Effective Spin Couplings in the Mott Insulator of the Honeycomb Lattice Hubbard Model

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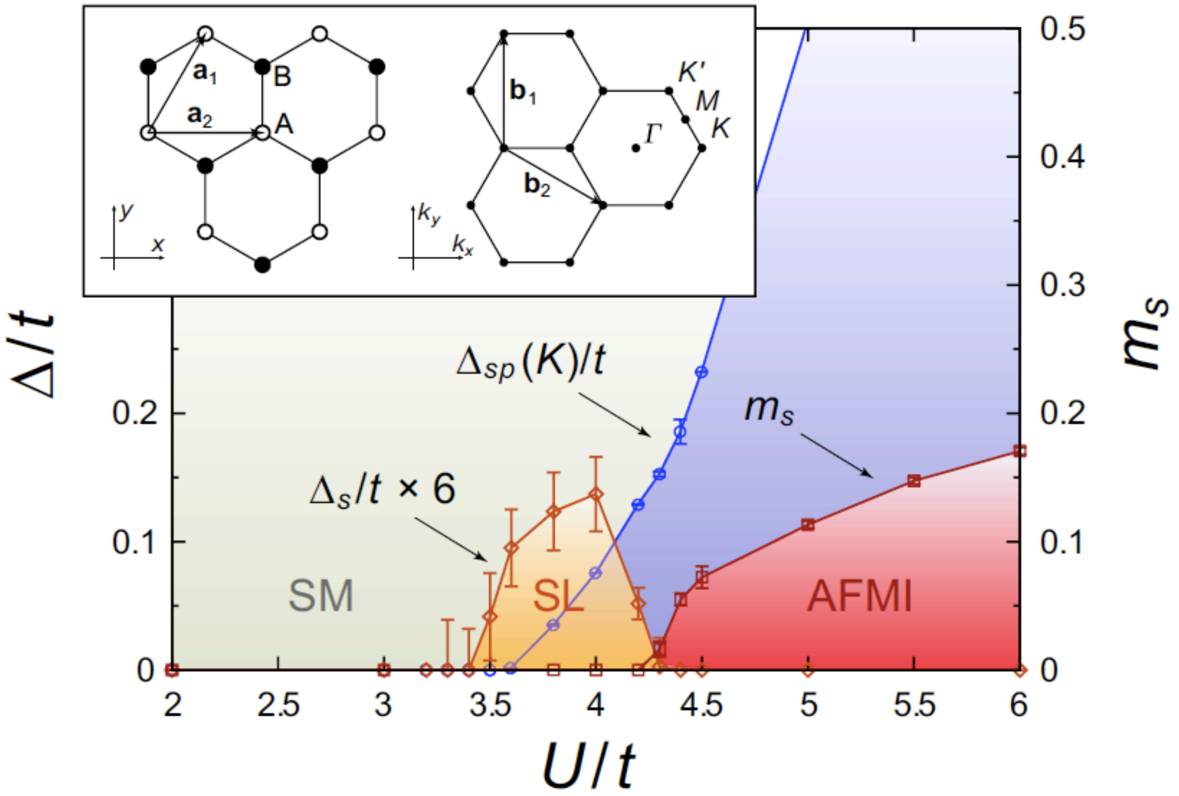
A.F. Albuquerque, D. Schwandt, B. Hetényi, S. Capponi, M. Mambrini, and A.M. Läuchli
Phys. Rev. B **84**, 024406 (2011)

H.Y. Yang, A. F. Albuquerque, S. Capponi, A. Läuchli, and K. P. Schmidt
arXiv:1207.1072

Original motivation

- Spin liquid phase has been found in QMC simulations

  Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad and A. Muramatsu, Nature 464, 847 (2010)



- We will hear more about it and recent controversy tomorrow !

  S. Sorella, Y. Otsuka, S. Yunoki, arXiv:1207.1783

Philosophy and Outline

- Assuming that a charge gap opens, there should exist a low-energy description only in terms of spin degrees of freedom
- Weak Mott-insulator behaviour means that mutiple-spin (ring exchange ?) terms could play a role
- Similar studies have been quite successful for the triangular lattice case
  - For instance, see talk by Kanoda for experimental review
  - Theoretically, role of ring exchange has been quite studied

Li Ming et al. PRB (2000); Motrunich PRB (2005); Yang, Läuchli, Mila, and Schmidt, PRL (2010), ...

1) For the honeycomb, can we hope that a simple spin model will work ?

2) If not, what would be a more realistic spin model ?

Lowest order perturbation

- Can a simple J_1-J_2 spin-1/2 model describe a spin liquid phase ?
- Naive perturbation: $$J_1 = 4\frac{t^2}{U} - 16\frac{t^4}{U^3}, \; J_2 = 4\frac{t^4}{U^3}$$

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Nature of the Spin Liquid State of the Hubbard Model on a Honeycomb Lattice

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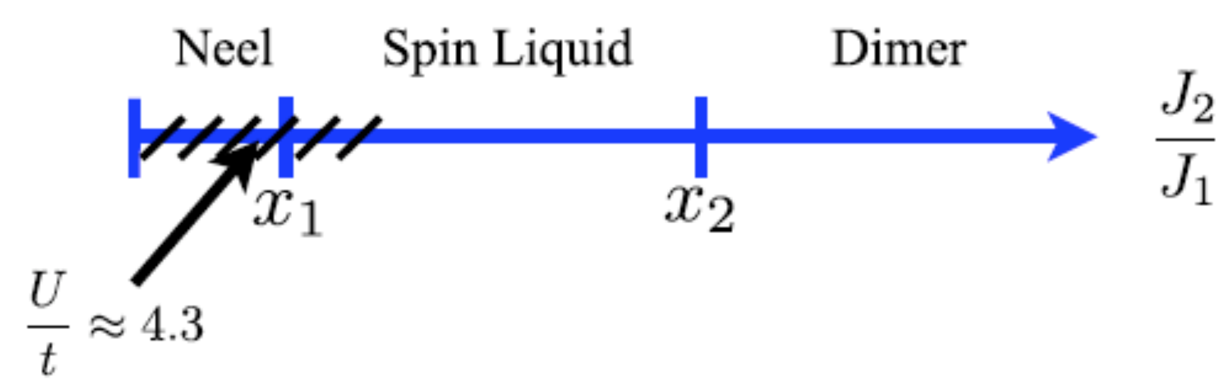
Recent numerical work [Z. Y. Meng *et al.*, Nature (London) **464**, 847 (2010)] indicates the existence of a spin liquid (SL) phase that intervenes between the antiferromagnetic and semimetallic phases of the half filled Hubbard model on a honeycomb lattice. To better understand the nature of this exotic phase, we study the quantum $J_1 - J_2$ spin model on the honeycomb lattice, which provides an effective description

- Variational calculation seems to agree with original QMC results:

  Néel phase is unstable beyond J_2/J_1 = 0.08 to a fully gapped spin liquid phase



Too good to be true ?

J_1-J_2 model has been extensively revisited. Let me cite:

- Exact Diagonalizations, short-range RVB, Quantum Dimer Models, ...

  Albuquerque et al. PRB (2011)

- Series Expansions: Oitmaa and Singh, PRB (2011)

- spin functional RG study Reuther, Abanin, and Thomale, PRB (2011)

- Variational QMC (again) Mezzacapo and Boninsegni, PRB (2012)

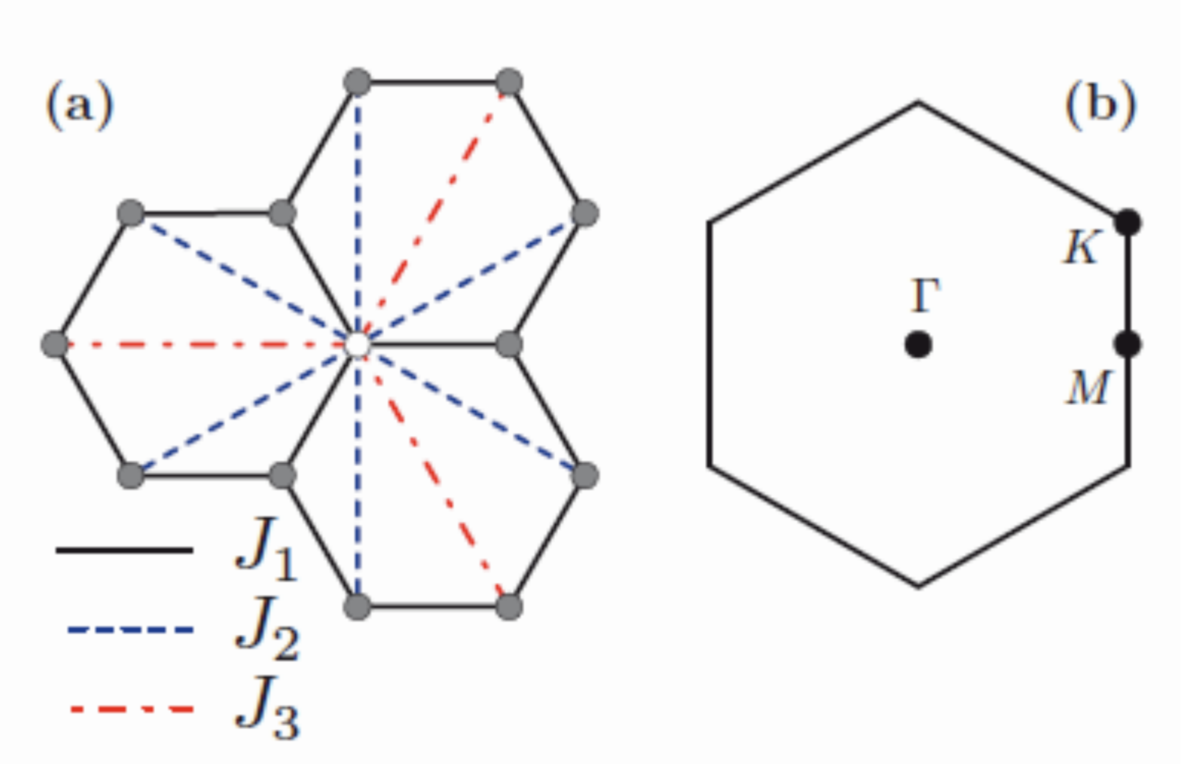
⇒ Néel order is **stable** beyond its classical value $J_2 > 1/6$

The validity of such a suggestion may have to be reconsidered in light of the results presented here, which indicate that the simple reduction of the physics of the Hubbard model to that of an effective spin-1/2 system, such as the $J_1 - J_2$, might not be achievable.

Simple Heisenberg model

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

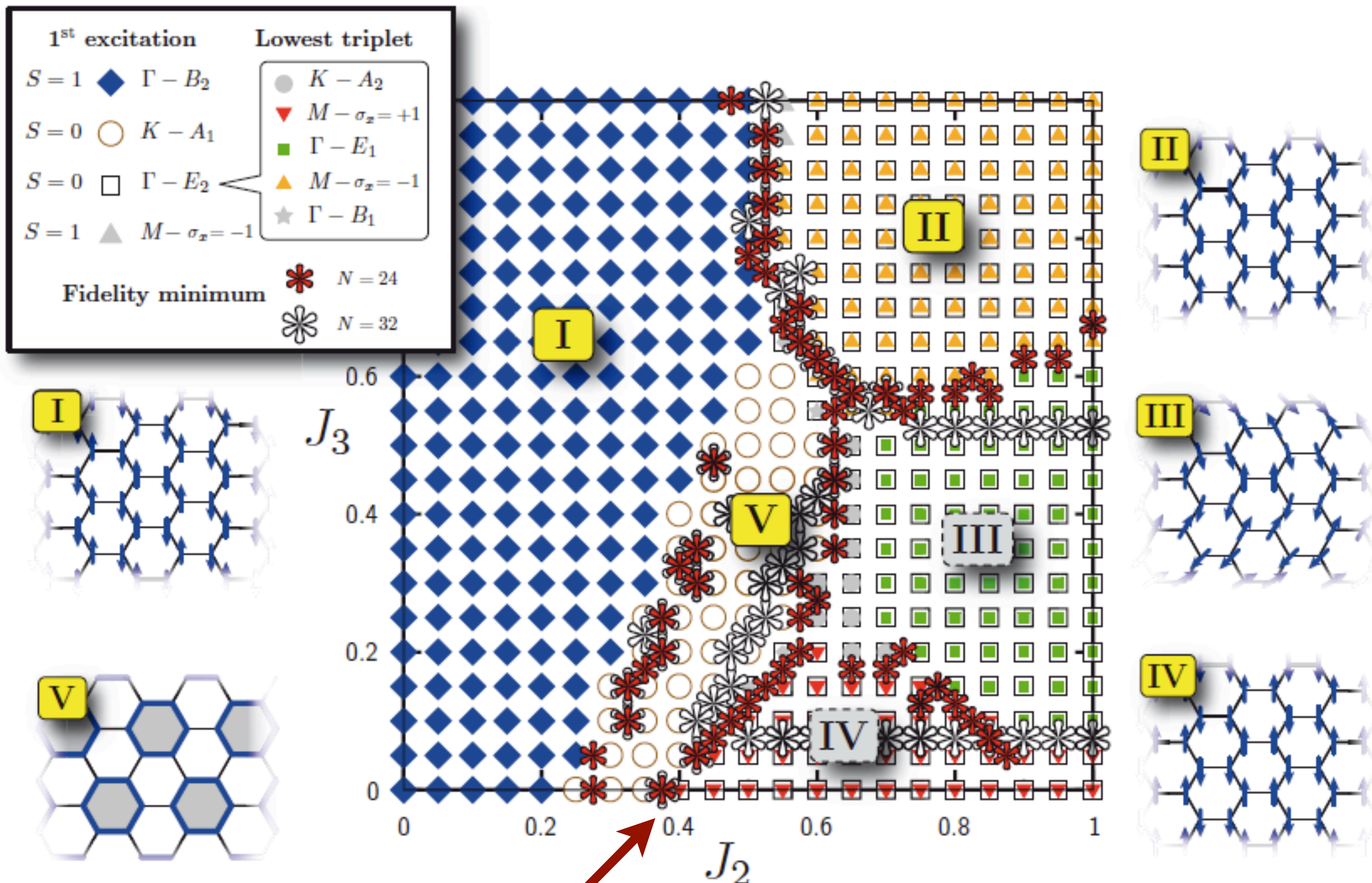
All coupling are antiferromagnetic (J_2 is frustrating, not J_3 !)



We extend the parameters space to stabilize some phases, as also found in the square lattice

M. Mambrini, A. Läuchli, D. Poilblanc, F. Mila, PRB (2006)

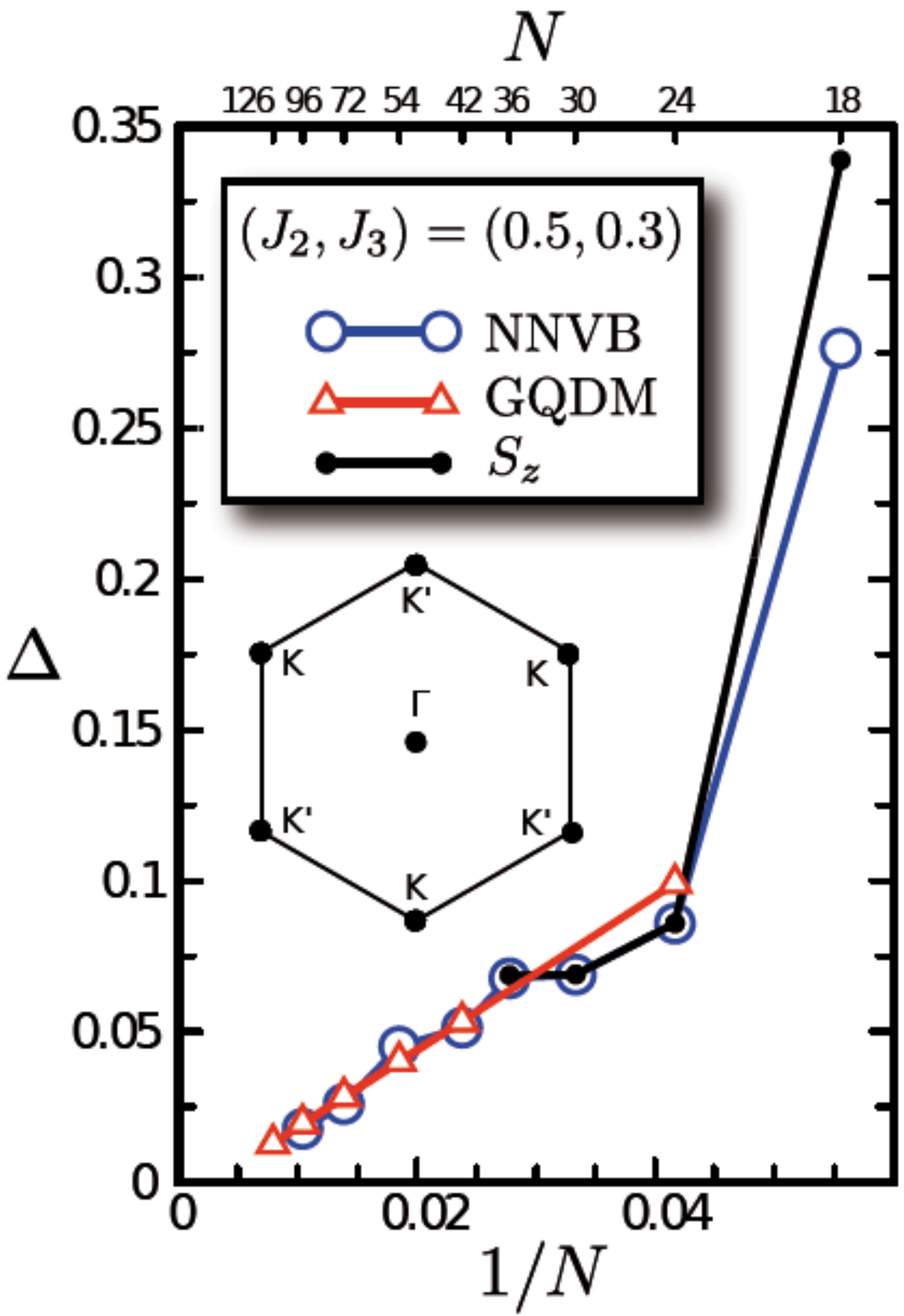
Interlude: Phase Diagram of the J1-J2-J3 model



Fidelity=GS overlap

Albuquerque et al. PRB (2011)

Interlude: what about the disordered phase ?



→ collapse of twofold degenerate level

→ possible plaquette VBC

→ GQDM shows less finite-size effects

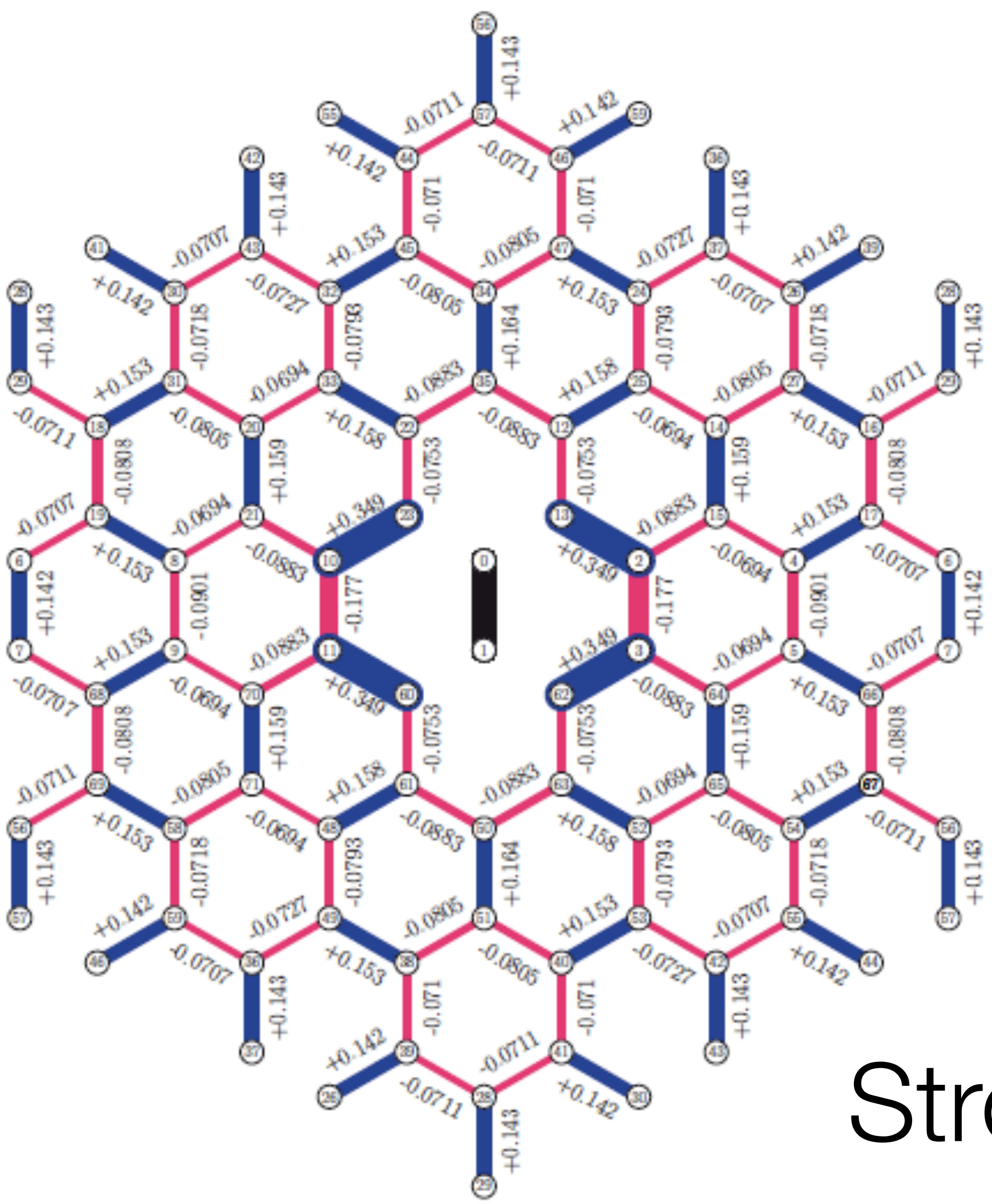
→ larger system sizes available

→ access non-standard observables

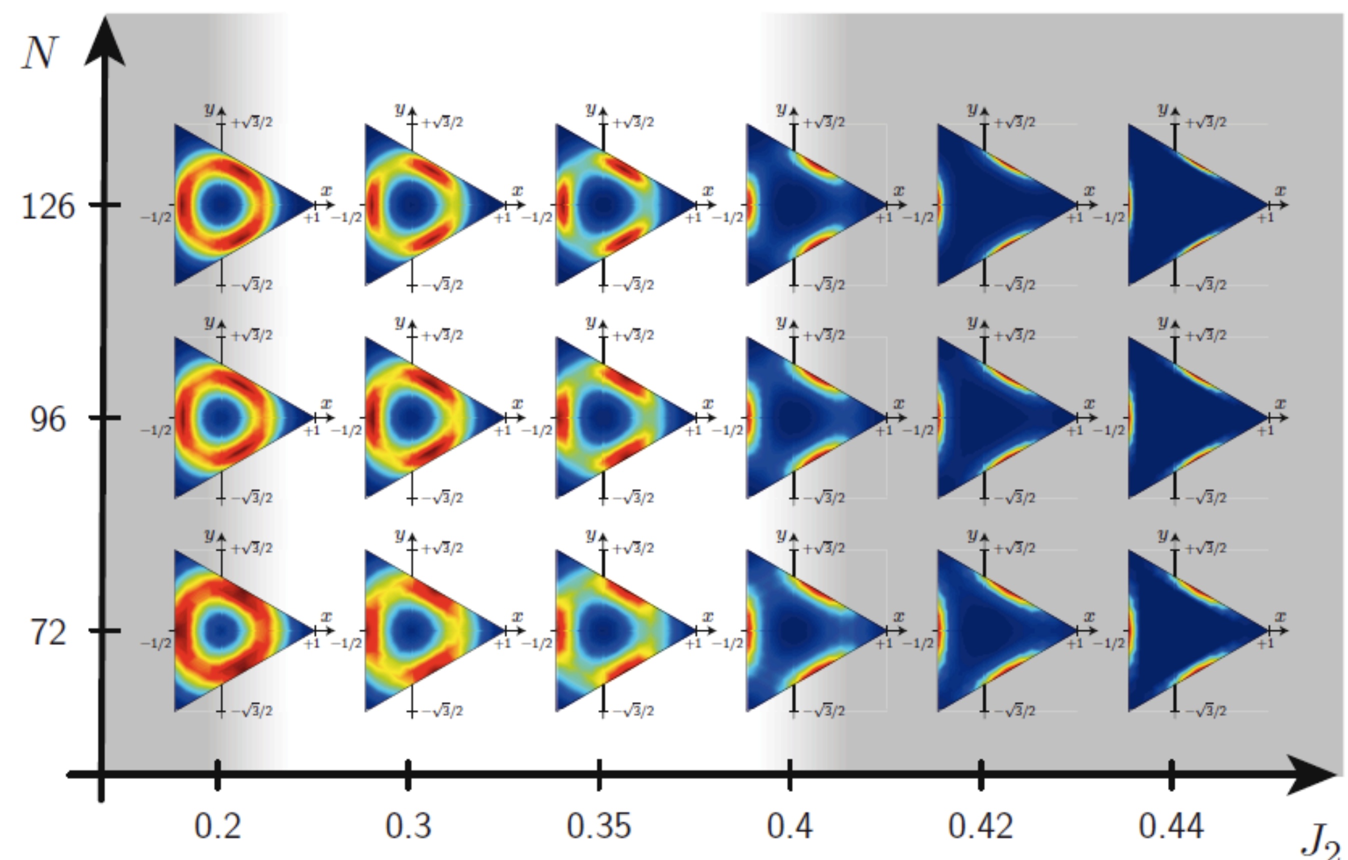
Interlude: what about the disordered phase ?

Dimer correlations in short-range RVB basis

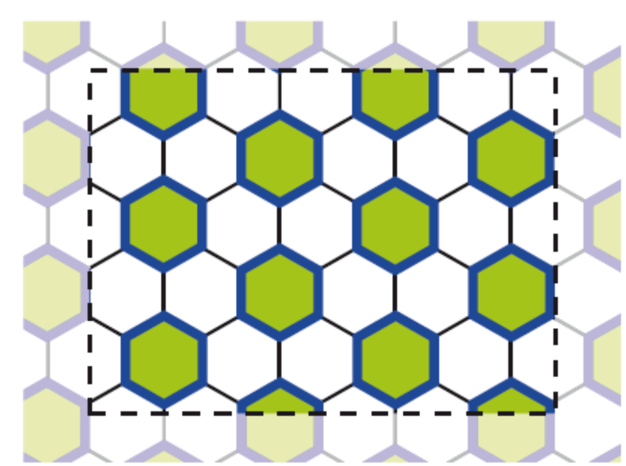
N=72 J_2=0.5 J_3=0.3



QDM effective model



Strong plaquette VBC



Albuquerque et al. PRB (2011)

Interlude: what about pure J1-J2 model ?

- It seems that VBC order is weaker and weaker as J_3 goes to 0
- DMRG seems compatible with a weak VBC as well

S. White (private communication)

- An XY version of this model might have a spin liquid phase

C. N. Varney, K. Sun, V. Galitski, and M. Rigol, PRL (2011)

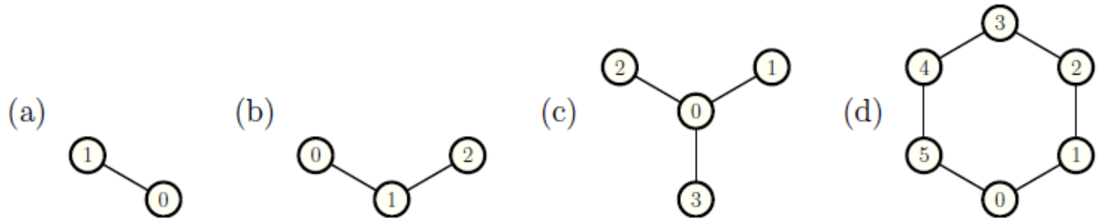
Towards a more realistic spin model...

Back to the problem: what is the spin model ?

We have used two non-perturbative techniques to derive an effective model

- Graph-based Continuous Unitary Transform — Yang and Schmidt, EPL (2011)
- Contractor Renormalization (CORE) — Morningstar and Weinstein, PRL (1994)

real-space RG-like technique

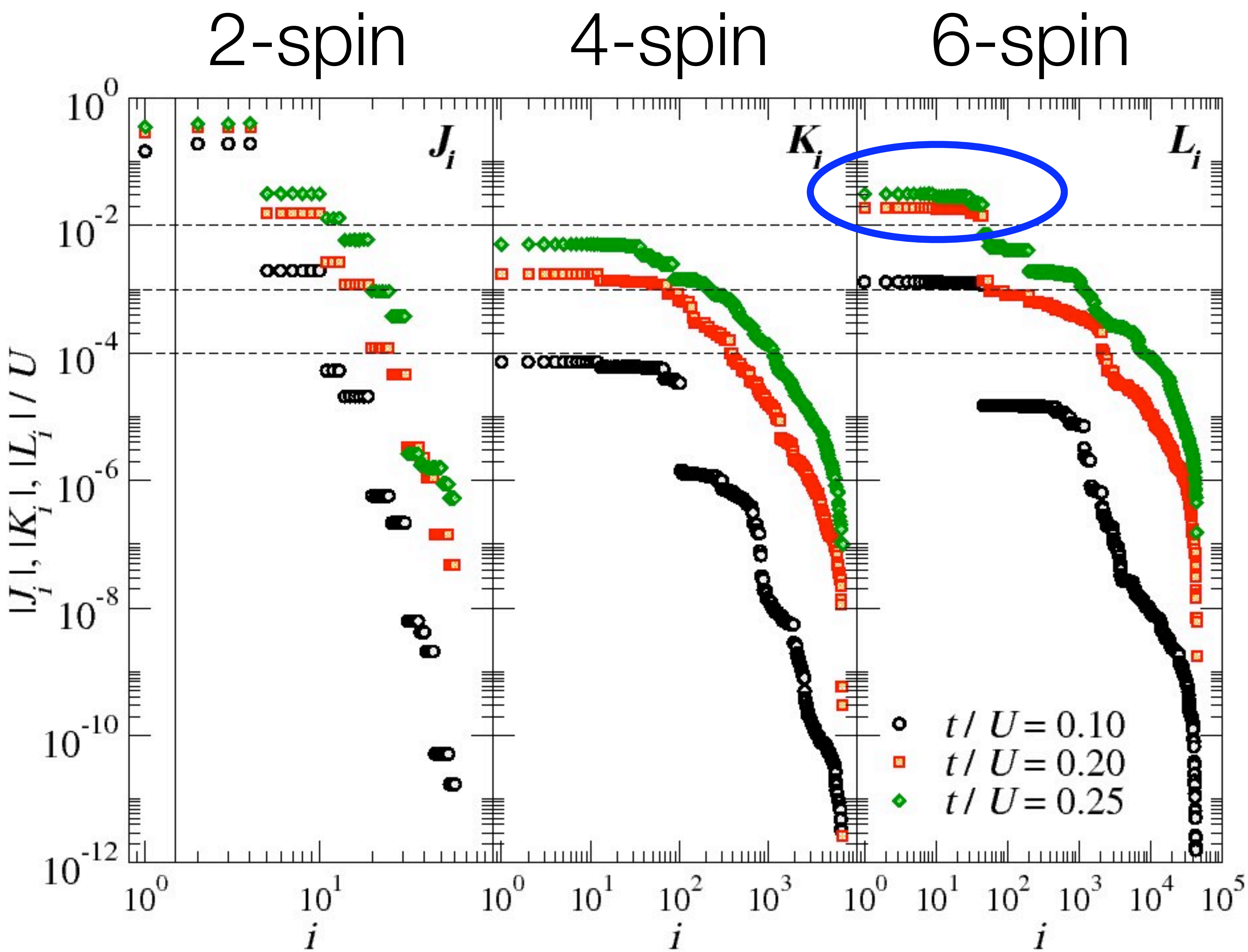


- Consider a graph expansion
- On each graph, knowledge of lowest eigenstates and energies of the Hubbard model allows to construct H_{eff}
- Use linked-cluster theorem to remove connected parts

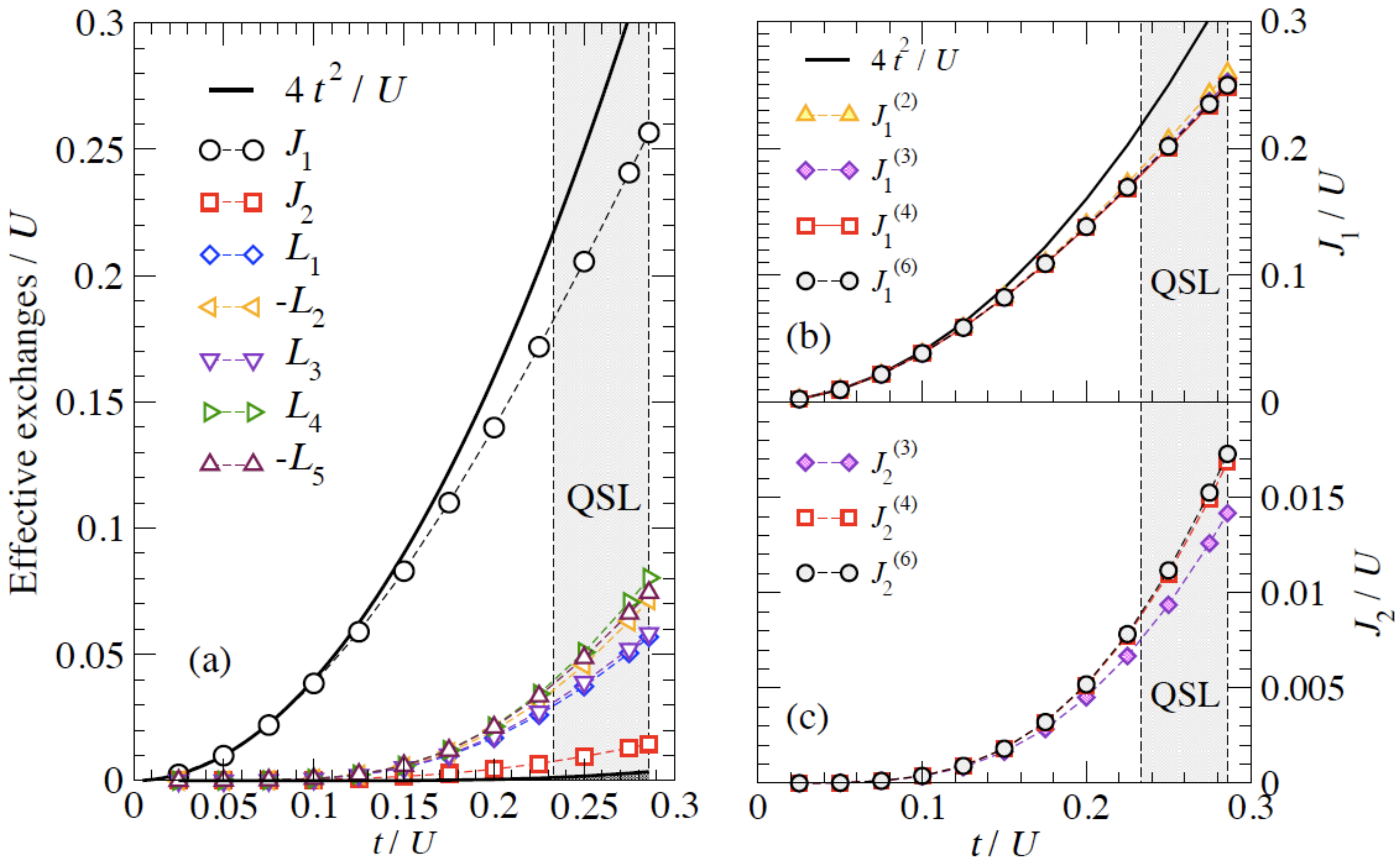
Both techniques give very similar results !

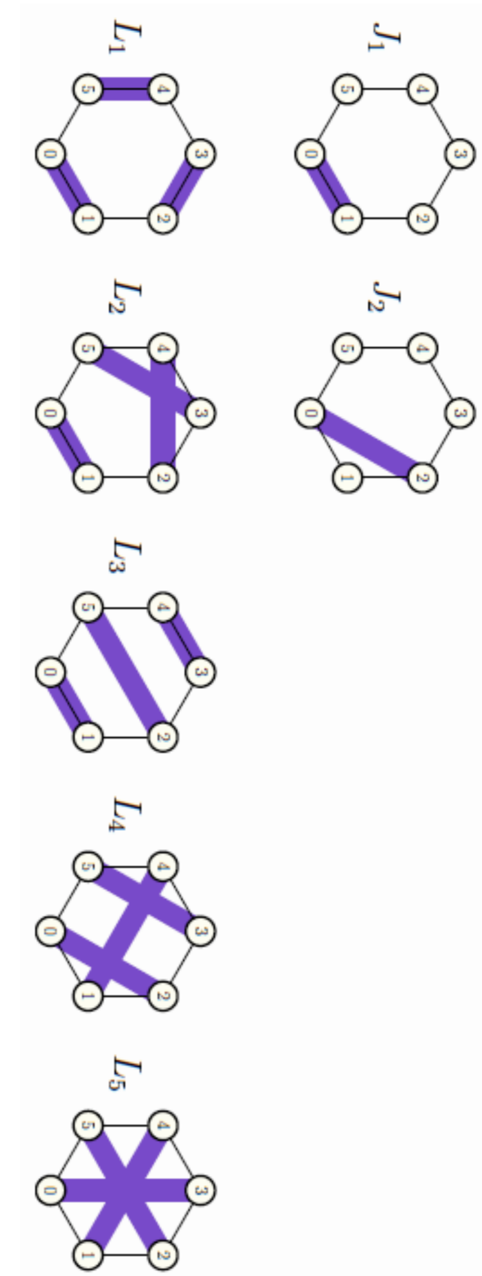
Yang et al. arXiv (2012)

gCUT results



CORE results:
Emergence of dominant multispin interactions





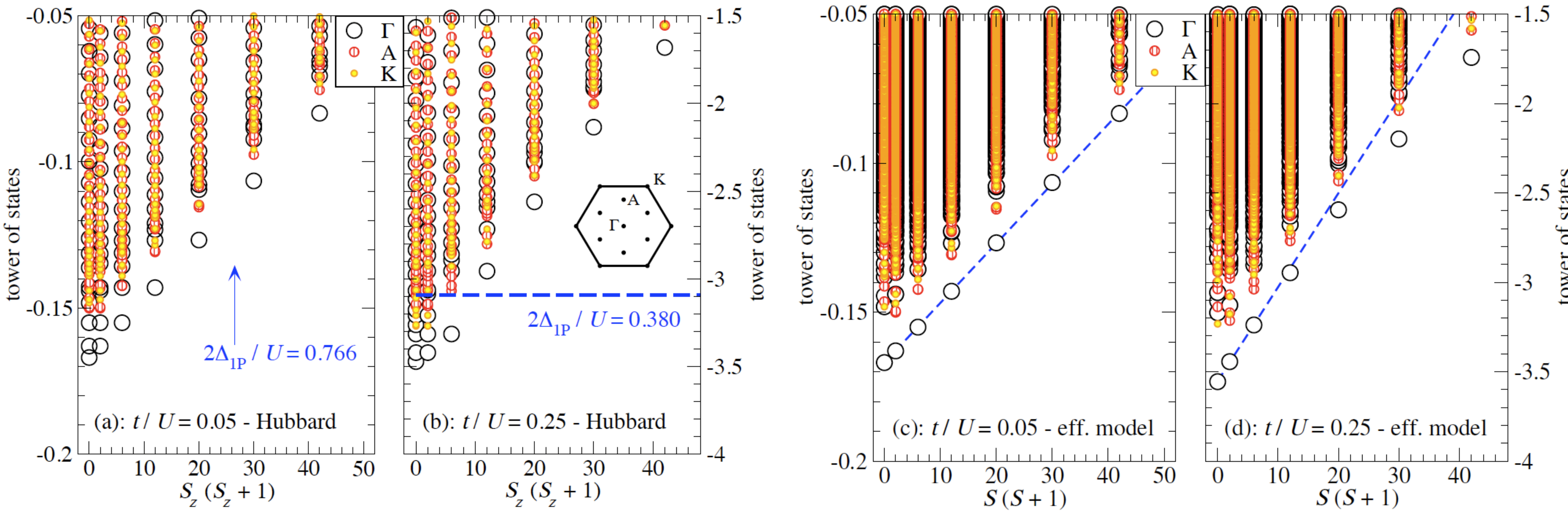
- negligible J_2
- fast convergence vs cluster expansion
- 6-spin terms are similar to permutation, but not completely since 4-spin terms are missing !?

Yang et al. arXiv (2012)

Numerical study of the “minimal” spin model

Hubbard model

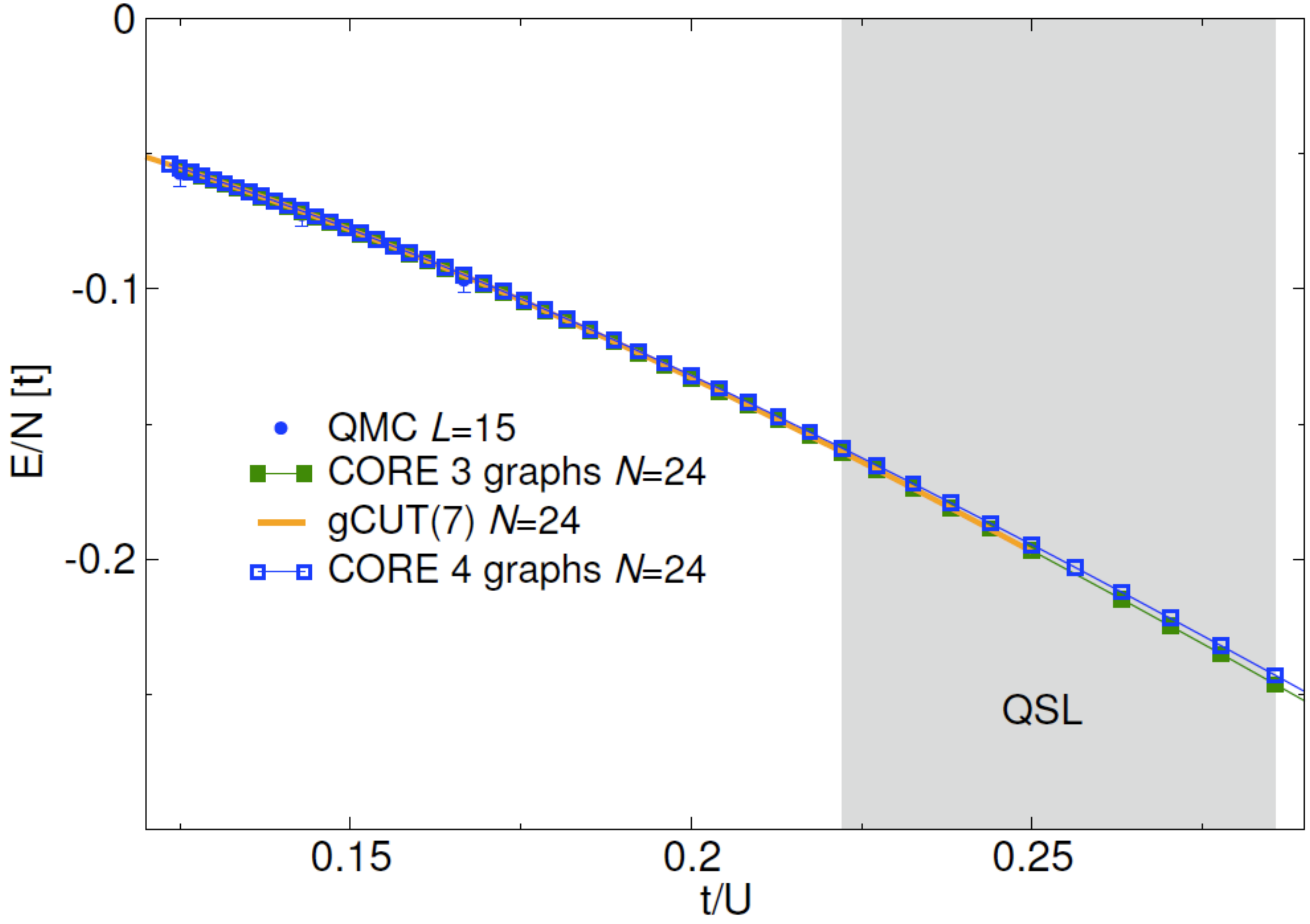
Effective spin model



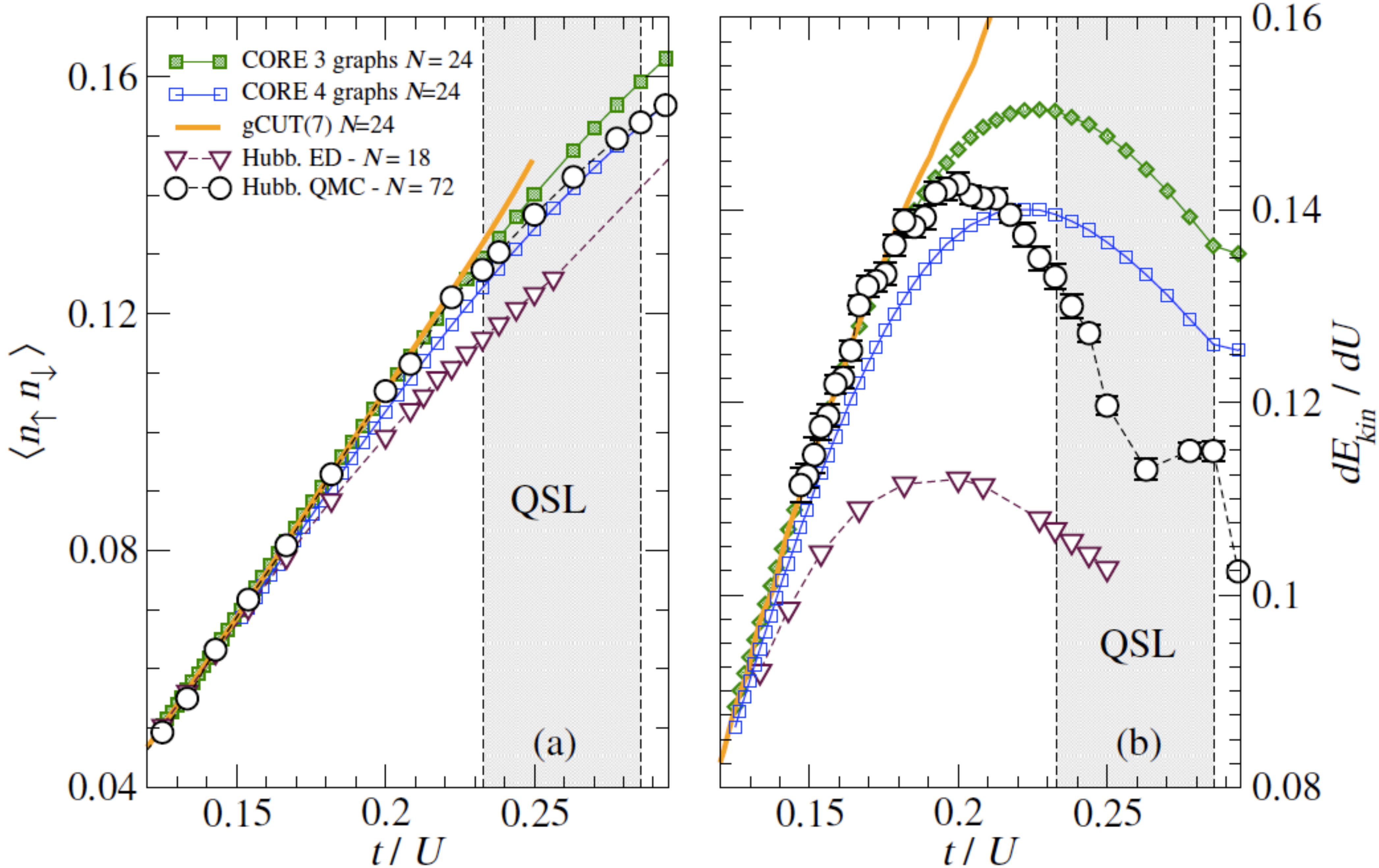
t/U=0.05: Consistent with Néel ordering

t/U=0.25: deviation from the expected S(S+1) excitations ?

Ground-state energy



Double occupancy and kinetic energy



Yang et al. arXiv (2012)

Conclusion

- Spin liquid phase is often found either with strong frustration and/or charge fluctuations ("weak" Mott insulators)
- Naive perturbation fails for the honeycomb: **J_1-J_2 is not accurate**
- Effective spin models contain **multi-spin interactions** (as found by two non-perturbative techniques), with some resemblance to permutation

Outlook

- Clearly, the large spin correlation length prevents any answer
- Maybe, one could stabilize a stronger Spin Liquid by deforming the spin model (ring exchange, XY ?) and then study it with various techniques
- No-go theorem: bipartite lattices QDM will not possess spin liquid phase

Not if one allows for longer bonds ! H. Yao and S. A. Kivelson, PRL (2012)