Symmetries and phases in the frustrated hexagonal lattice

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Work in collaboration with:

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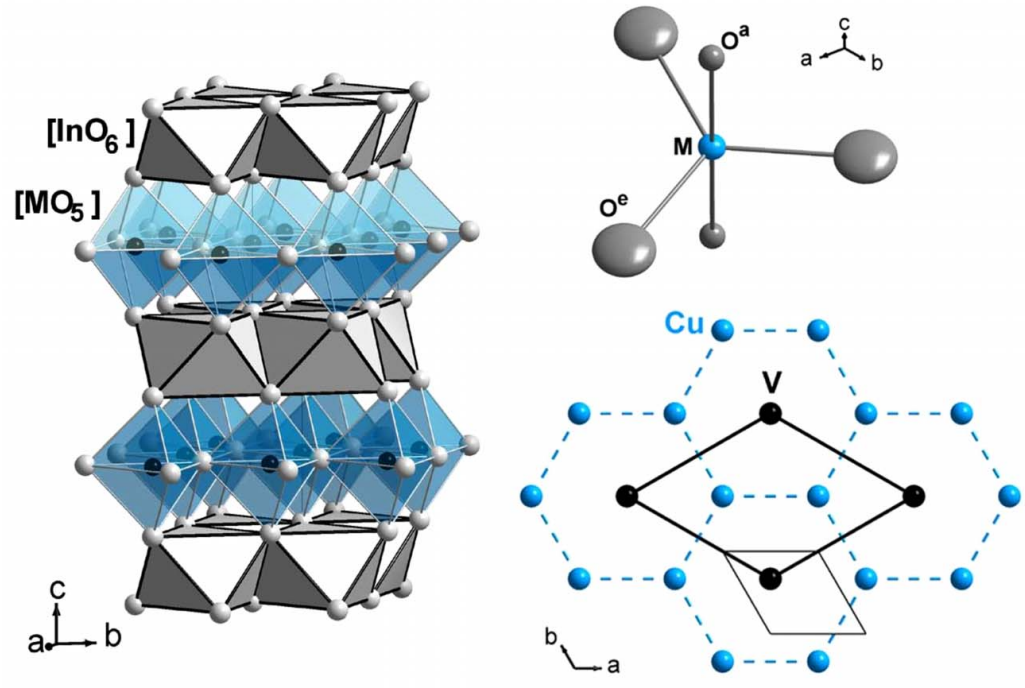
Plan of the Talk

- Motivation
- Quantum disordered phase from Schwinger bosons
- Magnetic field effects
- Results
- Conclusions

Experimental motivation

Hexagonal Heisenberg $InCu_{2/3}V_{1/3}O_3$ $\rightarrow$ short-range AF order $T < 50$K



- $Bi_3Mn_4O_{12}(NO_3)$ $\rightarrow$ $S = 3/2$ honeycomb frustrated Heisenberg no magnetic order down to 0.4 K

- Family of compounds $BaM_2(XO_4)_2$ with $M = Co, Ni$ and $X = P, As$ $\rightarrow$ frustrated honeycomb lattices with spin $S = 1/2$ for Co and $S = 1$ for Ni

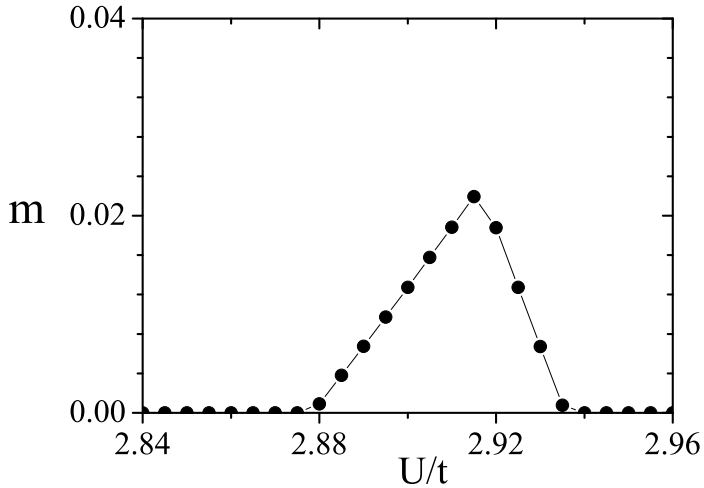
- Spin-Gap System $Na_3Cu_2SbO_6$ $\rightarrow$ Distorted $J_1 - J_3$ honeycomb under debate

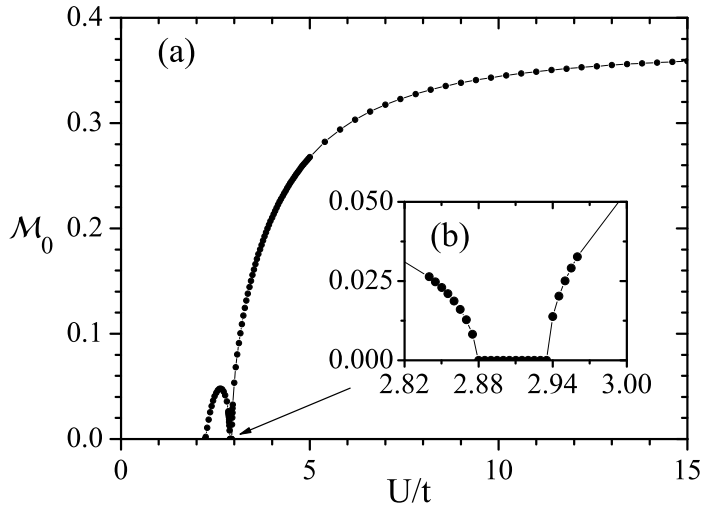
Hubbard-honeycomb at half-filling

$$H = -t \sum_{<ij>,\sigma} [\mathbf{c}^{\dagger}_{i,\sigma}\mathbf{c}_{j,\sigma} + H.c.] + U \sum_{i} \mathbf{n}_{i,\uparrow}\mathbf{n}_{i,\downarrow}$$

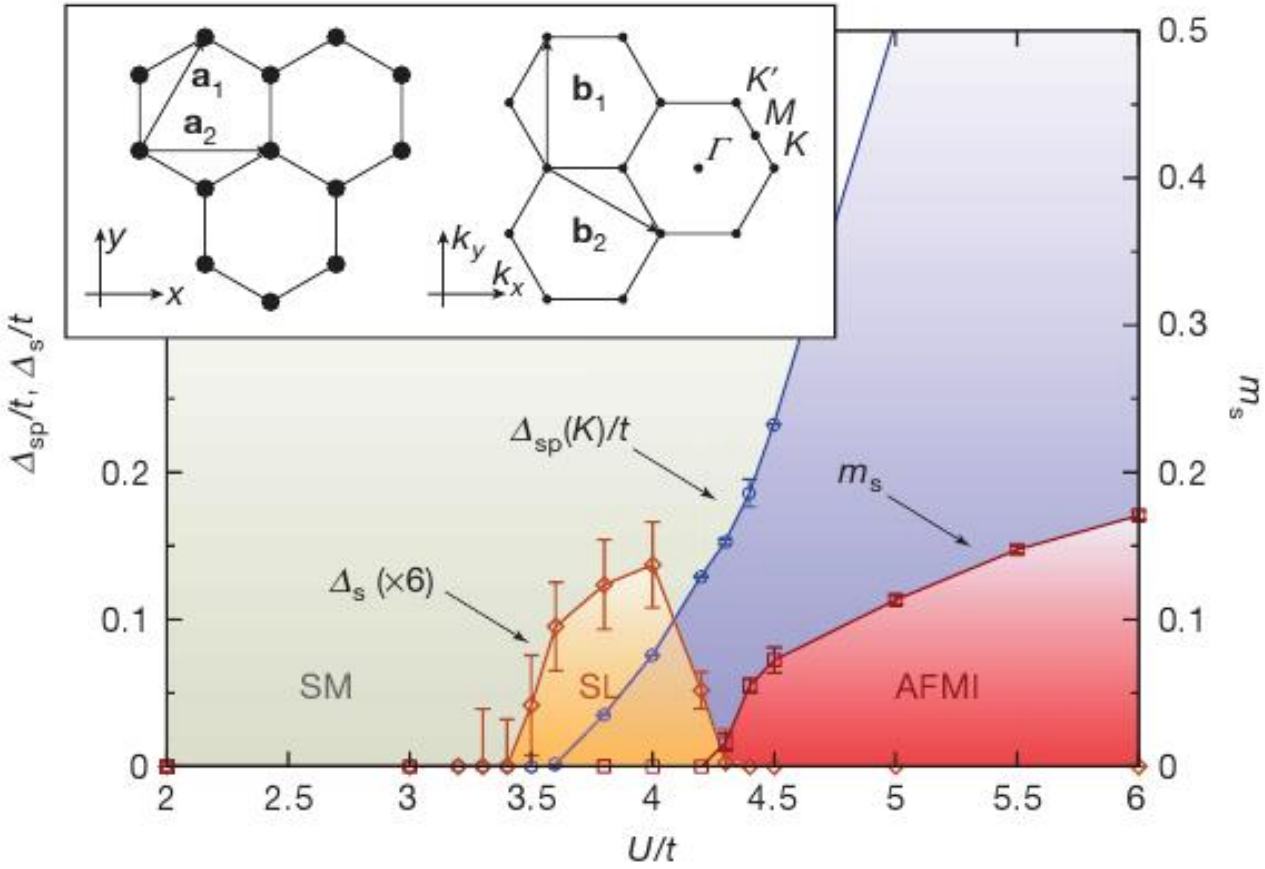
It maps into Heisenberg with J_1 ^{3}, ...

$O(3)$ nonlinear σ model (Sun-K e the AFMI

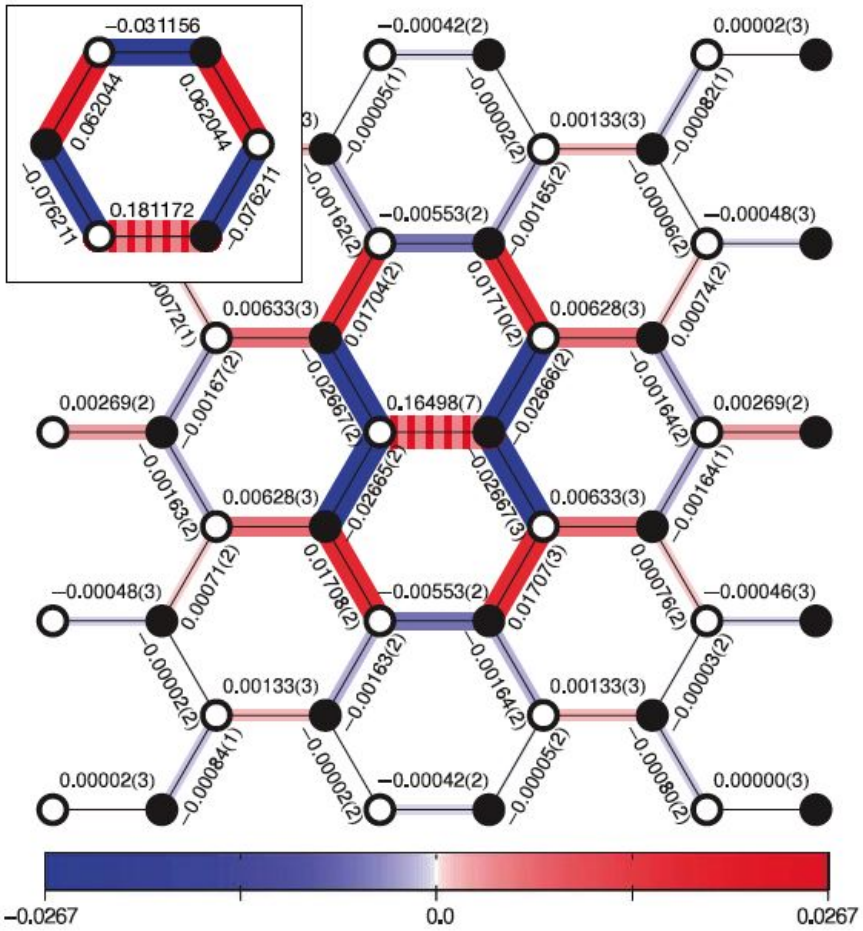




Z. Y. Meng *et al*, Nature 2010



Dimer-dimer correlations



Compared to the half-filled Hubbard $J_1 \sim t^2/U$, $J_2 \sim t^4/U^3$

$$\rightarrow \alpha \sim \frac{J_2}{J_1} \sim \frac{t}{U}^{2} \sim \frac{1}{16}$$

Higher orders (J_3, plaquette, etc.) are O(α^2)

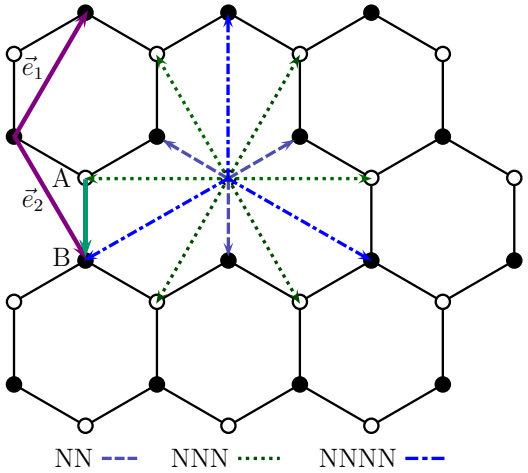
Motivation

From experiments: Study of the frustrated Heisenberg on honeycomb

From theory: How to get disorder in a pure spin system on honeycomb

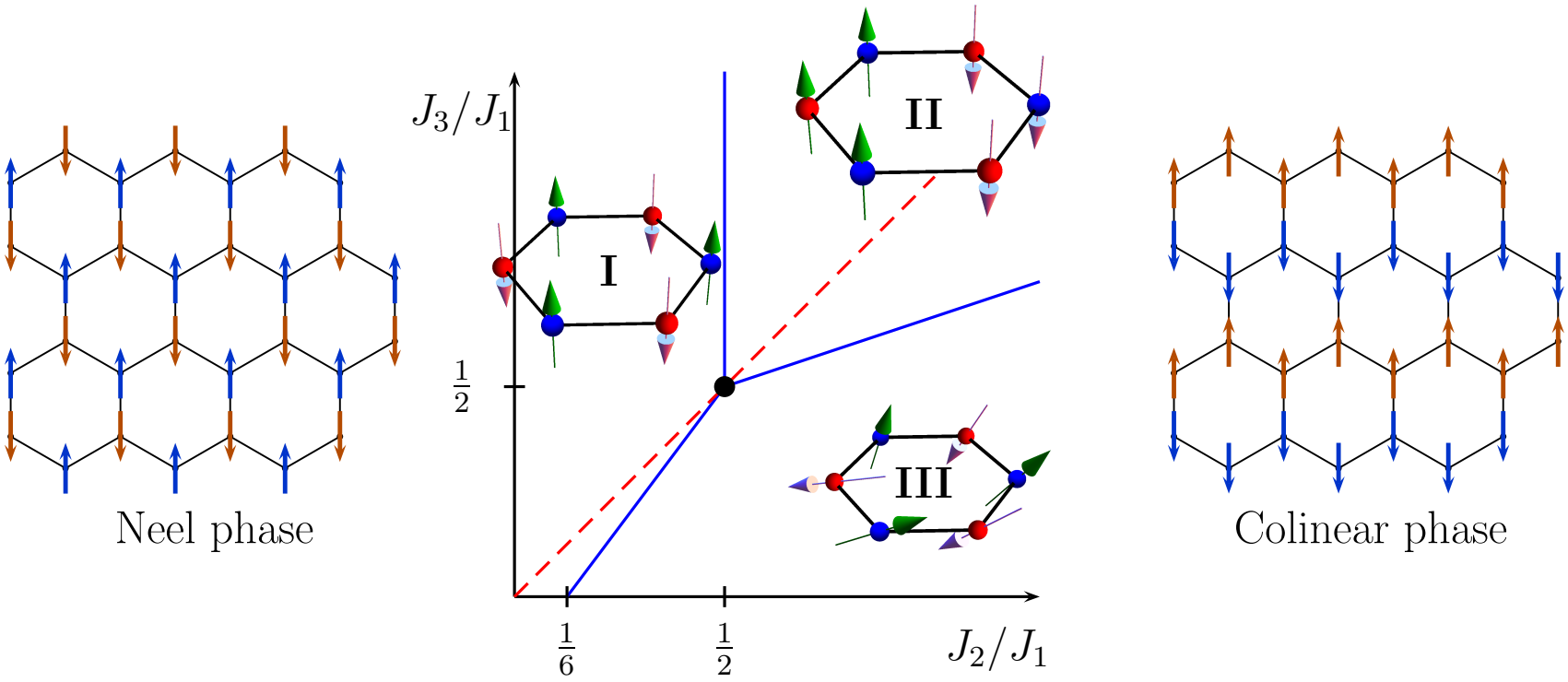
Is it possible or does one need doubly occupied states?

The model



$$H = J_1 \sum_{NN} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j + J_2 \sum_{NNN} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j + J_3 \sum_{NNNN} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j$$

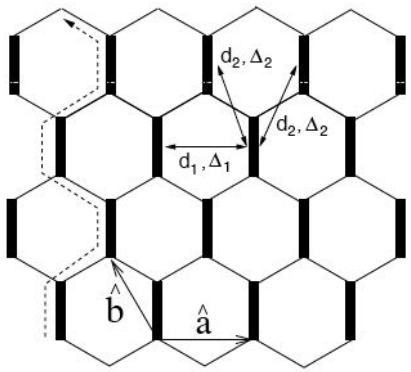
Classical phase diagram (Lhuillier *et al*)



Quantum $J_1 - J_2$ (Mulder $et\ al$ 2010, Mattsson-Frojdh PRB 1994)

Clasically: Néel $\rightarrow$ degenerate spiral at $J_2/J_1 = 1/6$

In the quantum case: Néel (Baskaran $et\ al$) $\rightarrow$ to



From bond operators for $J_2/J_1 \gtrsim 1/4$

The method: Schwinger bosons

Spin operators at each site are replaced by two species of bosons via:

$$
\begin{aligned}
\mathbf{S}^{+}_{\vec{x}} &= \mathbf{b}^{\dagger}_{\vec{x}\uparrow}\mathbf{b}_{\vec{x}\downarrow} \\
\mathbf{S}^{-}_{\vec{x}} &= \mathbf{b}^{\dagger}_{\vec{x}\downarrow}\mathbf{b}_{\vec{x}\uparrow} \\
\mathbf{S}^{z}_{\vec{x}} &= \frac{1}{2}(\mathbf{b}^{\dagger}_{\vec{x}\uparrow}\mathbf{b}_{\vec{x}\uparrow} - \mathbf{b}^{\dagger}_{\vec{x}\downarrow}\mathbf{b}_{\vec{x}\downarrow})
\end{aligned}
$$

Which is a faithful representation of the SU(2) algebra if one takes into account the constraint

$$
2S = \mathbf{b}^{\dagger}_{\vec{x}\uparrow}\mathbf{b}_{\vec{x}\uparrow} + \mathbf{b}^{\dagger}_{\vec{x}\downarrow}\mathbf{b}_{\vec{x}\downarrow}
$$

The spin-spin interaction can be written as

$$\vec{\mathbf{S}}_{\vec{x}} \cdot \vec{\mathbf{S}}_{\vec{y}} =: \mathbf{B}^{\dagger}_{\vec{x},\vec{y}} \mathbf{B}_{\vec{x},\vec{y}} : - \mathbf{A}^{\dagger}_{\vec{x},\vec{y}} \mathbf{A}_{\vec{x},\vec{y}}$$

where $\mathbf{A}_{\vec{x},\vec{y}}$ and $\mathbf{B}^{\dagger}_{\vec{x},\vec{y}}$ are the $SU(2)$ invariants defined as

$$\begin{aligned} \mathbf{A}_{\vec{x},\vec{y}} &= \frac{1}{2} \sum_{\sigma} \sigma \mathbf{b}_{\vec{x},\sigma} \mathbf{b}_{\vec{y},-\sigma} \\ \mathbf{B}^{\dagger}_{\vec{x},\vec{y}} &= \frac{1}{2} \sum_{\sigma} \mathbf{b}^{\dagger}_{\vec{x},\sigma} \mathbf{b}_{\vec{y},\sigma} \end{aligned}$$

$\mathbf{A}_{\vec{x},\vec{y}}$ creates a spin singlet pair between sites $\vec{x}$ and $\vec{y}$

$\mathbf{B}_{\vec{x},\vec{y}}$ intersite coherent hopping of Schwinger bosons

Advantages

- Fluctuations can be included leading to interesting QFT's
- Only one constraint for a generic S
- Possible generalization to $Sp(N)$ adapted for a large N expansion
- Combine large S and N
- For ordered regions, MF provides already a good approximation.

SBMFT procedure

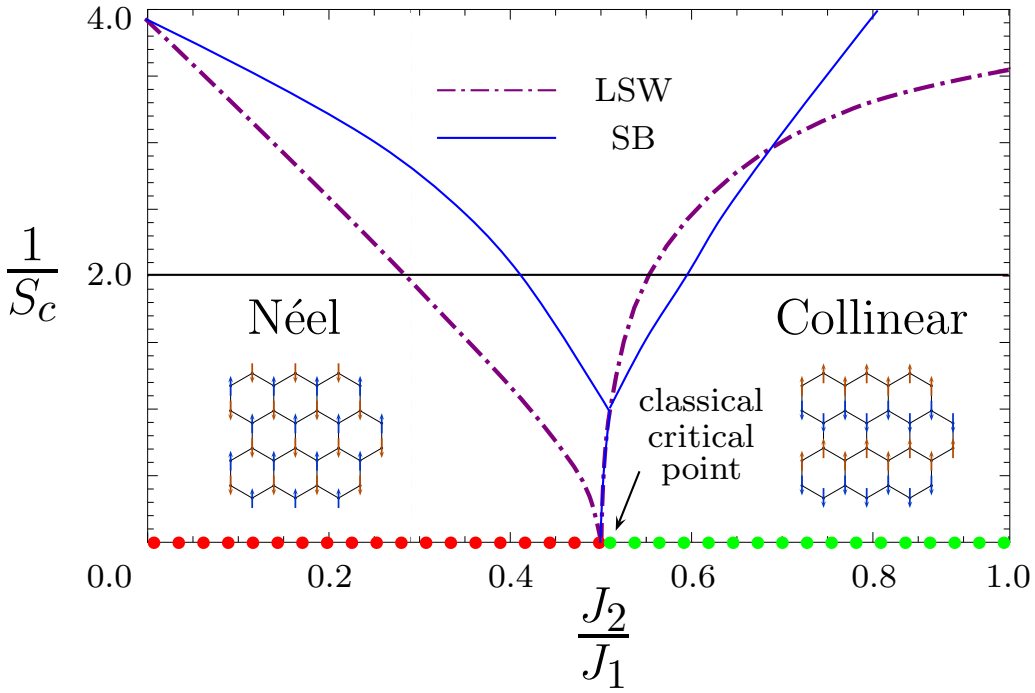
Given $J_2/J_1 \rightarrow$ classical values of the MF parameters $\rightarrow$

- $\rightarrow$ solve the constraint equation $\rightarrow \lambda_0^{(\alpha)}$
- $\rightarrow$ compute the energy $\rightarrow$ new values for the MF parameters
- $\rightarrow$ repeated until the energy and the MF parameters converge.

After convergence $\rightarrow$ compute the energy, spin-spin correlations and the gap of the excitations.

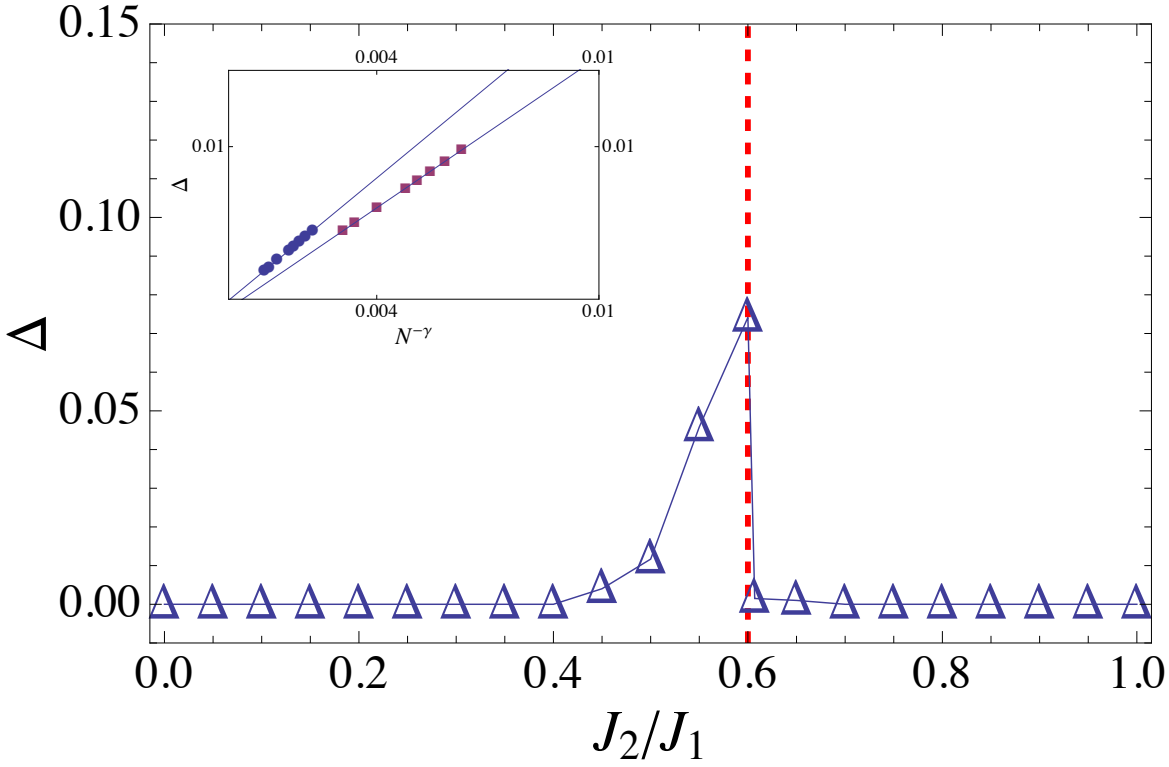
Results

Phase diagram in $1/S$

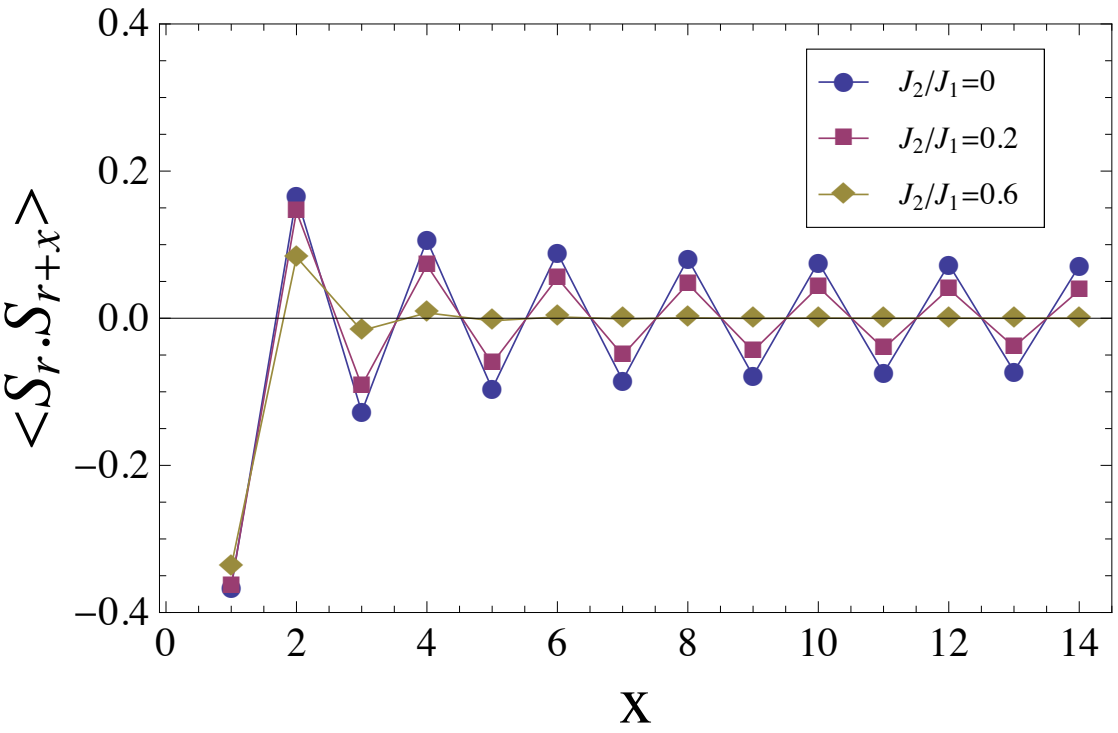


Thermodynamic limit from systems up to 3200 sites

Evolution of the quasiparticle gap from SBMFT

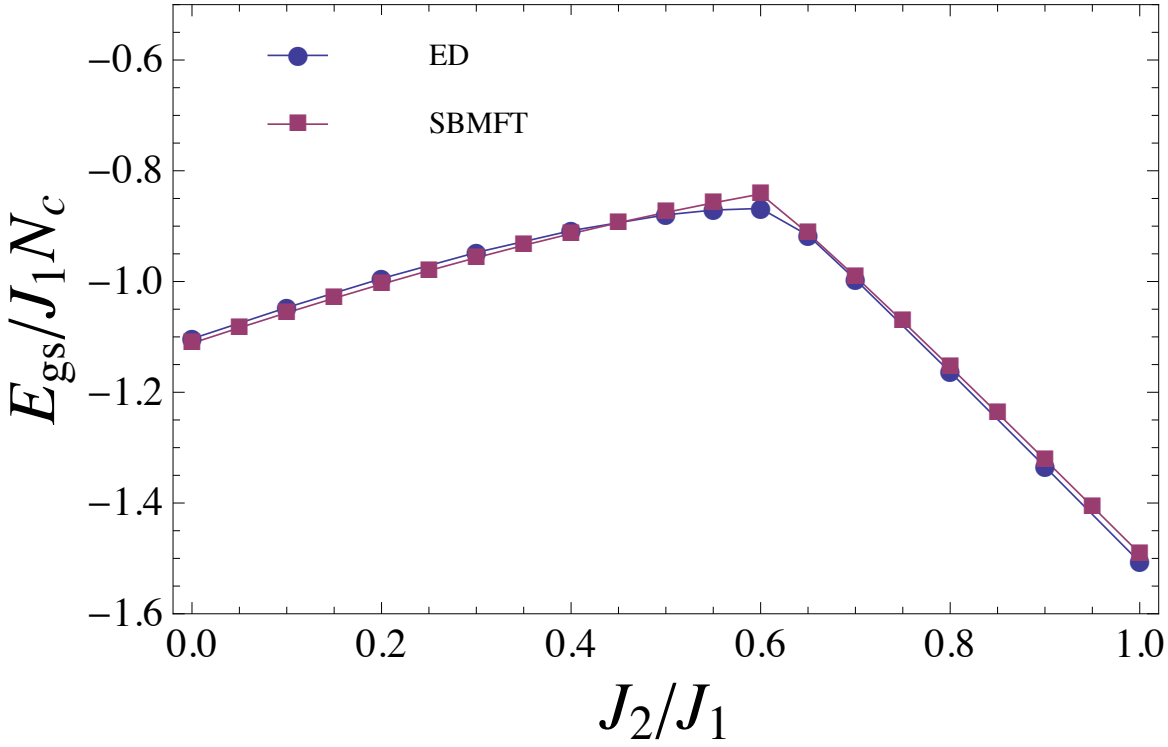


Spin-Spin correlation function vs distance X in the zig-zag direction.



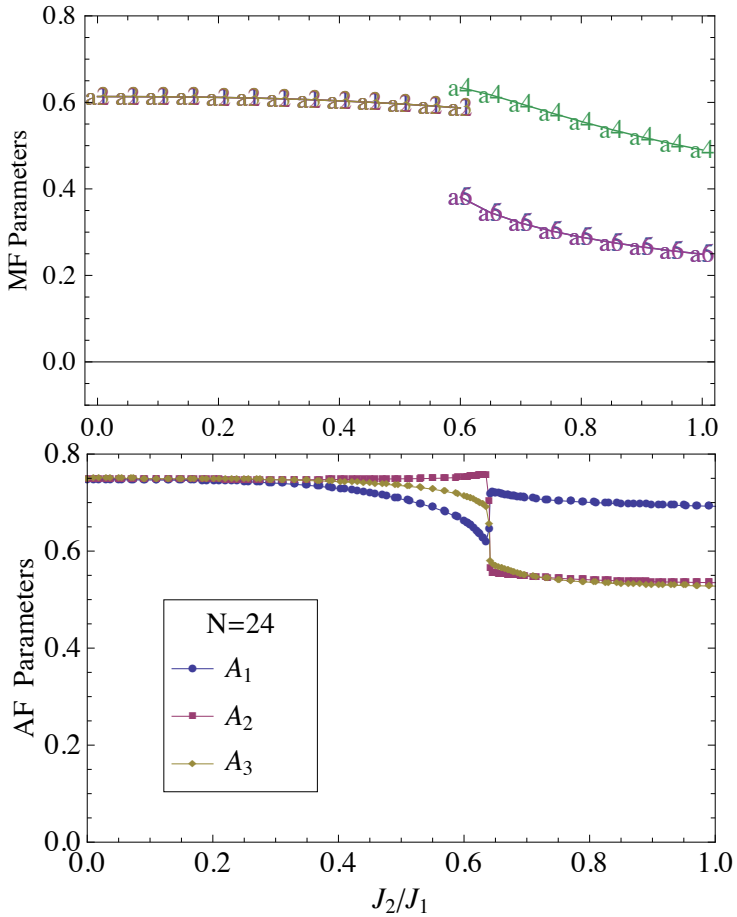
Néel LRO for $0 < J_2/J_1 \lesssim 0.55$ and SRO for $0.55 \lesssim J_2/J_1 \lesssim 0.6$

Ground state energy per unit cell as a function of the frustration for 32 sites



ED results (circles) vs. SBMFT (squares)

Antiferromagnetic mean field parameters A vs. J_2/J_1 (SBMFT (top) vs ED (bottom))



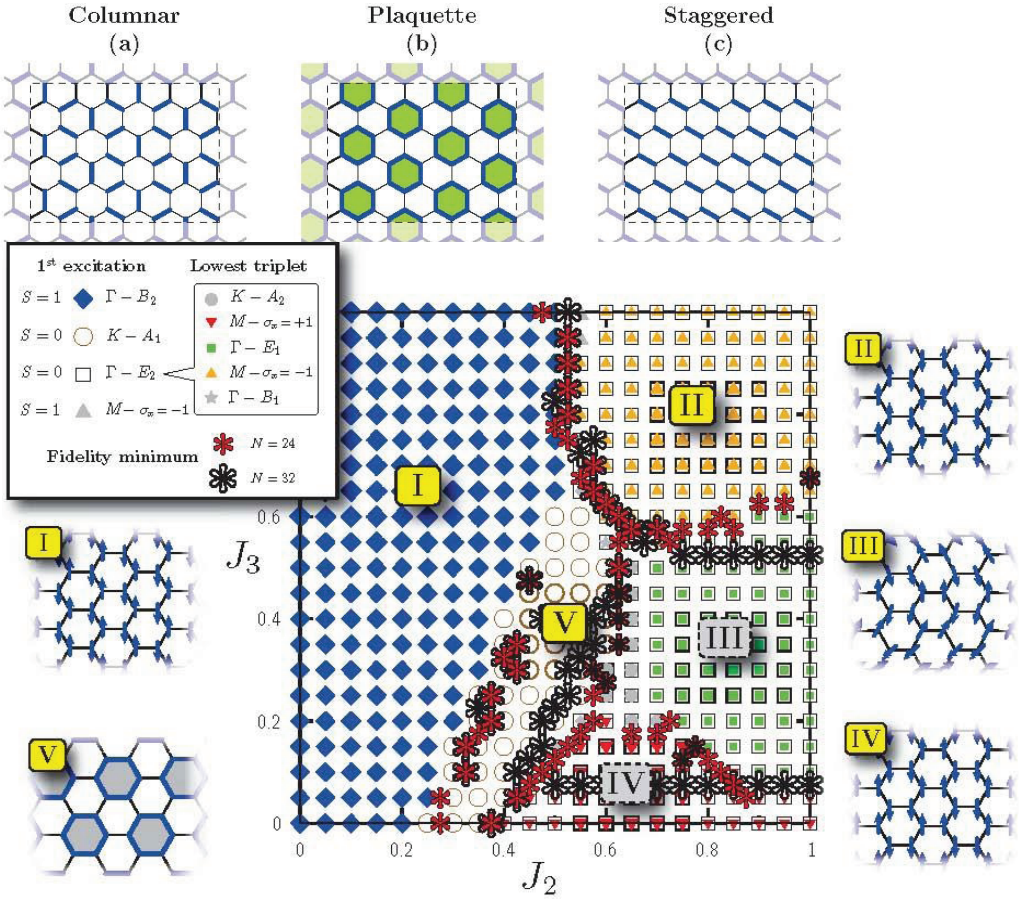
Discontinuity around $J_2/J_1 = 0.6 \rightarrow$ first order phase transition between Collinear LRO and Néel SRO

This discontinuous behavior is not a finite size effect

The same occurs for the ferromagnetic parameters B

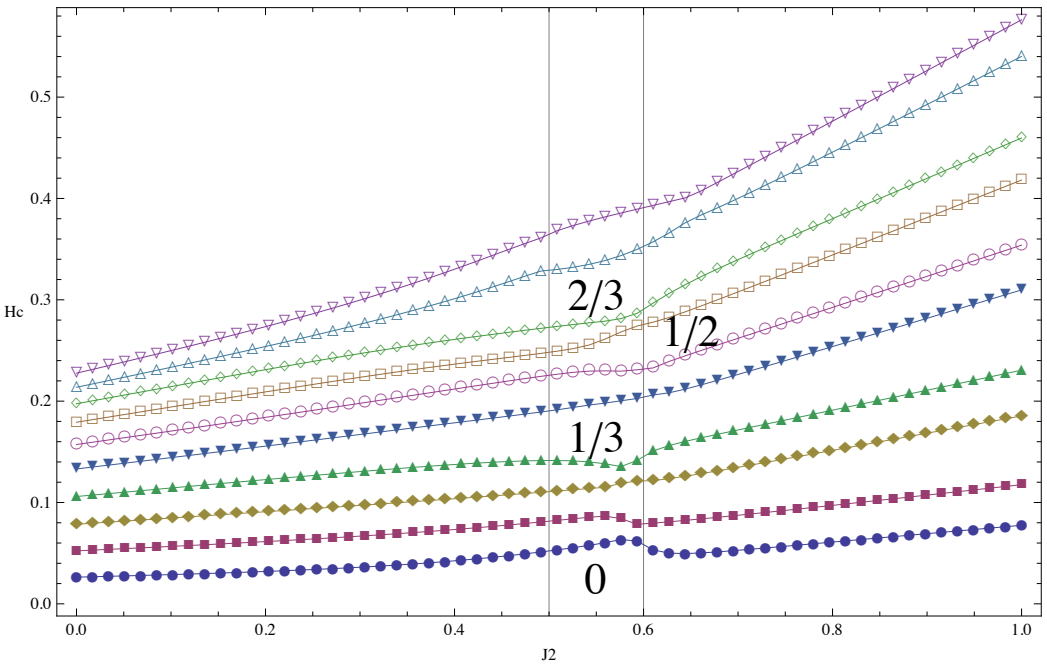
Nature of the disordered phase?

Possible candidates are



Phase diagram **(A.F. Albuquerque *et al* PRB 2011)**

Magnetization around the quantum disordered region



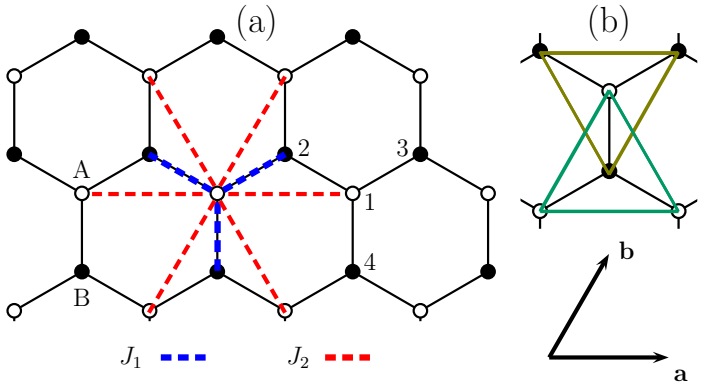
Two regions seem to emerge: plateaux at $\{0, 1/3, 2/3\}$ and $\{0, 1/2\}$

Classical spins in a magnetic field for $J_3 = 0$

$\mathbf{h} = 0$:

- Classically: Néel for $J_2 < J_1/6$ to infinite IC spiral states for $J_2 > J_1/6$
- $J_2 = J_1/2$ separates two different spirals
- Special degeneracy since the Hamiltonian can be written as a sum of the form

$$H = \text{cte} + \frac{J_1}{4} \sum_{\vee} \left(\mathbf{S}_{\vee}^2 - \frac{1}{J_1} \mathbf{h} \cdot \mathbf{S}_{\vee} \right) + \frac{J_1}{4} \sum_{\wedge} \left(\mathbf{S}_{\wedge}^2 - \frac{1}{J_1} \mathbf{h} \cdot \mathbf{S}_{\wedge} \right)$$



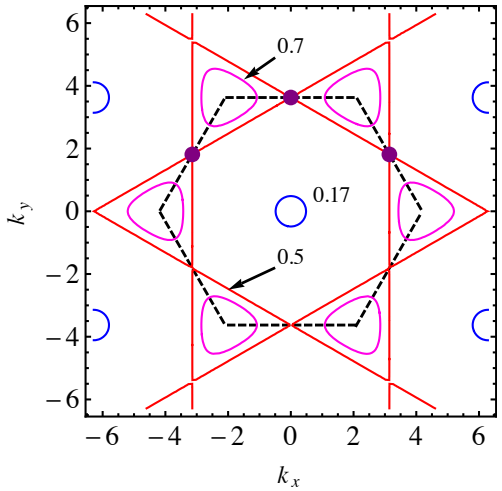
Hence the GS's satisfy

$$\mathbf{S}_{\vee} = \frac{\mathbf{h}}{2\, J_1}, \qquad \mathbf{S}_{\wedge} = \frac{\mathbf{h}}{2\, J_1}$$

on every $\wedge$ and $\vee$

Fluctuations

- Mulder *et al* in PRB 2010



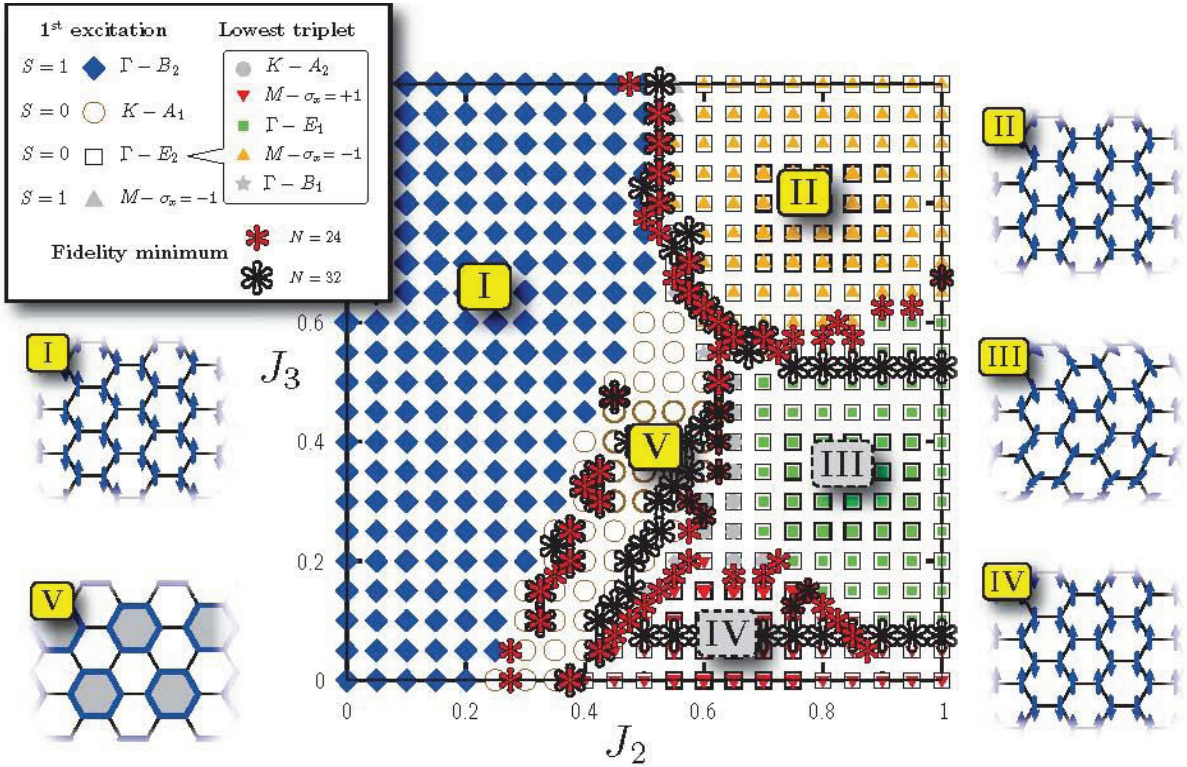
Quantum fluctuations select some directions (spiral OBD) $\rightarrow$ Valence bond solid (?) "nematic"
T restores the SU(2) symmetry, but the discrete rotational symmetry of the lattice remains broken

Transition to the PM phase in the universality class of the classical three-state

Potts (clock) model in 2D

- Albuquerque *et al* in PRB 2011

$J_3 = 0$: Néel $\rightarrow$ plaquette $\rightarrow$ collinear magnetically ordered



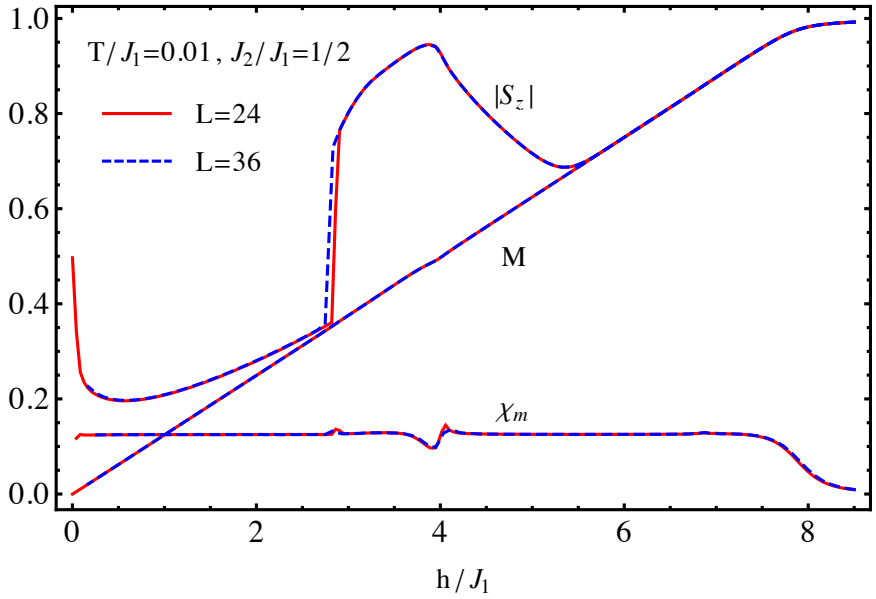
Hence, around $J_2 = J_1/2 \rightarrow$ collinear state with broken (spatial) Z_3

What happens if we turn on a magnetic field?

- For small fields, as in Mulder et al, fluctuations restore rotational order but leave the Z3 discrete symmetry in XY broken

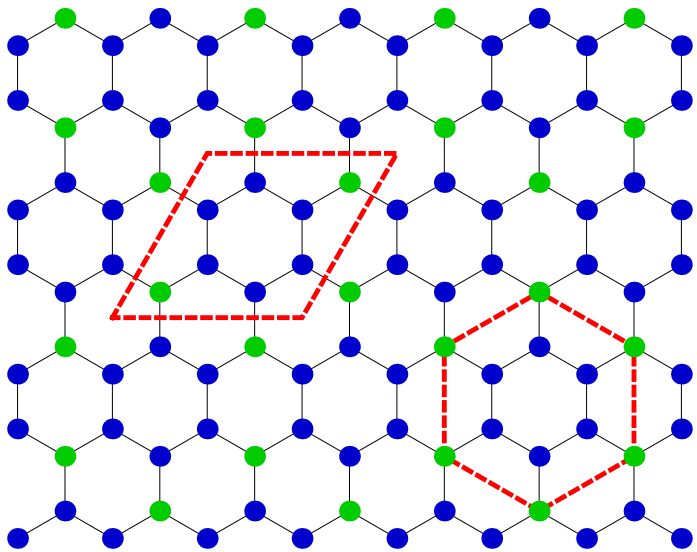
- The interesting thing is that for sufficiently large field, a transition occurs to a completely symmetric phase

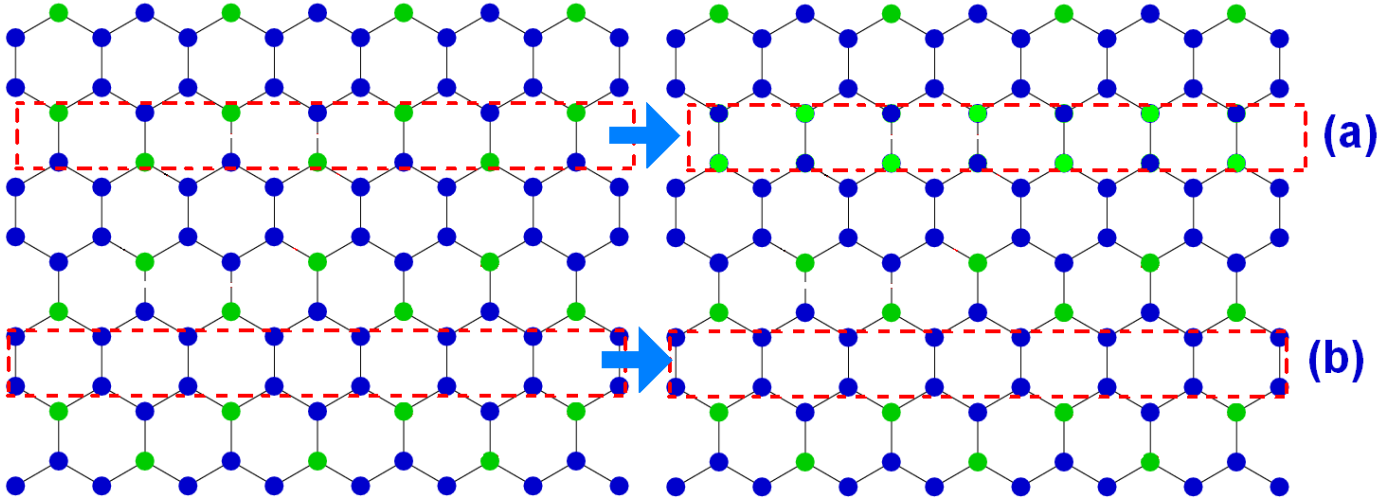
- $i.e.$ the broken discrete symmetry is restored in a finite magnetic field

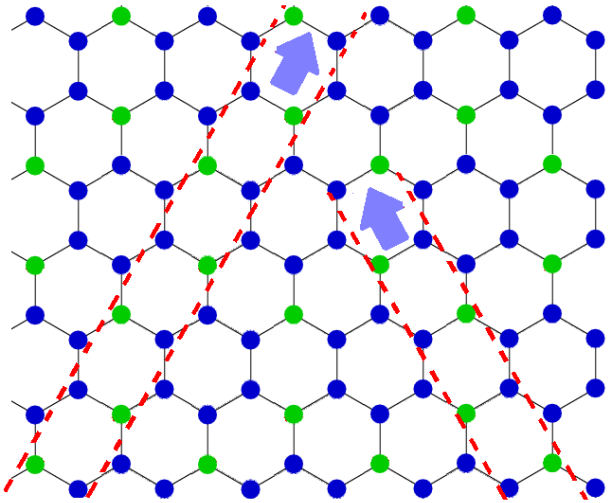


Magnetization, Susceptibility and $|S_z|$

Pattern within the plateaux region



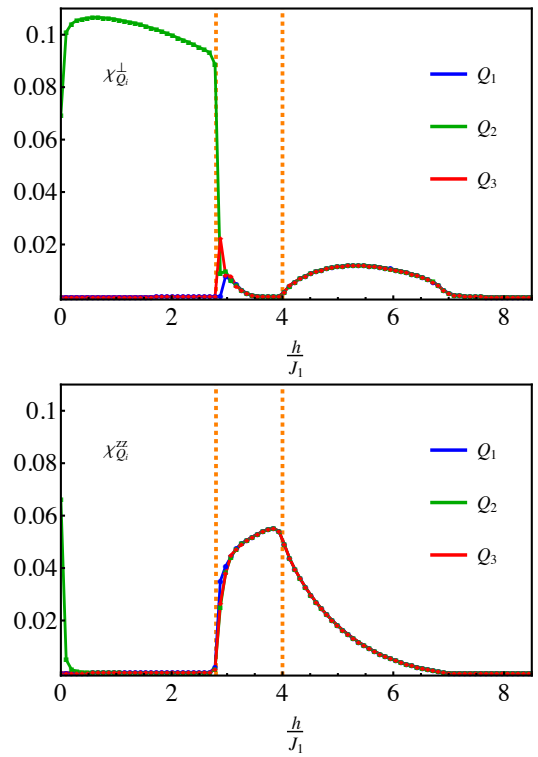

(a)
(b)



Structure factors

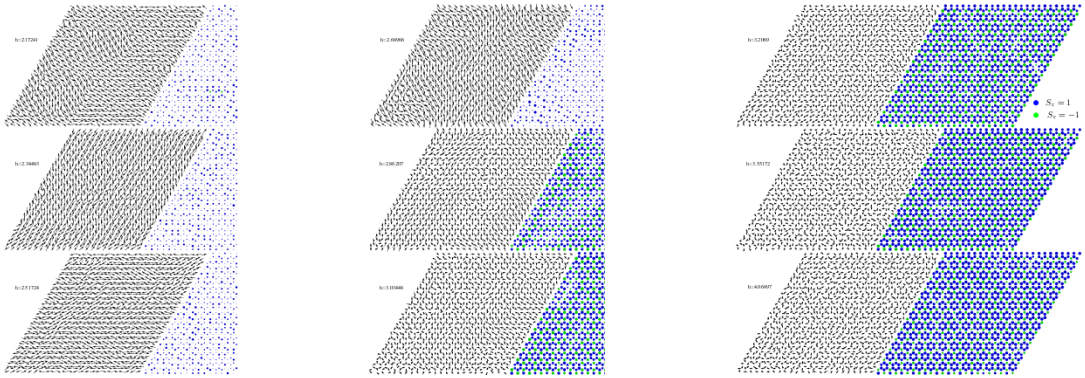
$$\chi_Q^{\perp} = \frac{1}{N^2}\sum_{i,j}\langle S_i^x S_j^x + S_i^y S_j^y\rangle\, e^{Q(i-j)}$$

$$\chi_Q^{zz} = \frac{1}{N^2}\sum_{i,j}\langle S_i^z S_j^z\rangle\, e^{Q(i-j)}$$

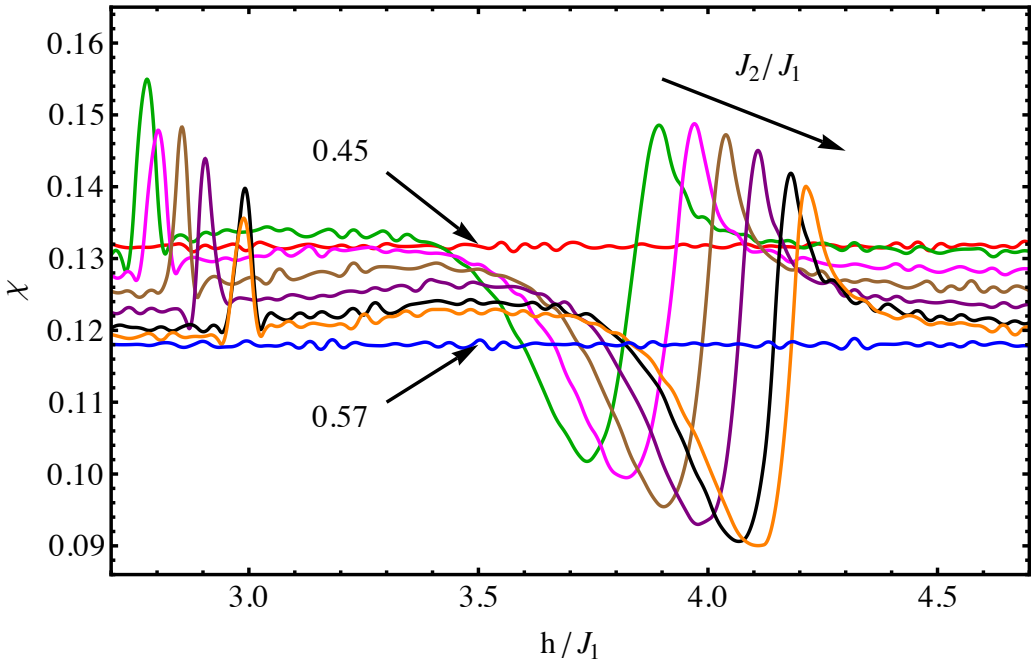


Supplementary material

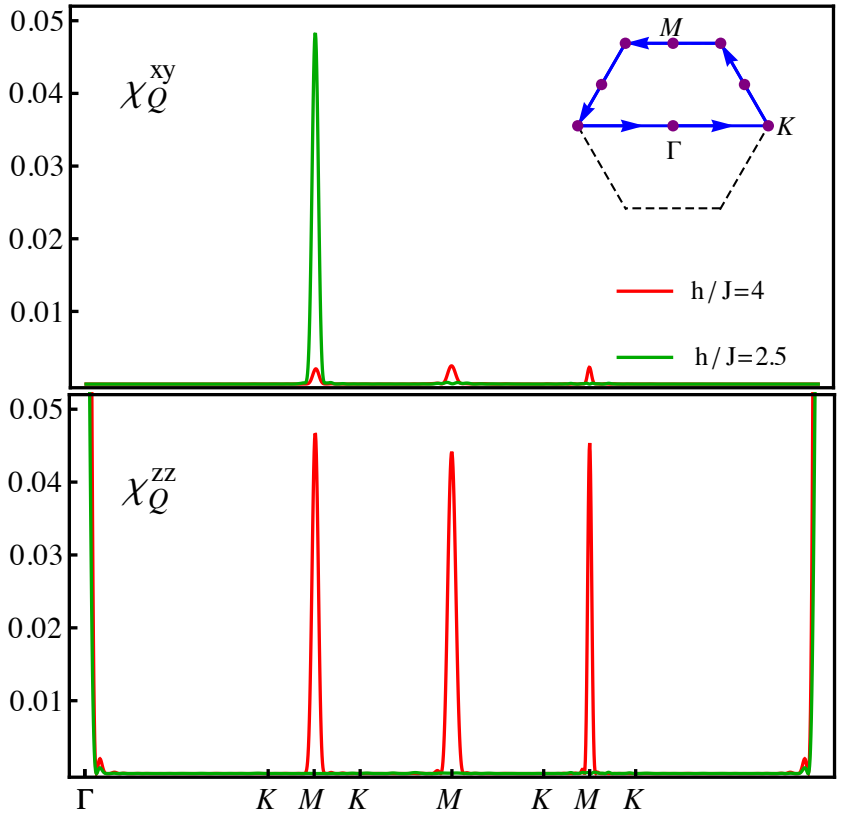
- MonteCarlo snapshots



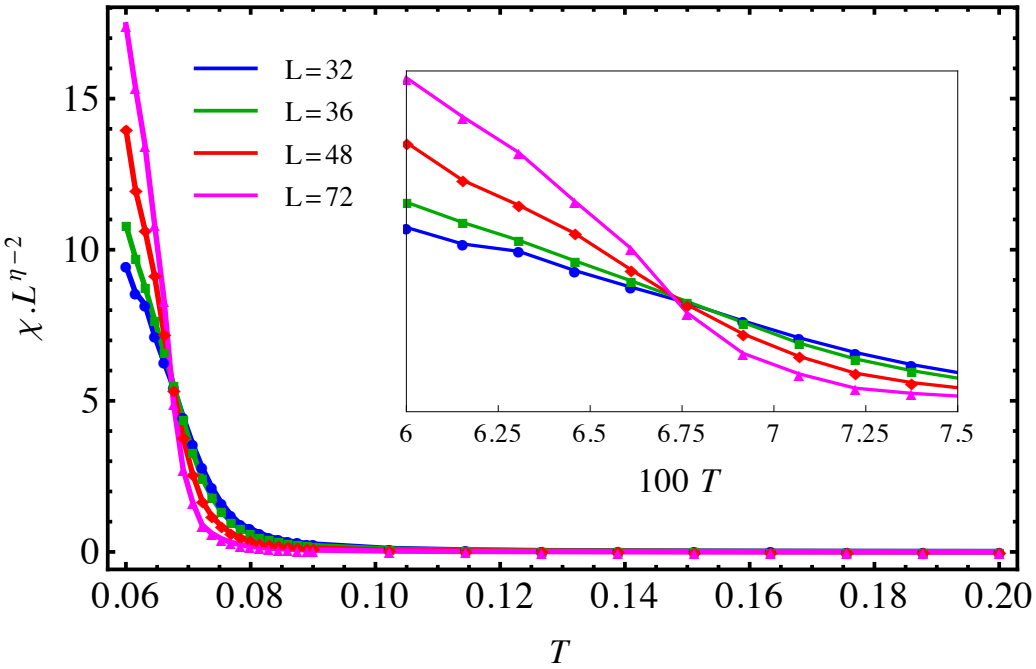
- Susceptibility around $J_2/J_1 = 0.5$



- Peaks of the structure factor



- $H = 0$ susceptibility vs. T and Binder cumulant



Conclusions and future work

- Heisenberg on the hexagonal lattice shows an interesting disordered phase which could be relevant to some materials

- Schwinger-bosons technique gives encouraging results

- Include fluctuations:

  – On top of SBMFT
  – Using bond operators, given the structure of the different GS's

- Interesting magnetization properties: OBD, pseudo-plateau, emerging symmetries,...

- Connection with the half-filled Hubbard