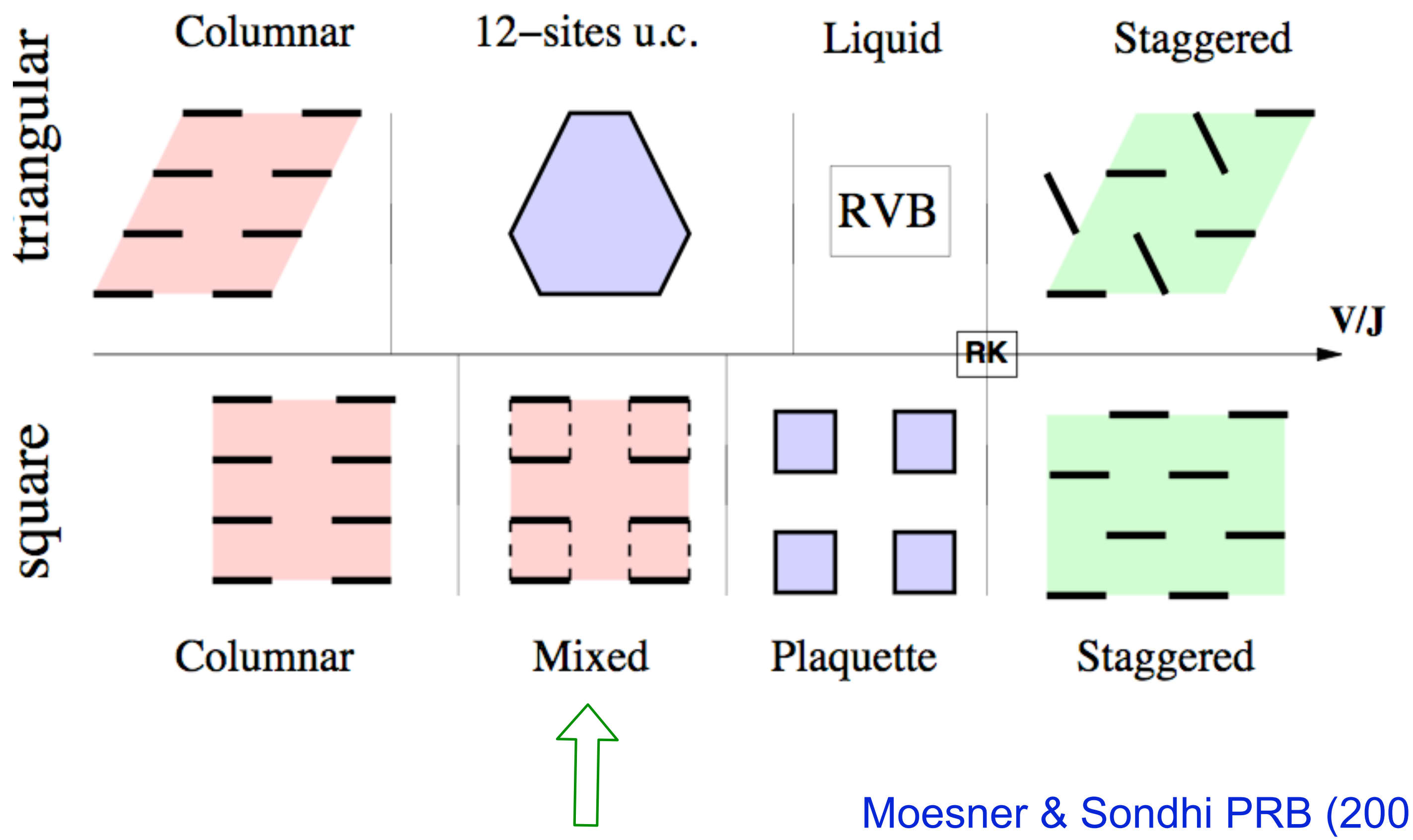


Finite correlation length
Exponential decay
of dimer-dimer correlations

Degeneracy from "topological order"
GS have different "winding numbers" {



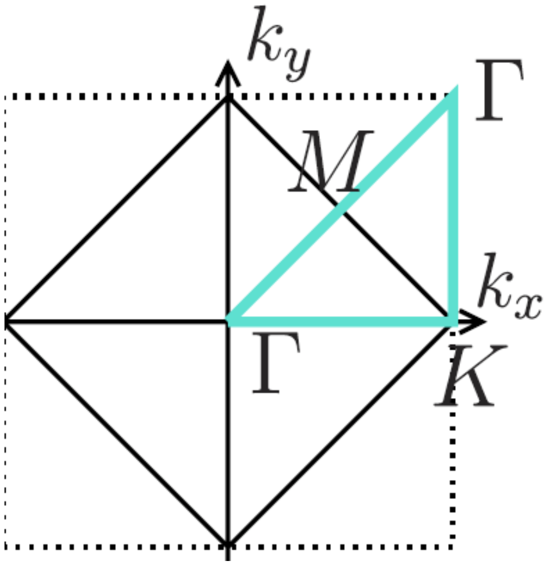
Rich phase diagrams at zero doping: “valence bond crystals” and RVB phases



Ralko, Poilblanc & Moesner, PRL (2008)

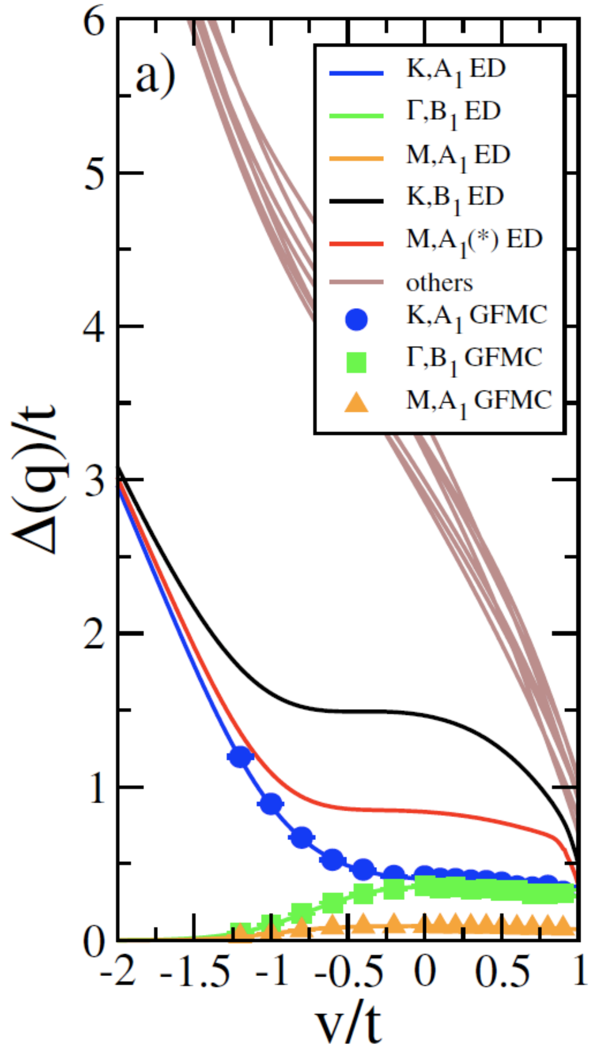
Moesner & Sondhi PRB (2001)
Syljuasen, PRB (2006)

Symmetry analysis



Order	Γ, A_1	Γ, B_1	M, A_1	K, A_1	K, B_1	M, A_1 (*)
Columnar	√	√	√			
Plaquette	√		√	√		
Mixed	√	√	√	√	√	√

Lanczos exact diagonalizations 8x8



Green's function QMC (T=0)

$$G = \lambda - H$$

$$\lim_{n \to \infty} G^n |\psi_T\rangle = |\psi_0\rangle$$

Define series: $\langle x' | \phi_{n+1} \rangle = \sum_x \langle x' | G | x \rangle \langle x | \phi_n \rangle$

$G_{x',x} = p_{x',x} b_x$ used as probability for stochastic Markow process

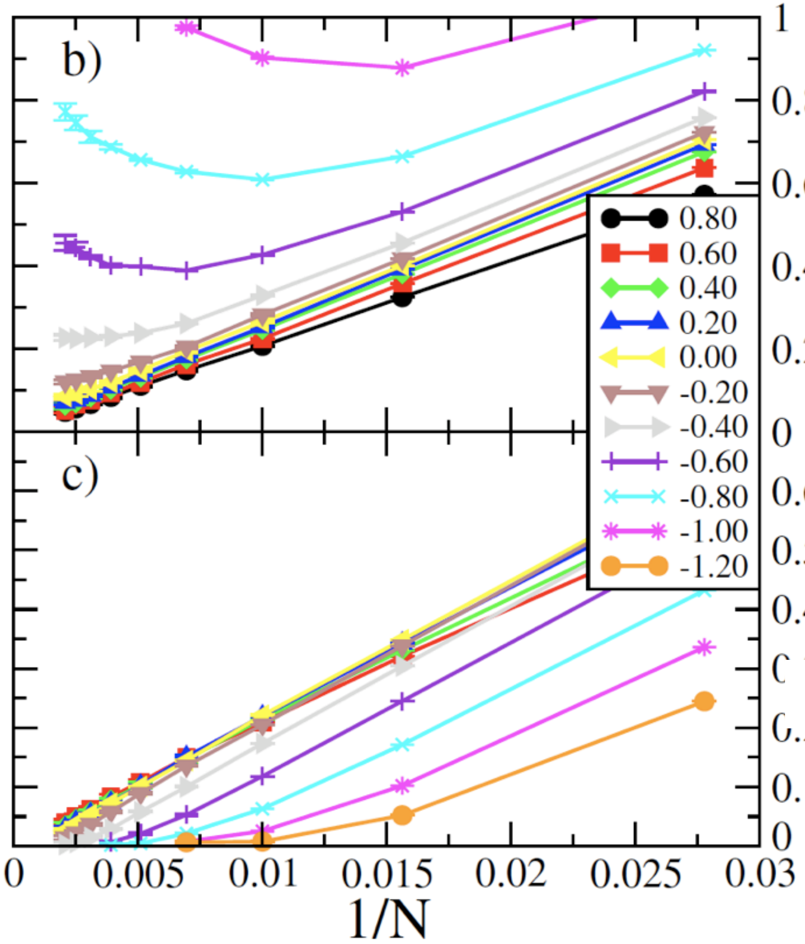
⇨ STATISTICAL SAMPLING

GFMC dynamical quantities

$$D(q,\tau) = \frac{\langle \Psi_G | P_\alpha(-q) e^{-H\tau} P_\alpha(q) | \Psi_0 \rangle}{\langle \Psi_G | e^{-H\tau} | \Psi_0 \rangle}$$

K,A_1

Γ,B_1



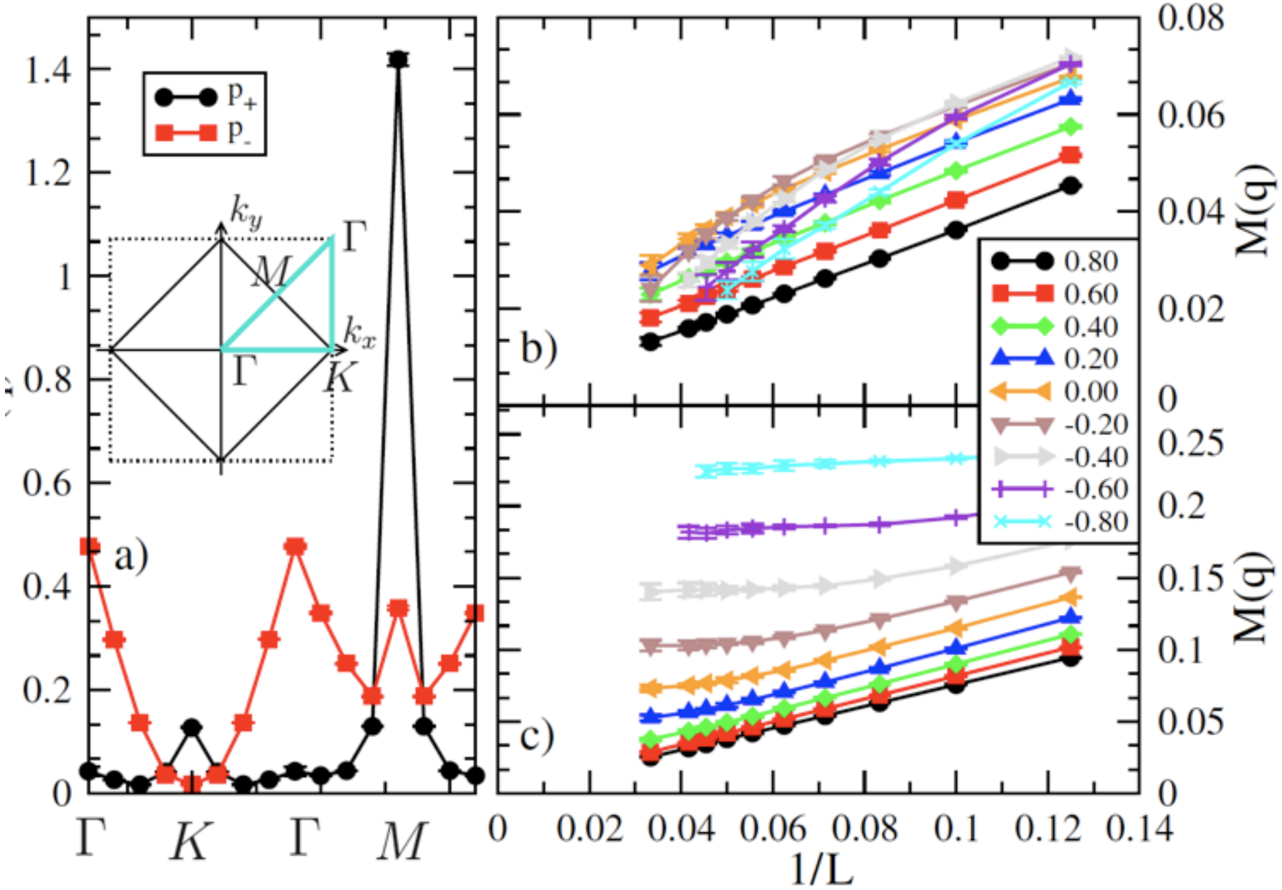
Up to 22 x 22 lattices

$$P_+ = d(i)d(j) + d(k)d(l)$$

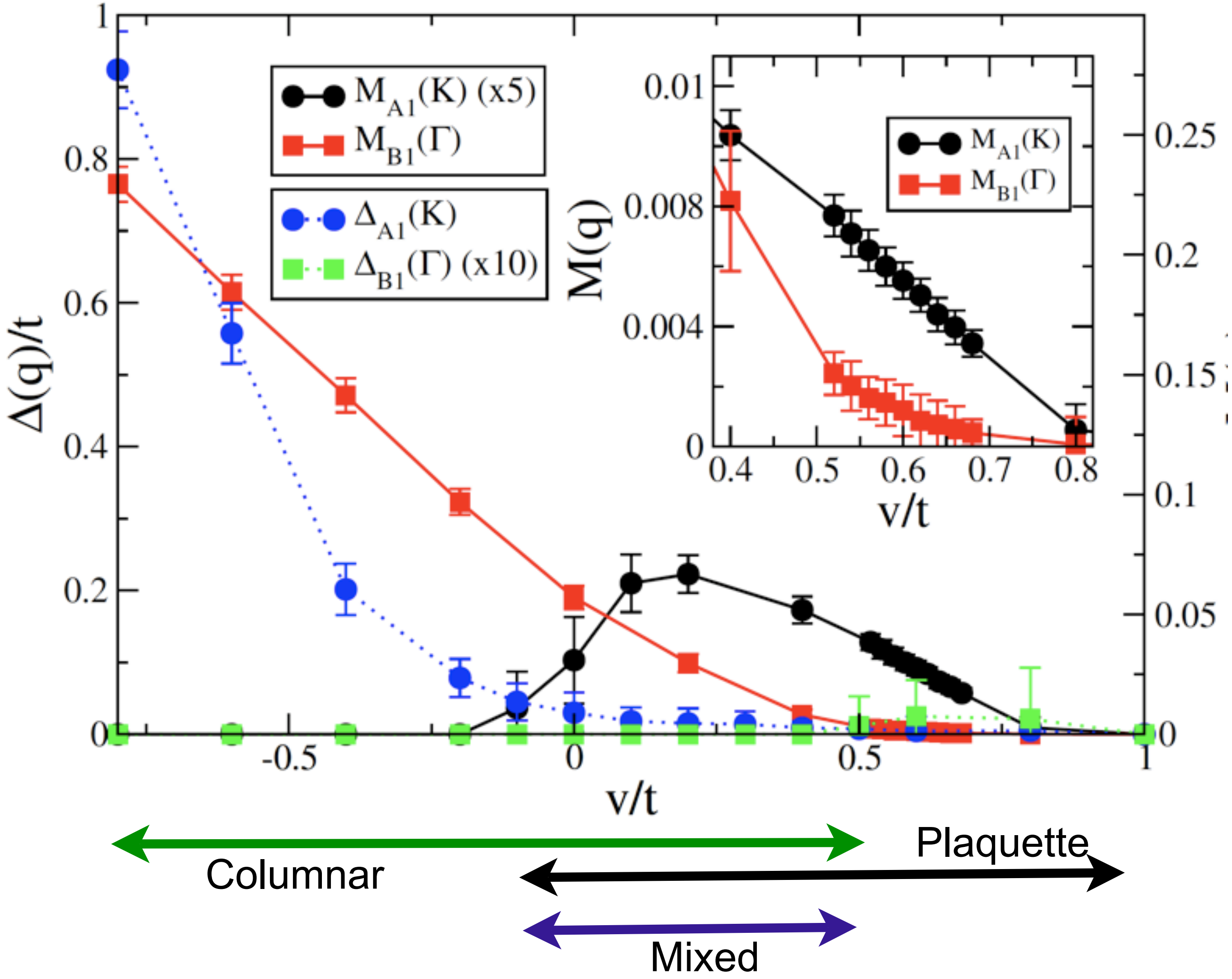
$$P_- = d(i)d(j) - d(k)d(l)$$

Structure factors

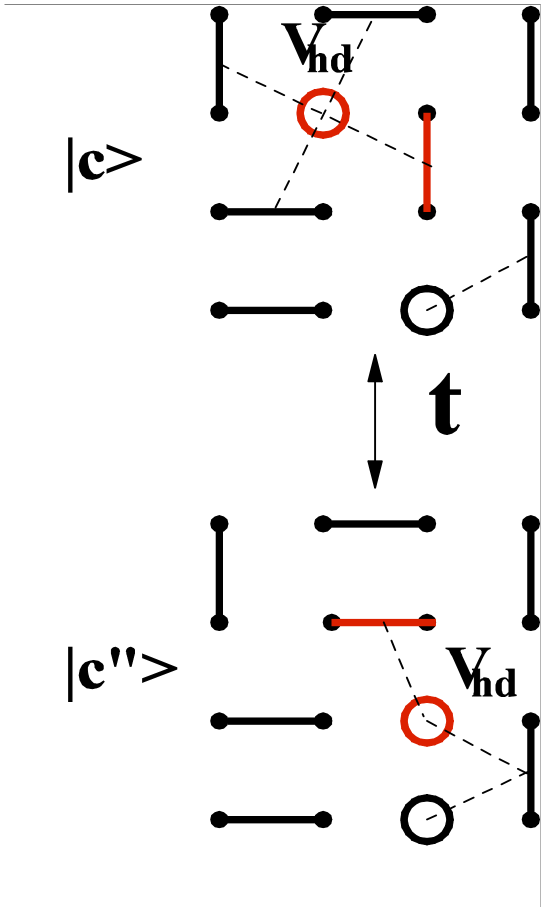
$$I(q) = \frac{\langle \Psi_0 | P_\alpha(-q) P_\alpha(q) | \psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \qquad M(q) = \sqrt{I(q)}/L$$



Phase diagram



Motion of “monomers”

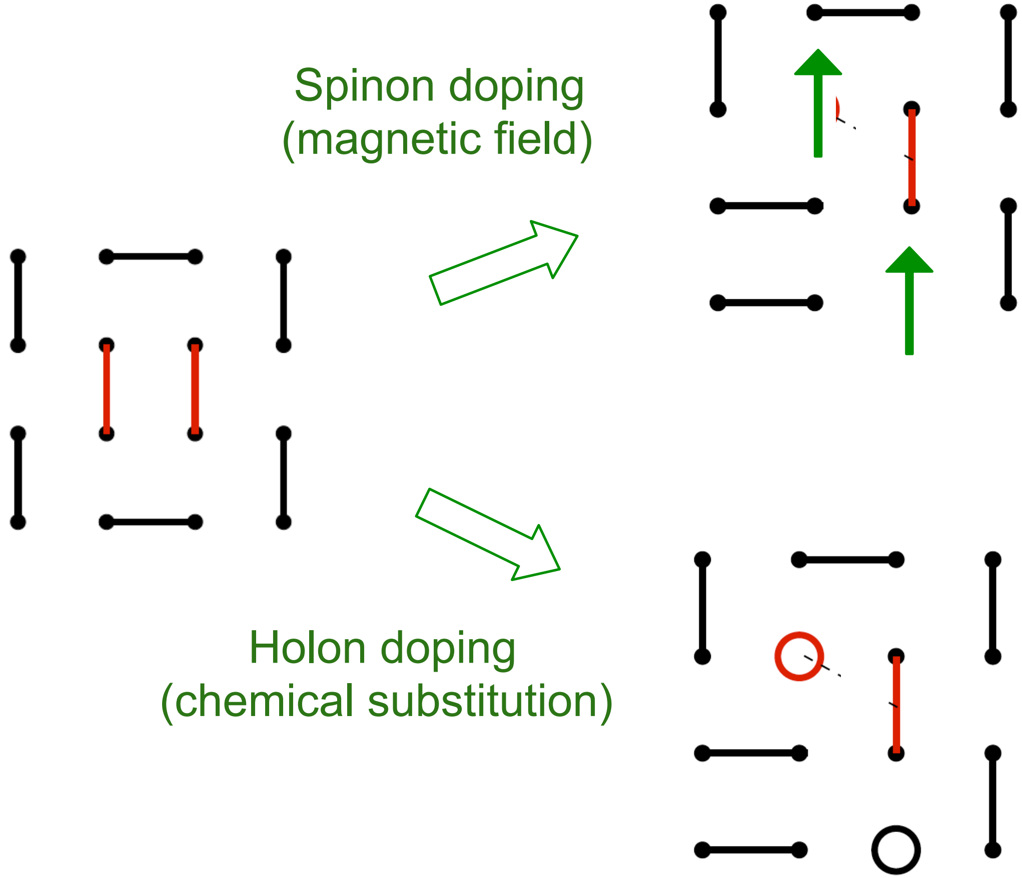


Inject monomers (by pairs) & add new term to H:

$$-t \sum_{c,c''} |c\rangle\langle c''|$$

« Monomer » doping

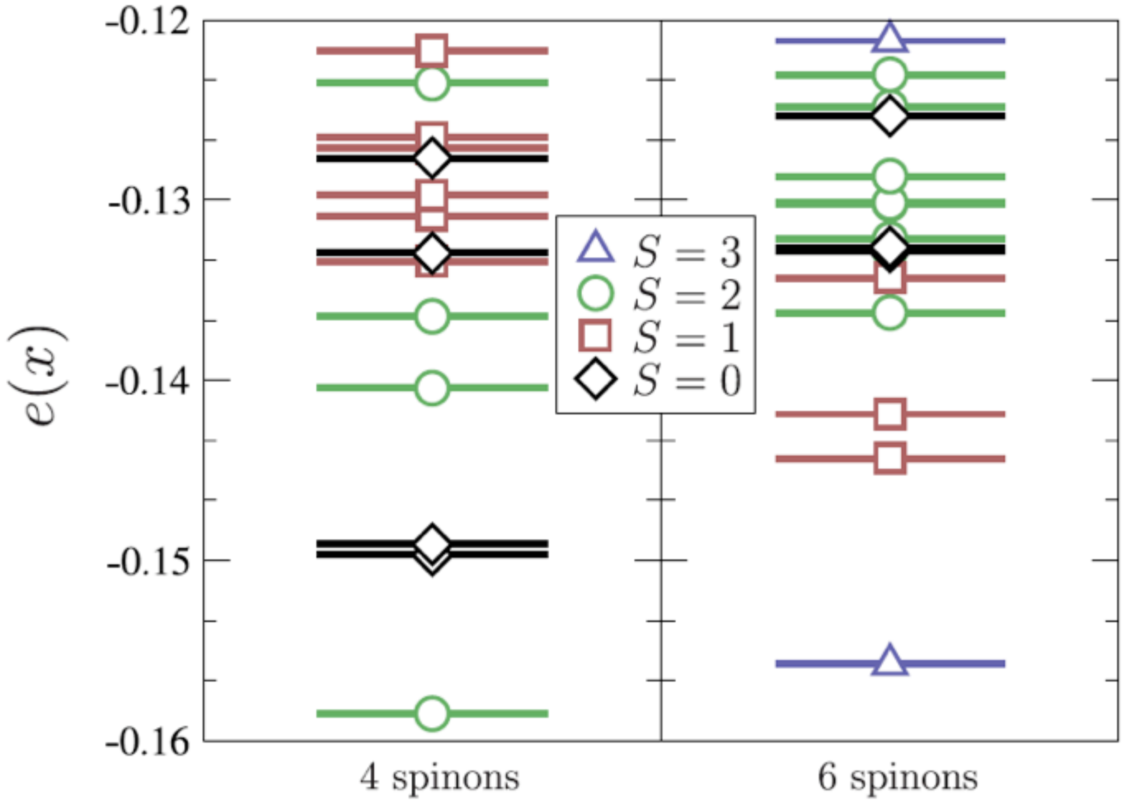
$$-g\mu_B H\sum_i S_i^z = -\frac{h}{2}N(n_\uparrow - n_\downarrow)$$



Ralko, Becca & DP, PRL (2008)

DP, PRL 100, 157206 (2007)

Spinons get fully polarized...



Spinon are polarized

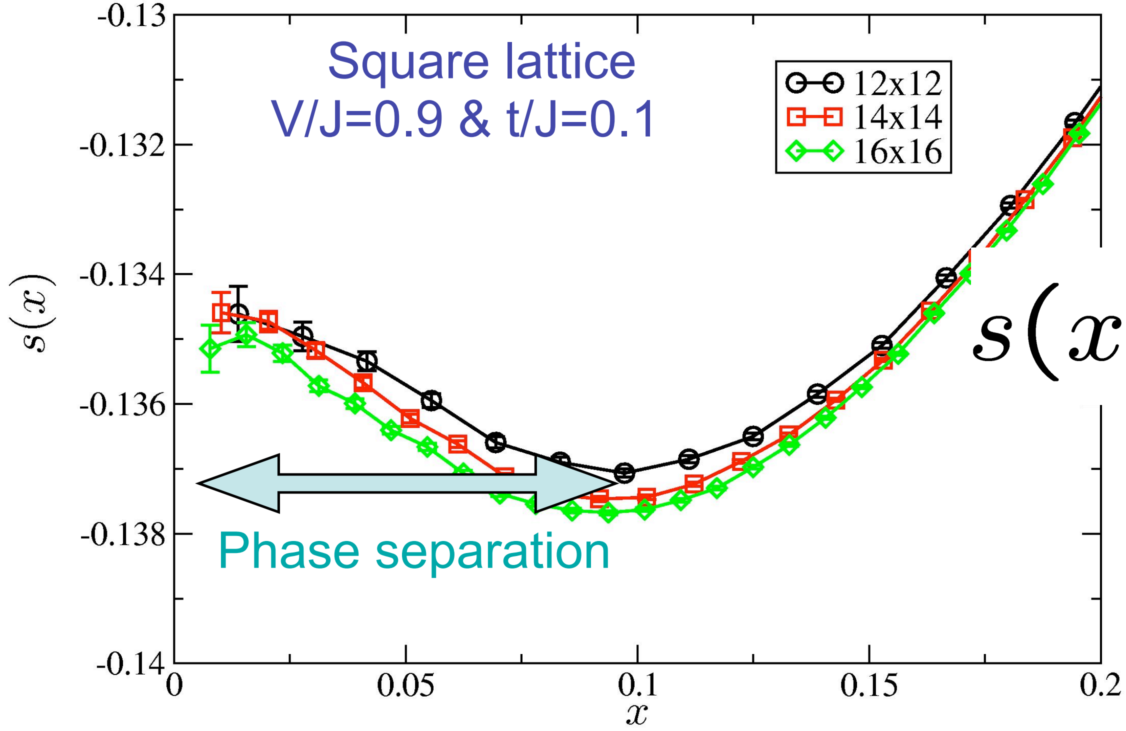
(« Nagaoka effect »)

Exact diagonalisations of small clusters

Maxwell construction for phase separation

(GFQMC)

J, t > 0 :
No “- sign problem”

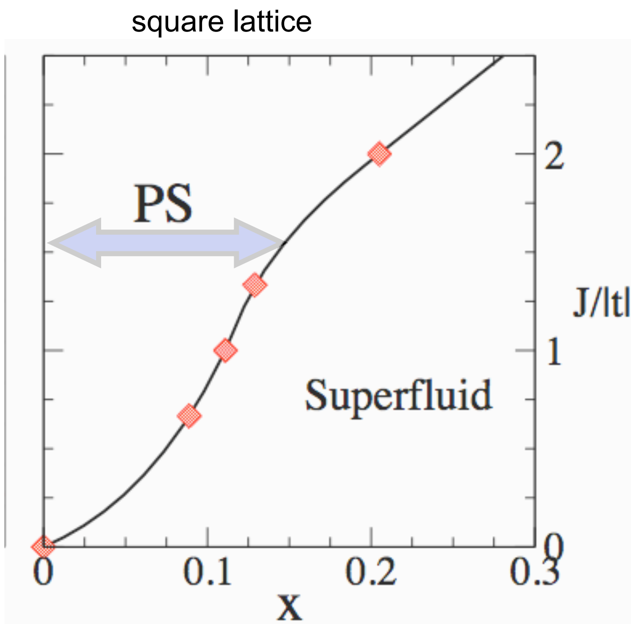


doping ratio

$$s(x) = \frac{e(x) - e(0)}{x}$$

A. Ralko et al., PRL (2007)

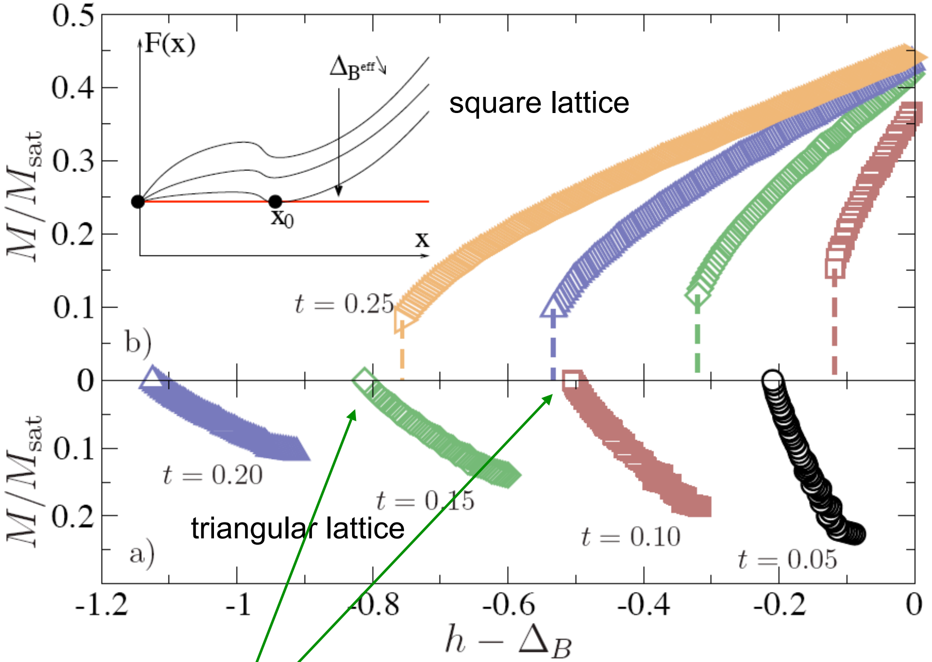
Phase diagram vs spinon doping / magnetic field



VBC insulator

J, t > 0 :
No “- sign problem”

GF Monte Carlo



boson condensation of spinons !

A. Ralko, F. Mila & DP, PRL (2007); A. Ralko, F. Becca, DP, PRL (2008)

Holon doping

⇒ The GS wavefunction acquires nodes !

A doped QDM with a minus sign problem

holon vs spinon doping ?

	monomers	definition of dimer operator	« bare » monomer statistics	Sign of J	« true » monomer statistics
Chemical doping	holons	$\frac{1}{\sqrt{2}}(f^\dagger_{i\uparrow}f^\dagger_{j\downarrow}+f^\dagger_{j\uparrow}f^\dagger_{i\downarrow})$	bosonic	J<0 non- - Frobenius	bosonic/ fermionic
Applied Magnetic field	spinons	$\frac{1}{\sqrt{2}}(b^\dagger_{i\uparrow}b^\dagger_{j\downarrow}-b^\dagger_{i\downarrow}b^\dagger_{j\uparrow})$	bosonic	J>0 Frobenius	bosonic

Input in Hamiltonian (↑ « bare » monomer statistics, Sign of J)

emerging (↑ « true » monomer statistics)

Statistics of the excitations of the resonating-valence-bond state

N. Read and B. Chakraborty

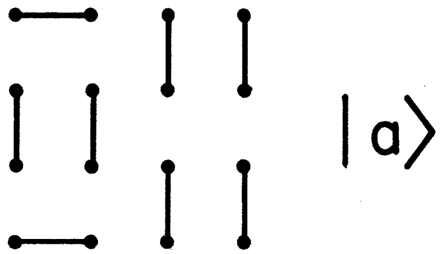
PRB 89'

By extending recent proposals for choosing the phases in resonating-valence-bond ground states to the case of excited states, we show for these wave functions that the hole excitations are charged, spinless fermions and the spin excitations are neutral, spin-$\frac{1}{2}$ bosons. We also show that for a sys-

Variational RVB

$$|\psi\rangle = \sum_{\text{configurations}} g_{i_1 j_1}(i_1 j_1) g_{i_2 j_2}(i_2, j_2) \cdots |0\rangle$$

here $g_{ij} = 0$ if i, j are not nearest neighbors.



$$(ij) = (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)/\sqrt{2}$$

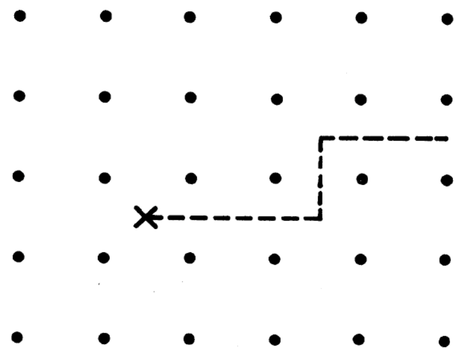


FIG. 2. X is the center of a vortex, in a plaquette of the lattice; the dashed line is the "cut": the g_{ij} factor for a link crossing the cut is multiplied by -1.

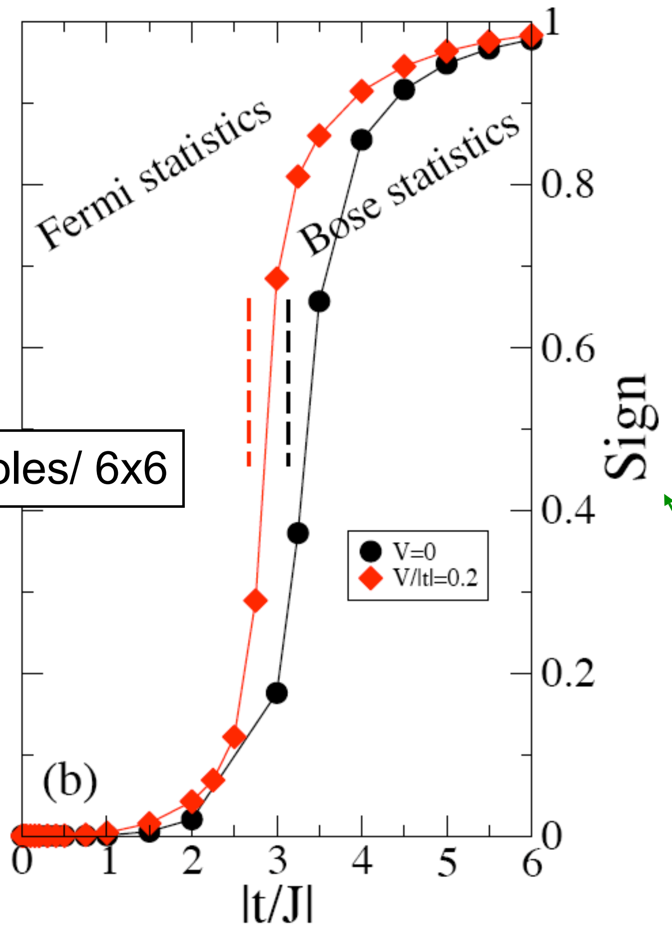
Role of topological defects:
vortex or Z_2 vison

Holon (boson) + vortex ⟹ spinless fermion !

Holon doped QDM

Physical case:
J<0

QMC replaced by
Lanczos Exact Diagonalizations



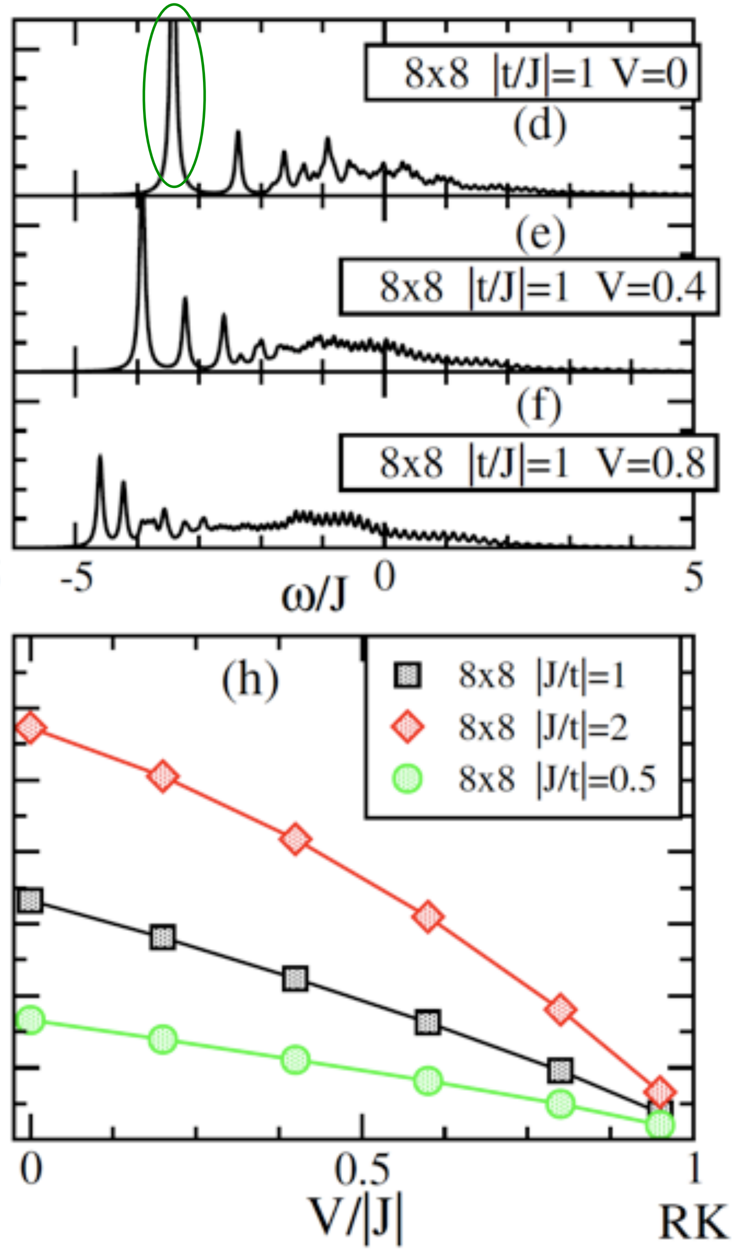
6 holes/ 6x6

Holon (boson) + « vison »

spinless fermion

$$\mathrm{Sign_R} = \sum_{\mathcal{C}} \left| \sum_{c\in\mathcal{C}} \langle\Psi_0|c_\mathrm{R}\rangle\, |\langle\Psi_0|c_\mathrm{R}\rangle| \right| / \sum_{c} |\langle\Psi_0|c_\mathrm{R}\rangle|^2$$

2-holon bound-state in d-wave channel



2-holon propagator

“string picture”

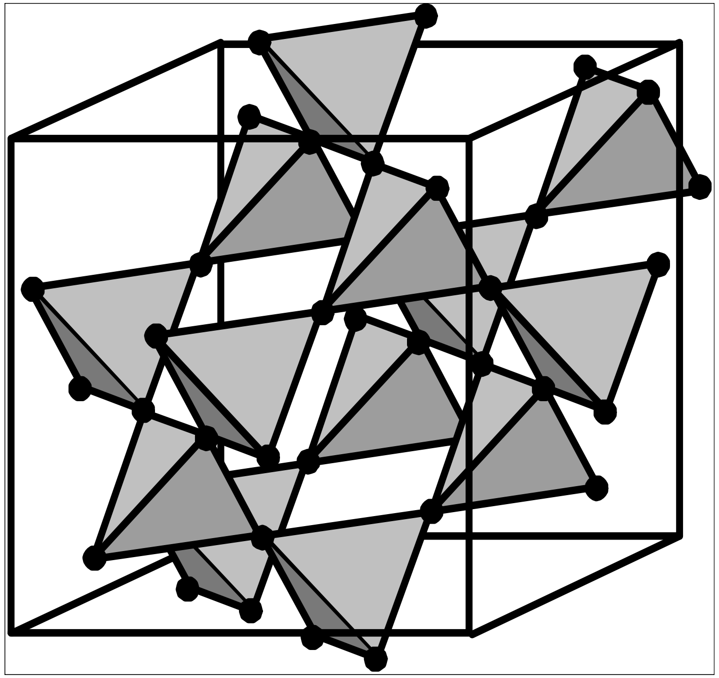
Summary / Conclusions

- Can replace efficiently "microscopic" models since easier to simulate
- To do list:
  - for frustrated magnets, carry out systematic "loop" expansion => more complicated QDM's but minus-sign problem can still be avoided !
  - doped systems: optics, transport, impurity doping, connection with Z_2 gauge field theory…

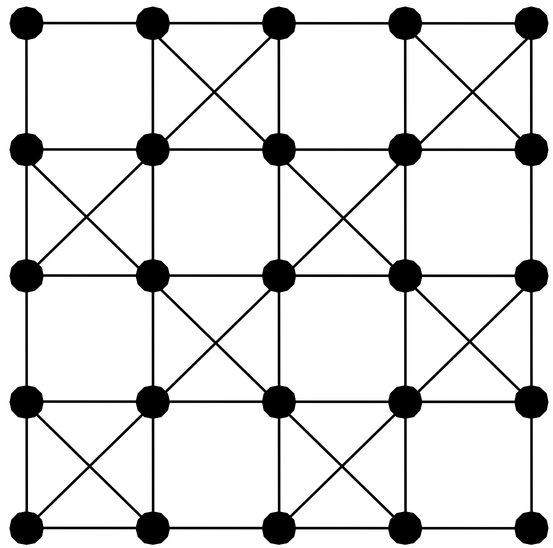
Collaborators

- Arnaud Ralko (Post-doc -> Institut Néel, Grenoble)
- Fabien Trousselet (PhD)
- Roderich Moessner (Dresden)
- Matthieu Mambrini (Toulouse)
- Karlo Penc (Budapest)
- Nic Shannon (Bristol)
- Federico Becca (Trieste)
- Frédéric Mila (Lausanne)

Pyrochlore lattice

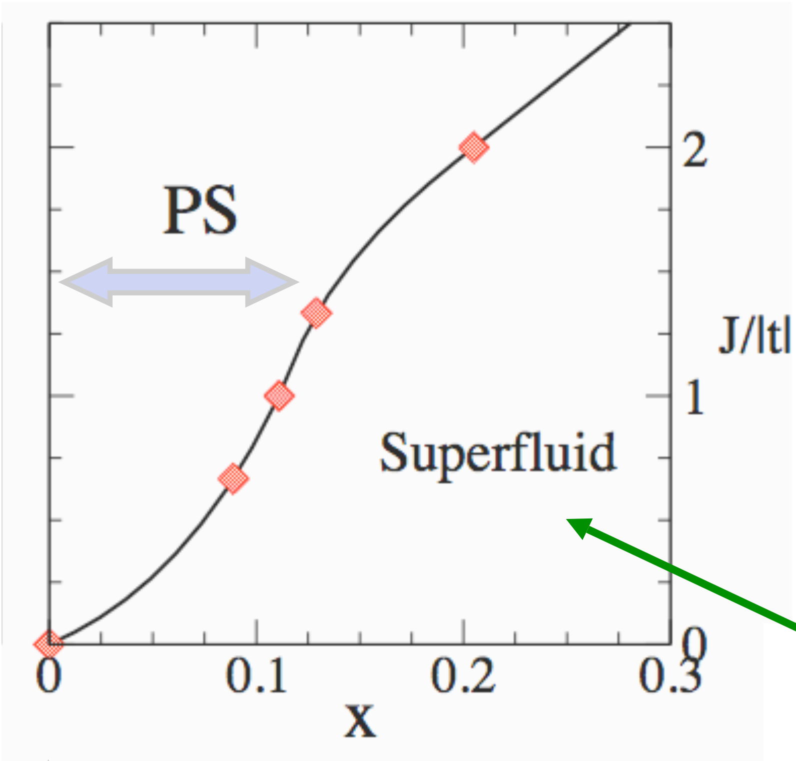


Checkerboard lattice



A lattice for theorists !

Phase diagram vs doping

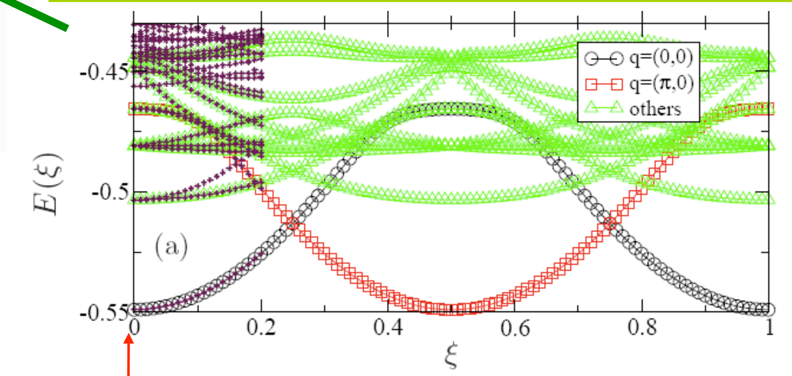


VBC insulator

Role of gauge field

Flux quantization: in terms of h/2e

2e-Cooper pairs



0-flux

1/2-flux quantum