3rd International Workshop on Quantum Condensation (QC11), 4 - 15 July, 2011
HongKong University of Science and Technology

Spin-½ Frustrated Heisenberg J_1-J_2 Model on Square Lattice: Plaquette Renormalized Tensor Network Study

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Jul. 6, 2011

Outline

A. Introduction: open debate in this model

B. Method: Plaquette renormalized tensor network

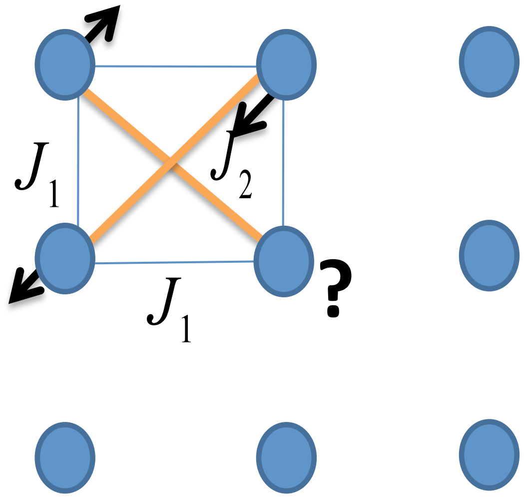
C. Results and discussions

D. Summary

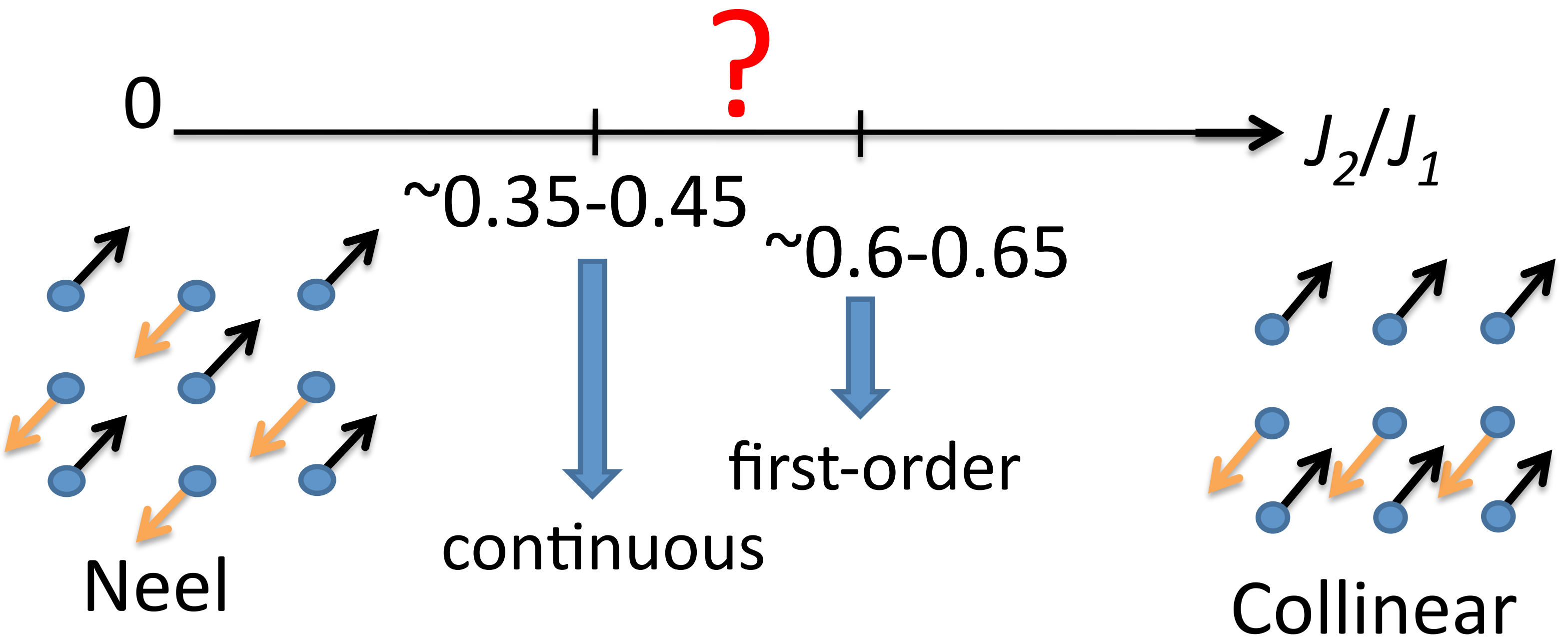
A. Introduction

1. Model Hamiltonian:

$$H = \sum_{\langle ij \rangle} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\langle\langle ij \rangle\rangle} J_2 \vec{S}_i \cdot \vec{S}_j$$



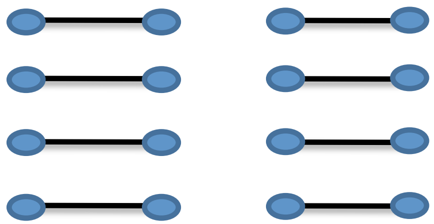
2. Phase diagram of this model on square lattice:



Questions:

a. phase order of intermediate region

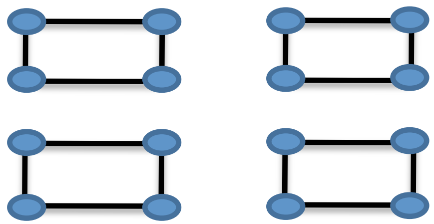
1.> column dimer



V. Murg, F. Verstraete and J. Cirac, Phys. Rev. B 79, 195119 (2009)

:projected entangled pair states (PEPS), structure factors

2.> plaquette



M. Zhitomirsky, Phys. Rev. B 54, 9007 (1996)
:ground state energy comparison

M. Mambrini, Phys. Rev. B 74, 144422 (2006)
: exact diagonalization(ED) **N=32**

b. transition points

J. Richter and J. Schulenburg, Eur. Phys. J. B 73, 117 (2010) :ED and extrapolation: ~0.35 and ~0.66

J. Reuther and P. Wolfle, Phys. Rev. B 81, 144410 (2010): ~0.40-0.45 and ~0.66-0.68

Some researches:

1.

Eur. Phys. J. B **73**, 117–124 (2010)
DOI: 10.1140/epjb/e2009-00400-4

THE EUROPEAN PHYSICAL JOURNAL B

Regular Article

The spin-1/2 J_1–J_2 Heisenberg antiferromagnet on the square lattice: Exact diagonalization for N = 40 spins

J. Richter[1,a] and J. Schulenburg[2]

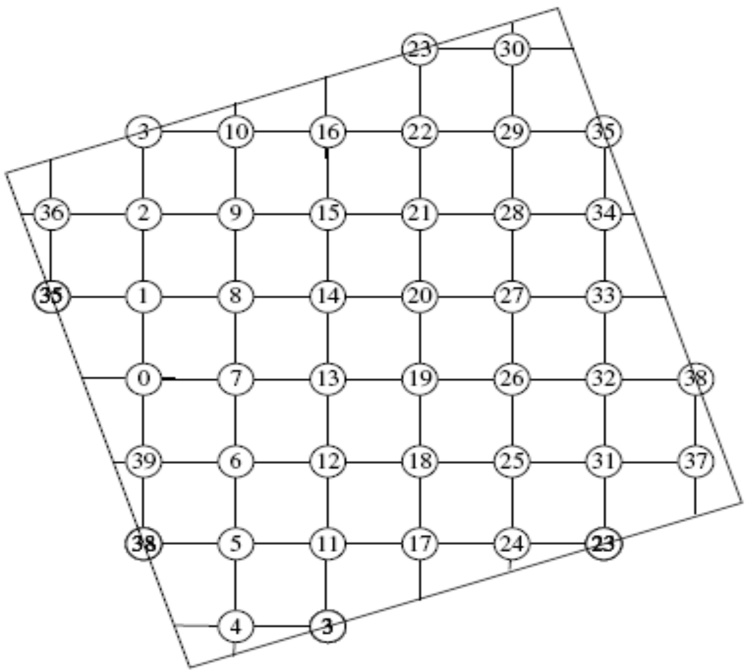
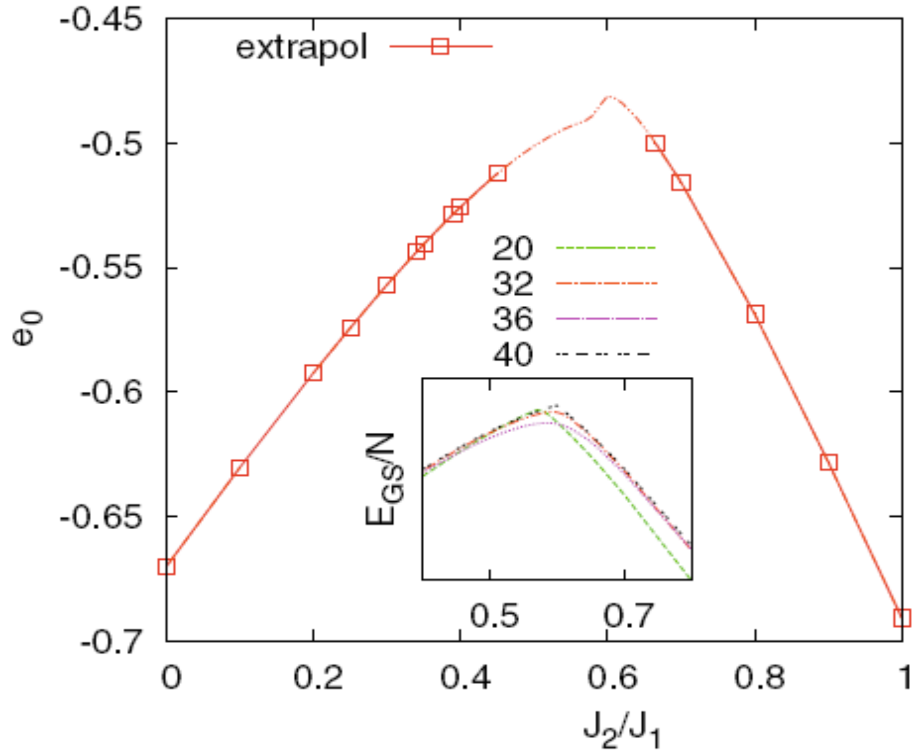


Fig. 1. The finite square lattice with $N = 40$ sites.



1.

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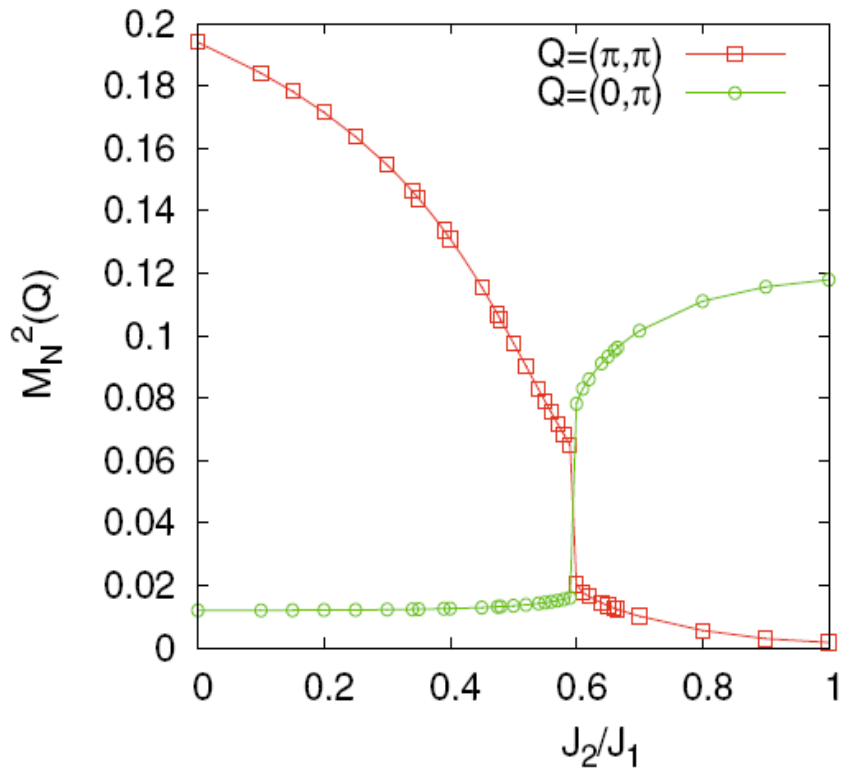
$$M^2 = \langle (\frac{1}{N}\sum_i e^{iQ\cdot R_i} s_i)^2 \rangle, \ Q = (\pi,\pi), (0,\pi)$$



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The European Physical Journal B

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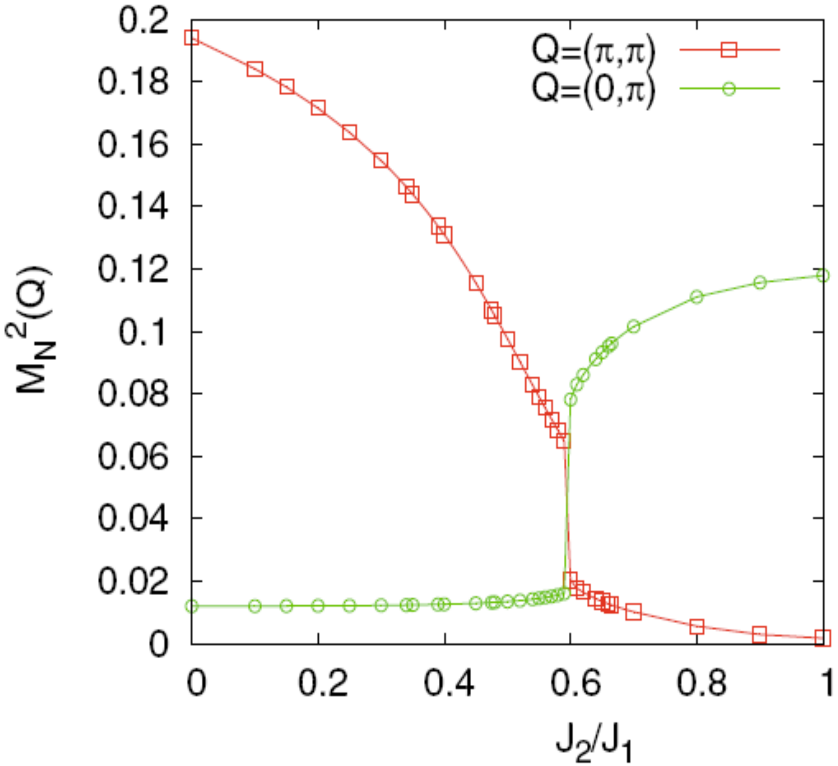
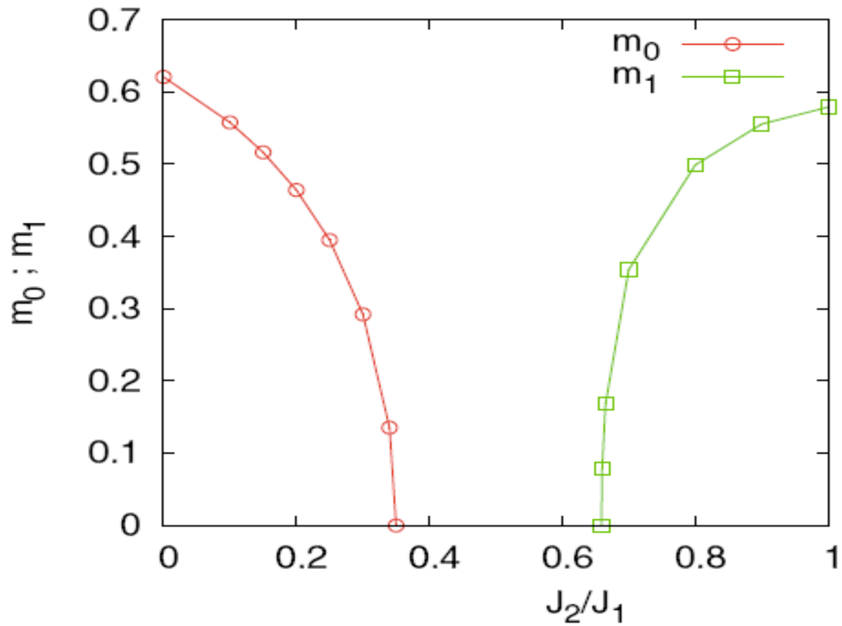


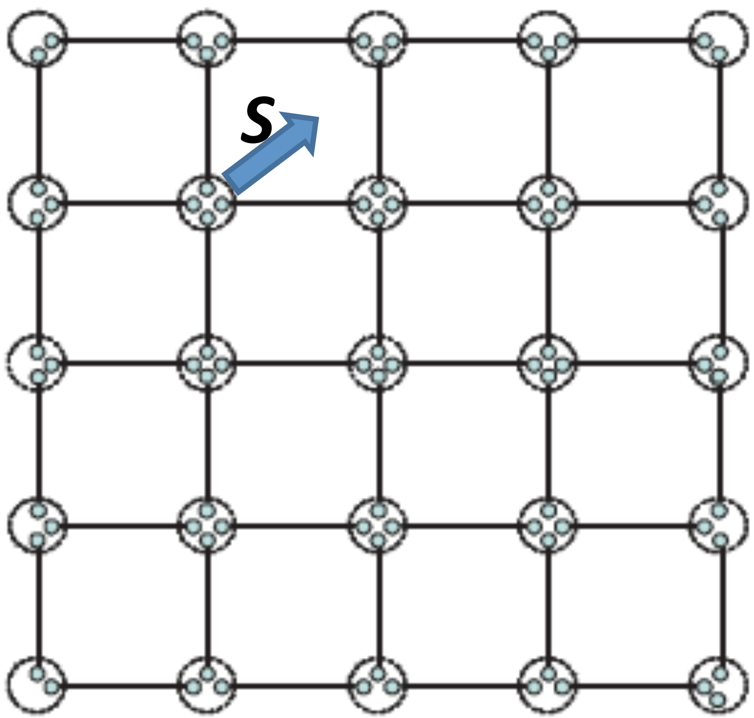


extrapolation: ~0.35 and ~0.66

PHYSICAL REVIEW B **79**, 195119 (2009)

2. **Exploring frustrated spin systems using projected entangled pair states**

V. Murg,[1] F. Verstraete,[2] and J. I. Cirac[1]



2-d PEPS, bond means entangled D-dimensional auxiliary spins, circle is the projector mapping inner auxiliary spins to physical spin.

PHYSICAL REVIEW B 79, 195119 (2009)

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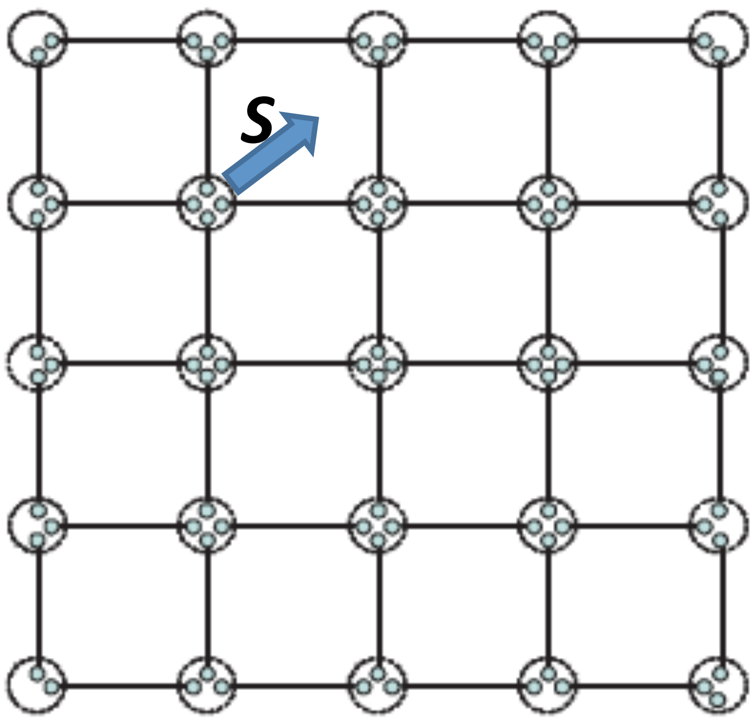

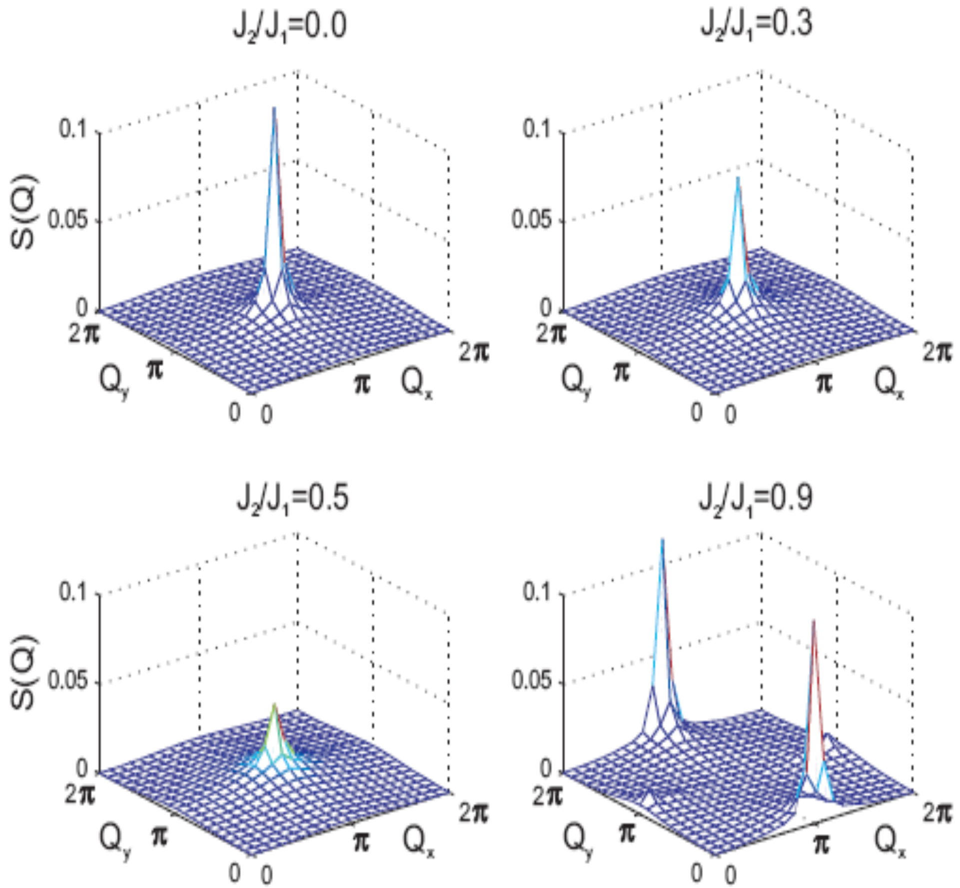

2-d PEPS, bond means entangled D-dimensional auxiliary spins, circle is the projector mapping inner auxiliary spins to physical spin.

D=3

PHYSICAL REVIEW B 79, 195119 (2009)

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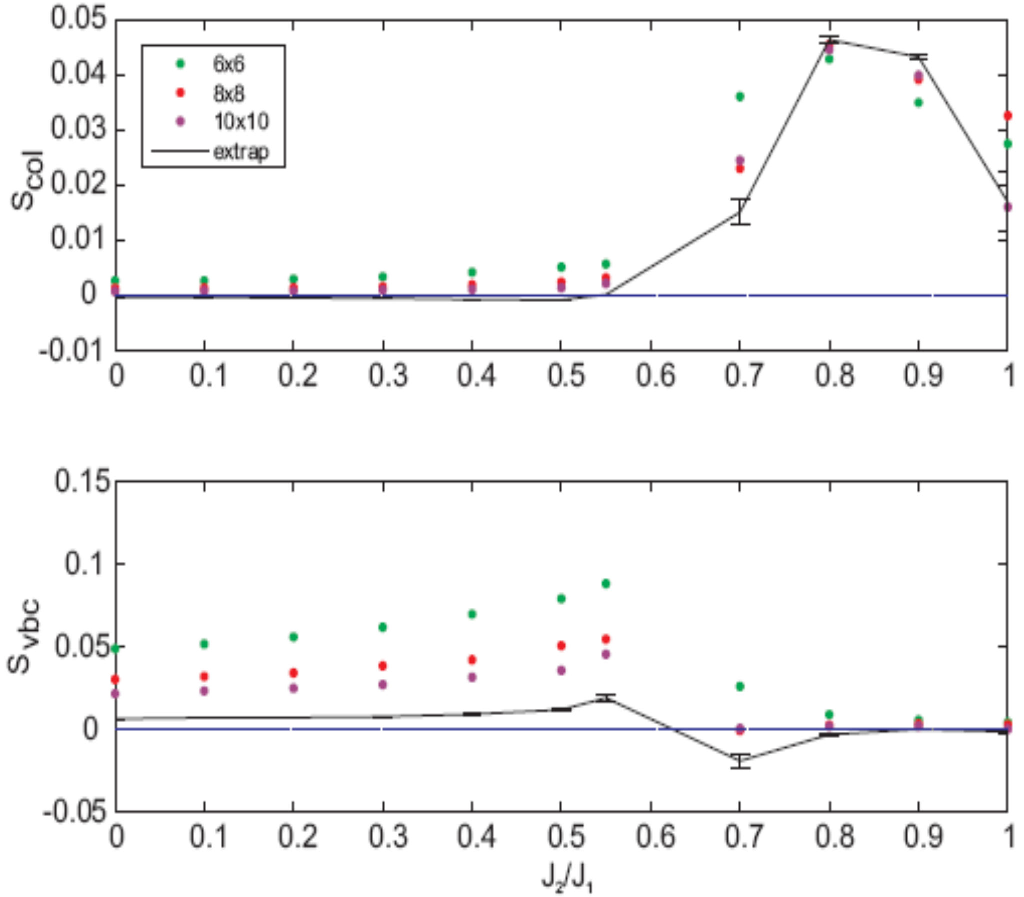
V. Murg,[1] F. Verstraete,[2] and J. I. Cirac[1]

$$S_\lambda = \frac{1}{N_B}\sum_{(k,l)} \varepsilon_\lambda(k,l)\left(\langle(\mathbf{s}_i\cdot\mathbf{s}_j)(\mathbf{s}_k\cdot\mathbf{s}_l)\rangle - \langle(\mathbf{s}_i\cdot\mathbf{s}_j)\rangle^2\right)$$



Plaquette: S(vbc) finite, S(col) 0

dimer: both finite

PHYSICAL REVIEW B 79, 195119 (2009)

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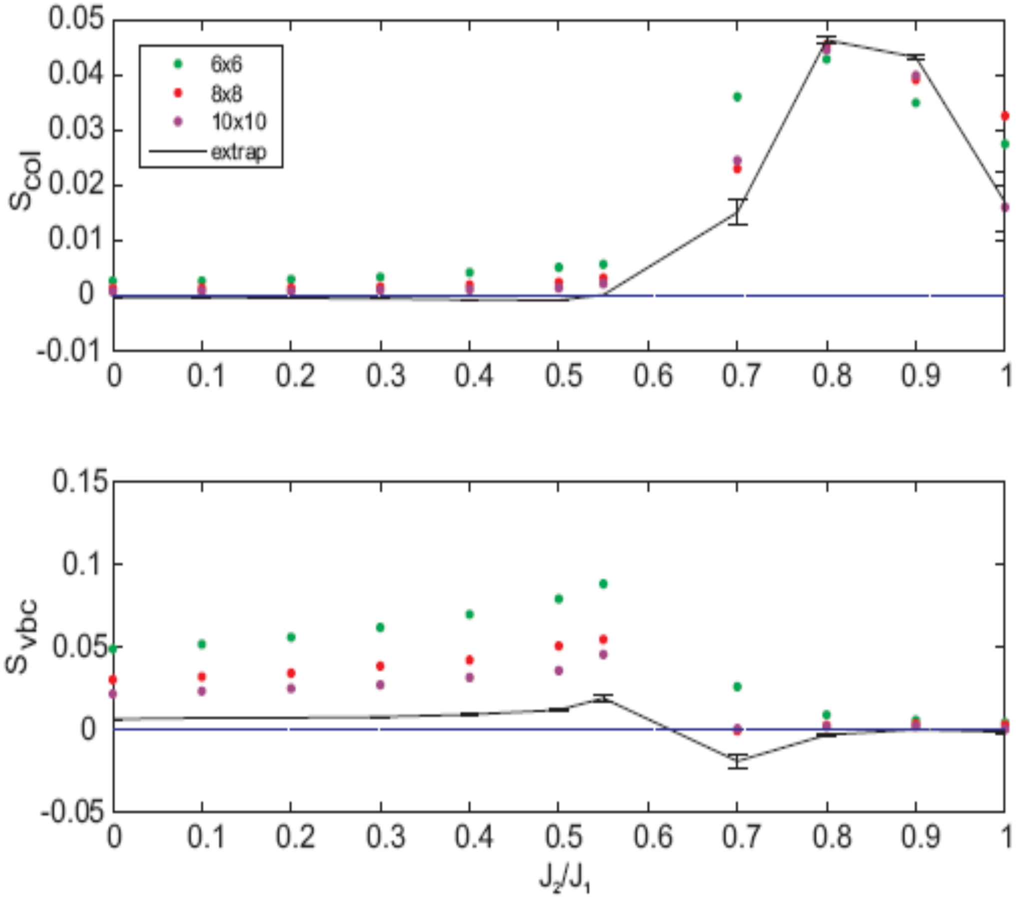
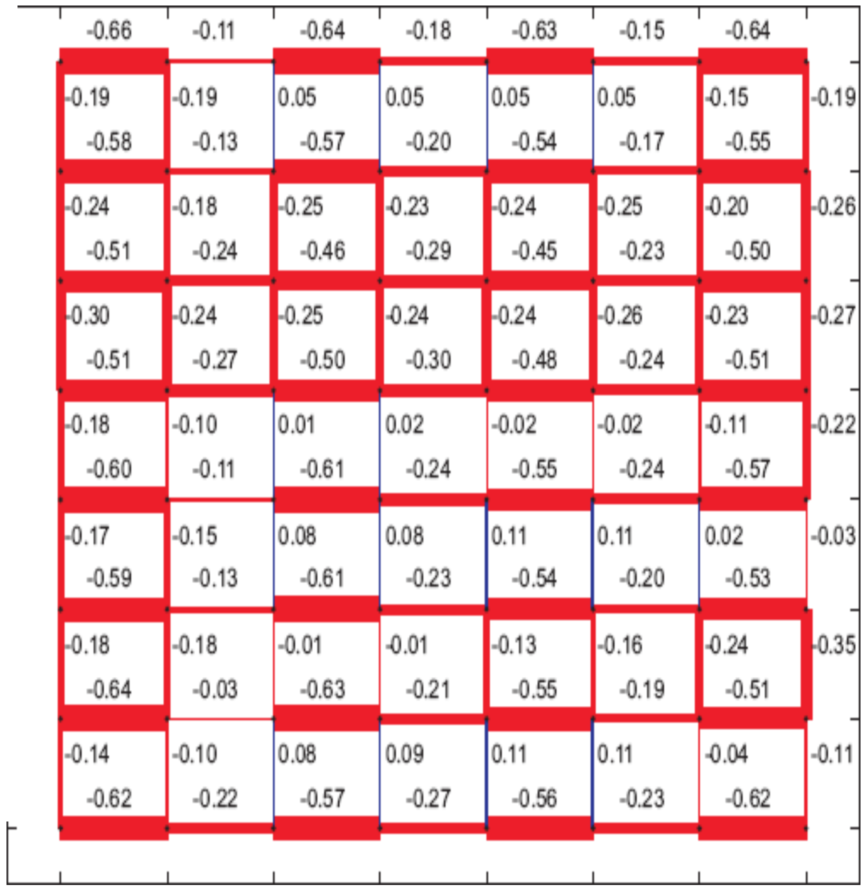


D=3,nearest spin-spin correlation at J2/J1=0.6



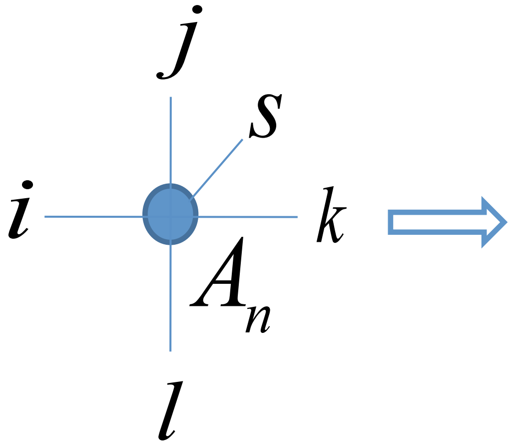
Plaquette: S(vbc) finite, S(col) 0

dimer: both finite

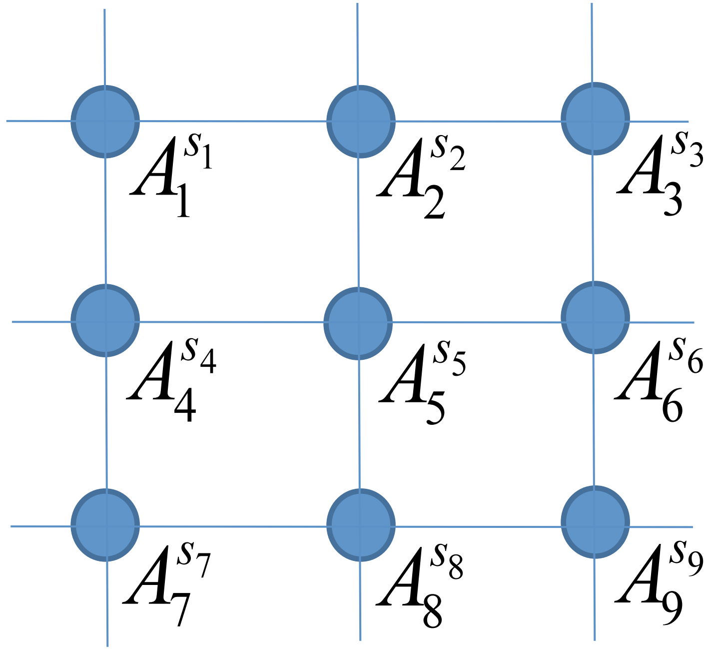
B. Method:
tensor network state (TNS)

Wave function interpretation: satisfying entropy area-law

2-d: Tensor network state (TNS)



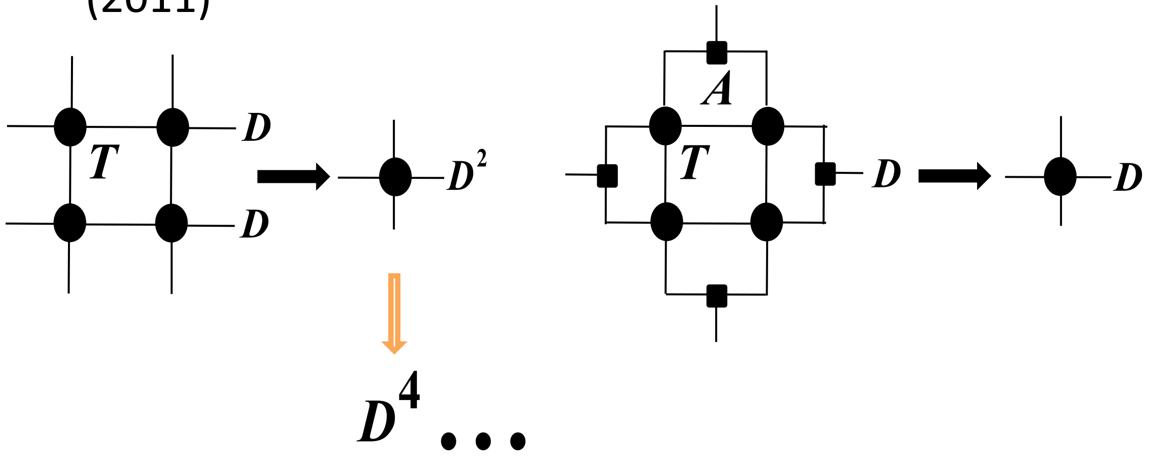
$$\left(A_n^{s_n}\right)_{ijkl}$$

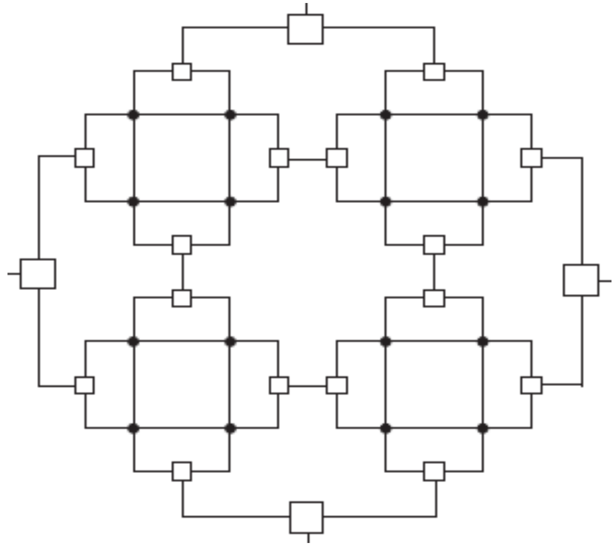


$$\left|\Phi\right\rangle = \sum_{\{s\}\{i\}} \left(A^{s_1}\right)_{i_1 i_2 i_3 i_4} \left(A^{s_2}\right)_{i_3 i_5 i_6 i_7} \cdots \left|s_1 s_2 \cdots\right\rangle$$

Plaquette renormalization

L. Wang, Y.-J. Kao and A. Sandvik, Phys. Rev. E 83, 056703 (2011)





$$|\Phi\rangle = \sum_{\{s\}} tTr(T_1^{s_1} \otimes T_2^{s_2} \otimes A_1 \cdots)|s_1 s_2 \cdots\rangle$$

Advantages: keep bond dimension (*D*) constant, small

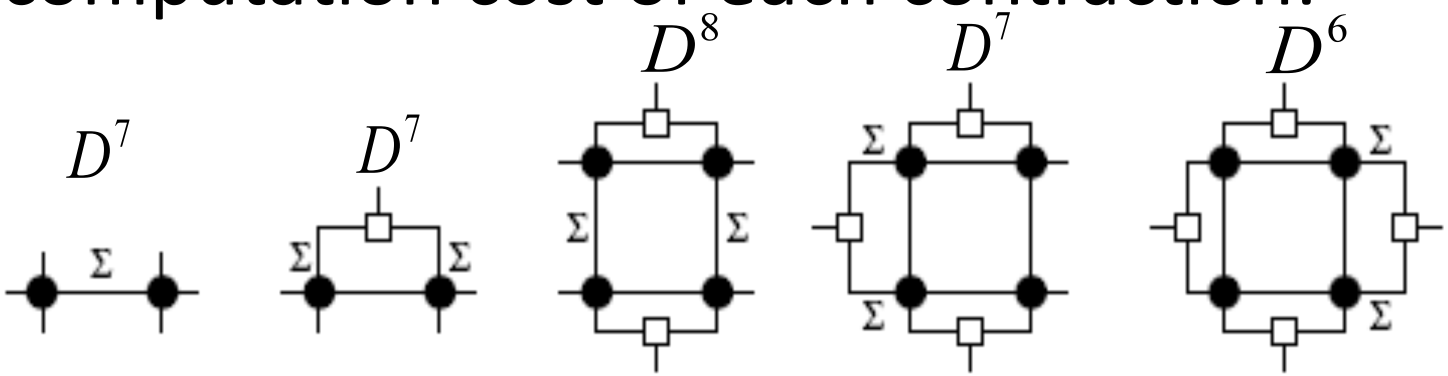
Disadvantages: entanglement (violates area-law)

Task: Determine the tensors ***T***s and ***A***s.

$$\left|\Phi_g\right\rangle = \sum_{\{s\}} tTr(T_1^{s_1} \otimes T_2^{s_2} \otimes A_1 \cdots)\left|s_1 s_2 \cdots\right\rangle$$

Method: variational, ground state energy

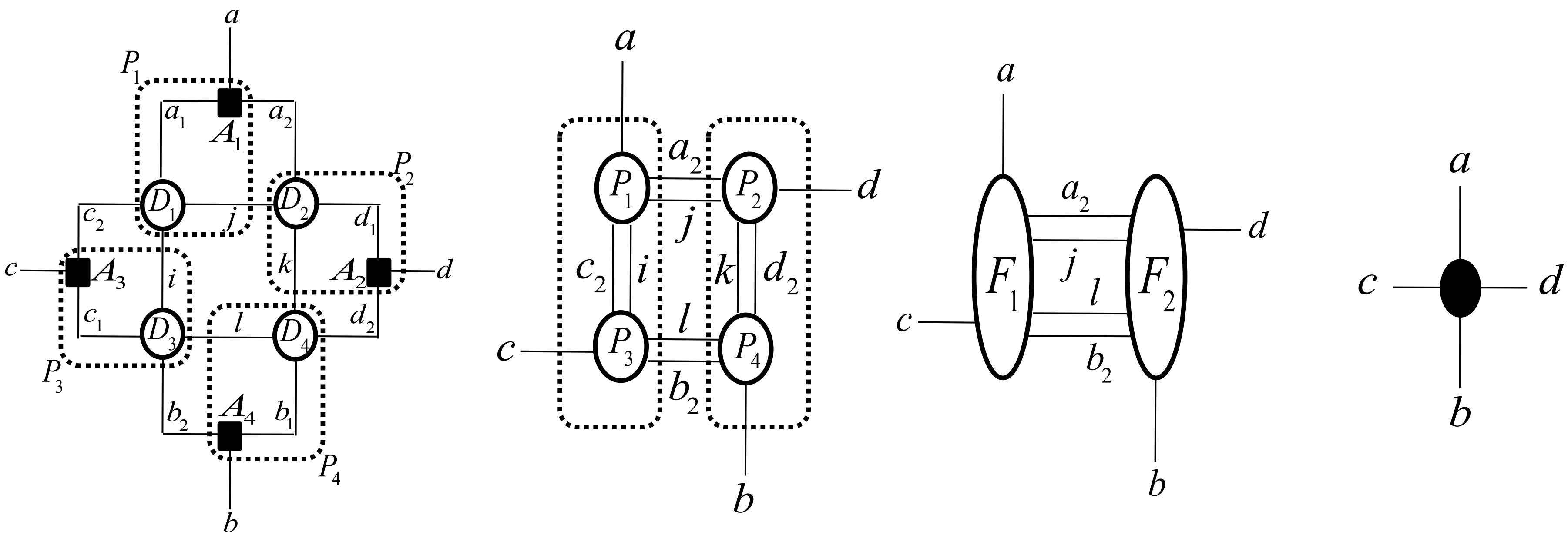
computation cost of each contraction:



L. Wang *et al.*, Phys. Rev. E 83, 056703 (2011)

Graphic processing unit (GPU) is needed for this.

contraction steps

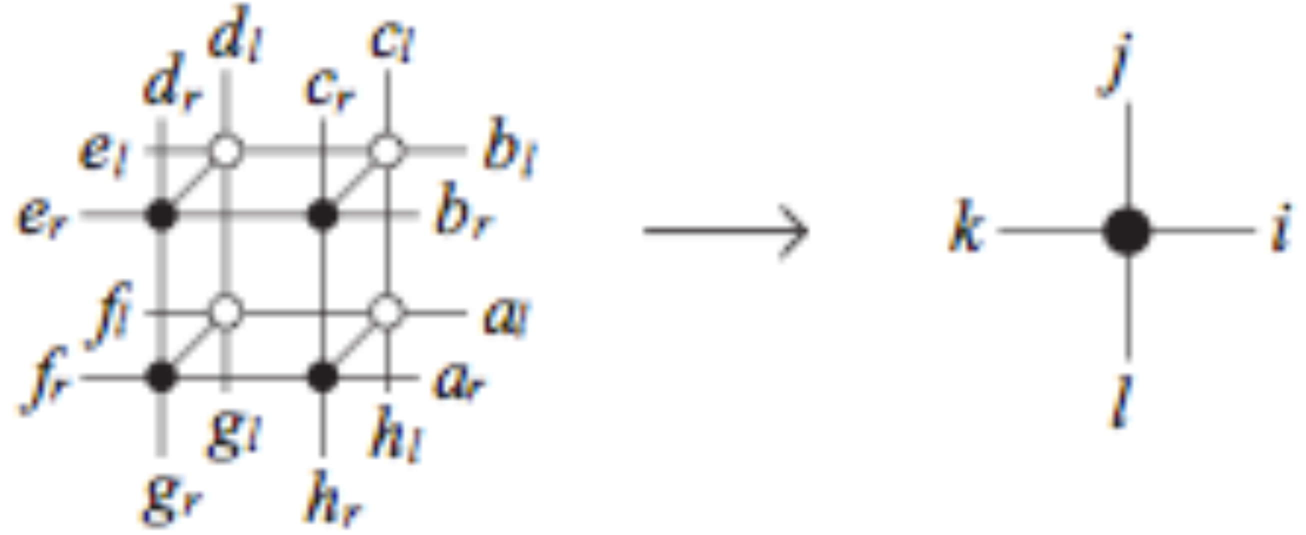


(1) (2) (3) (4)

maximal cost: D^7

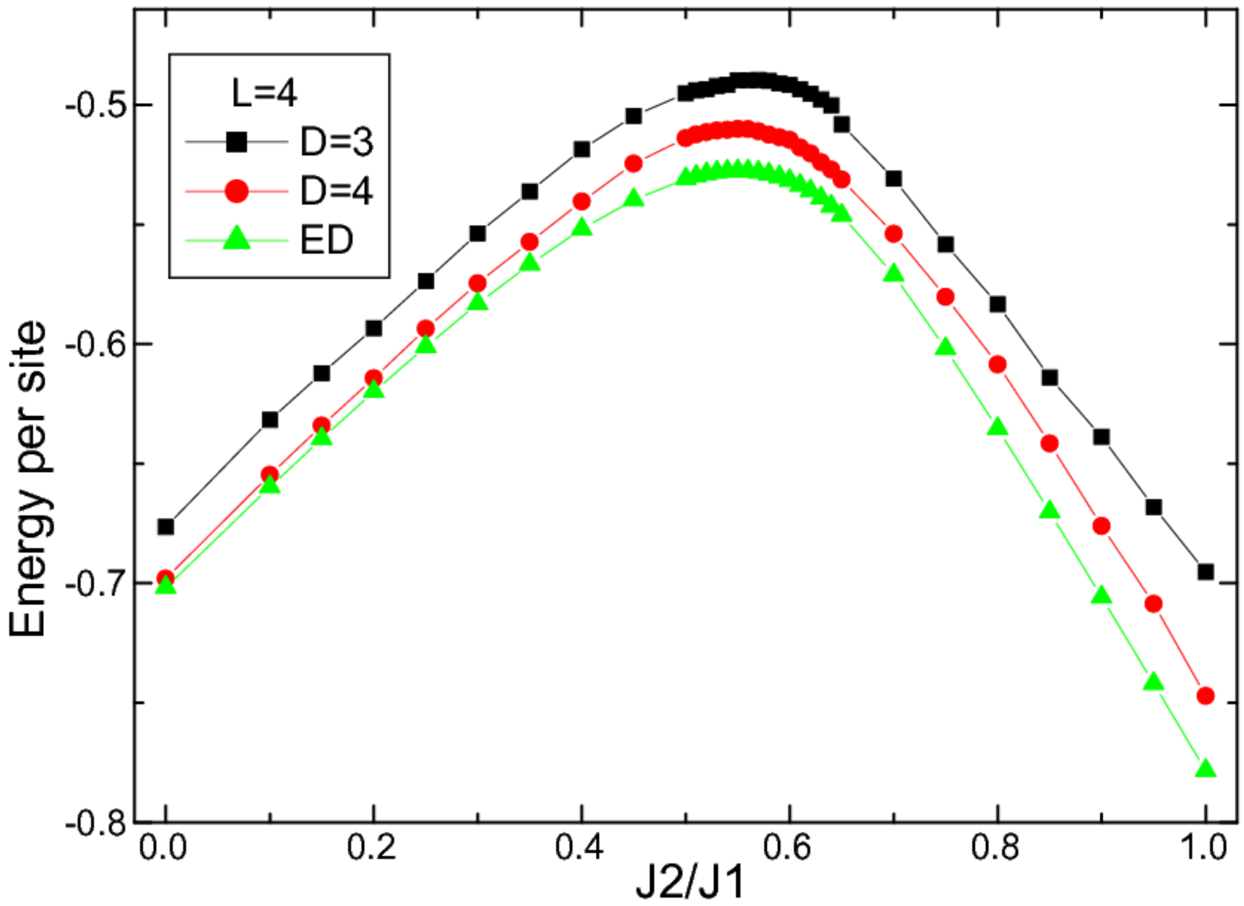
Norm or observables

$$D^{s}_{abcd} = \sum_{\sigma_s} T^{s*}_{ijkl}(\sigma_s) \otimes T^{s}_{mnop}(\sigma_s),$$



C. Results and discussions

ground state energy VS. J2/J1

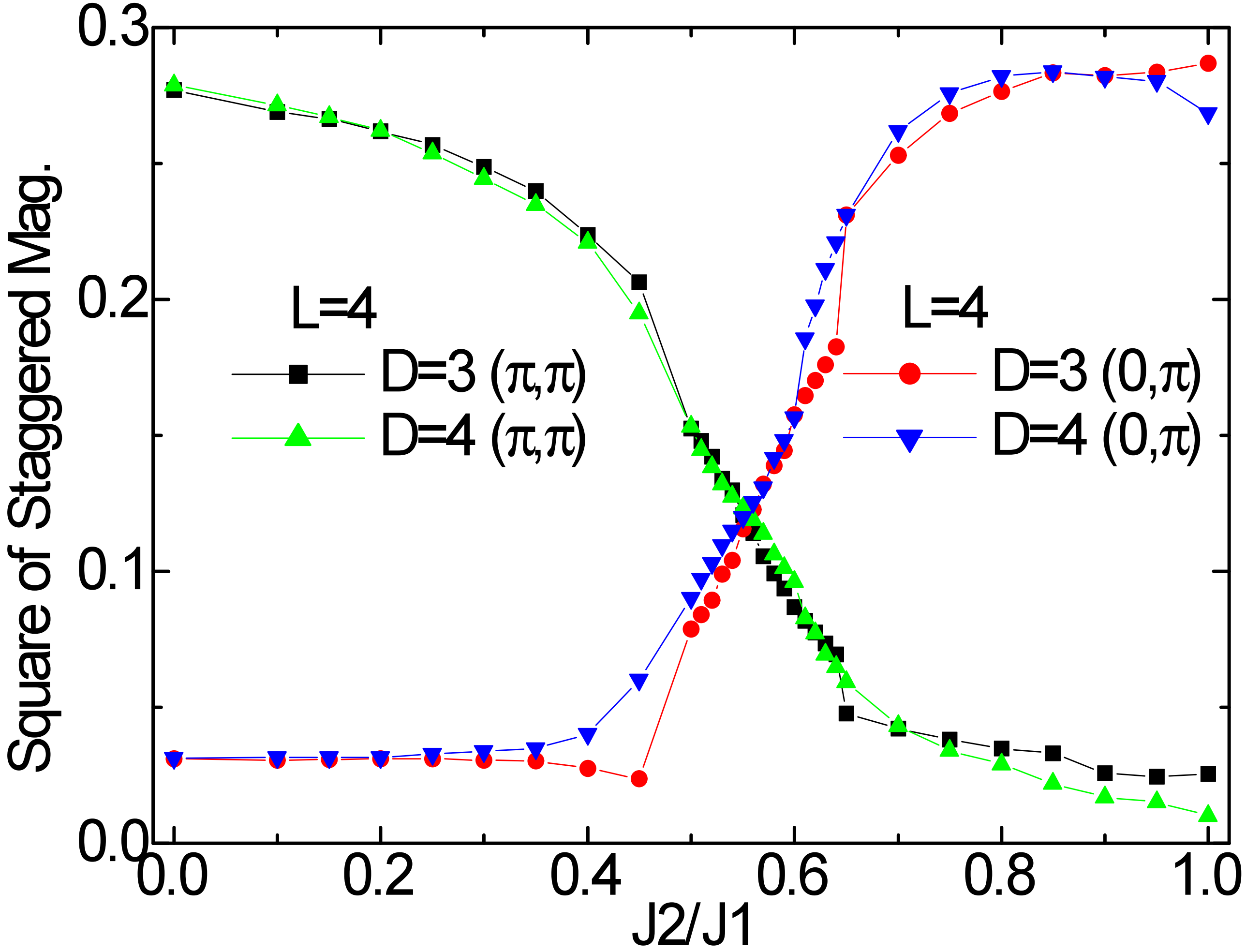


One transition point: ~0.55-0.6

J2/J1=0, Error: ~0.5%

ED: -0.701781, D=4: -0.69808

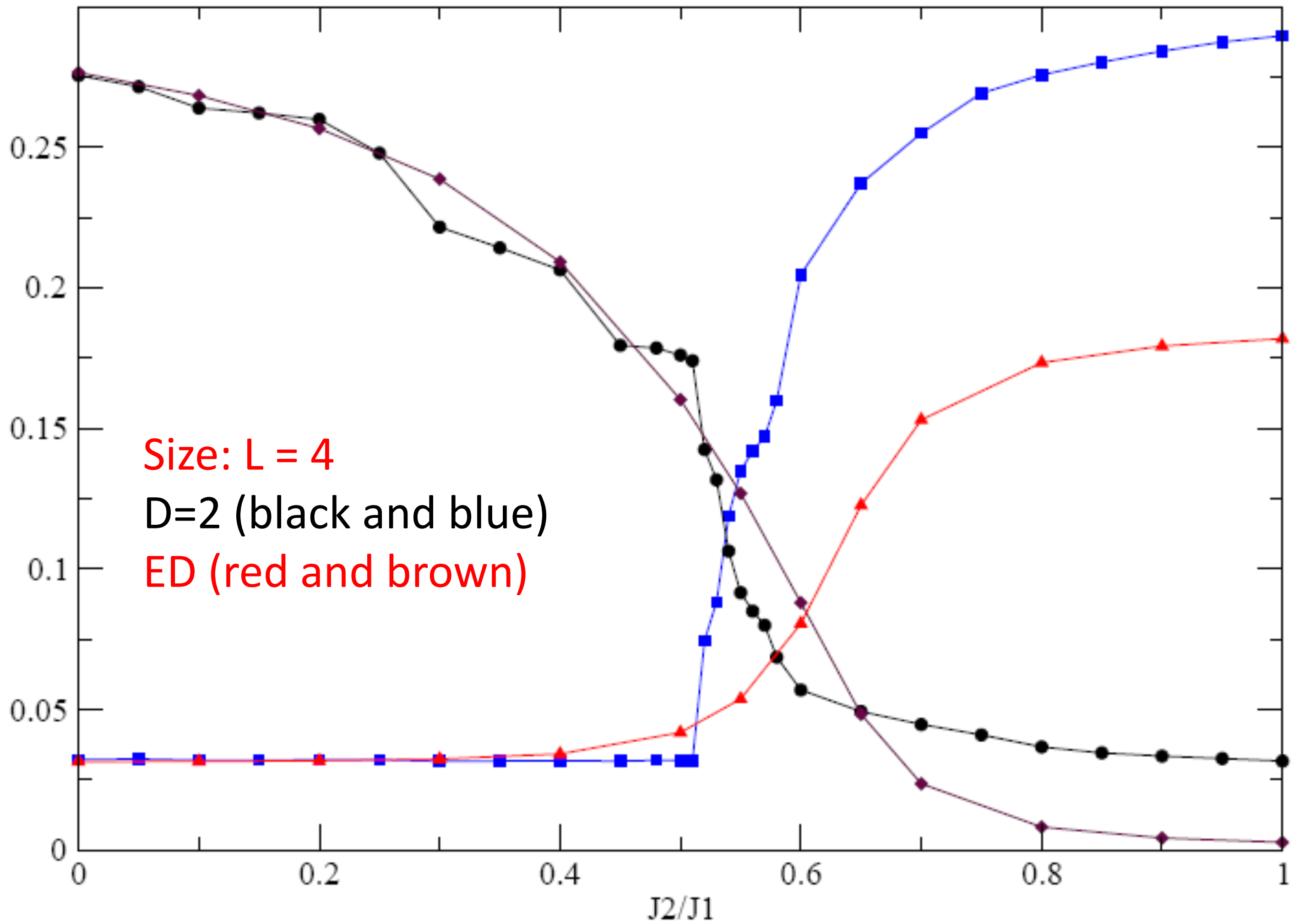
Magnetization square VS. J2/J1



One transition point: ~0.55, continuous

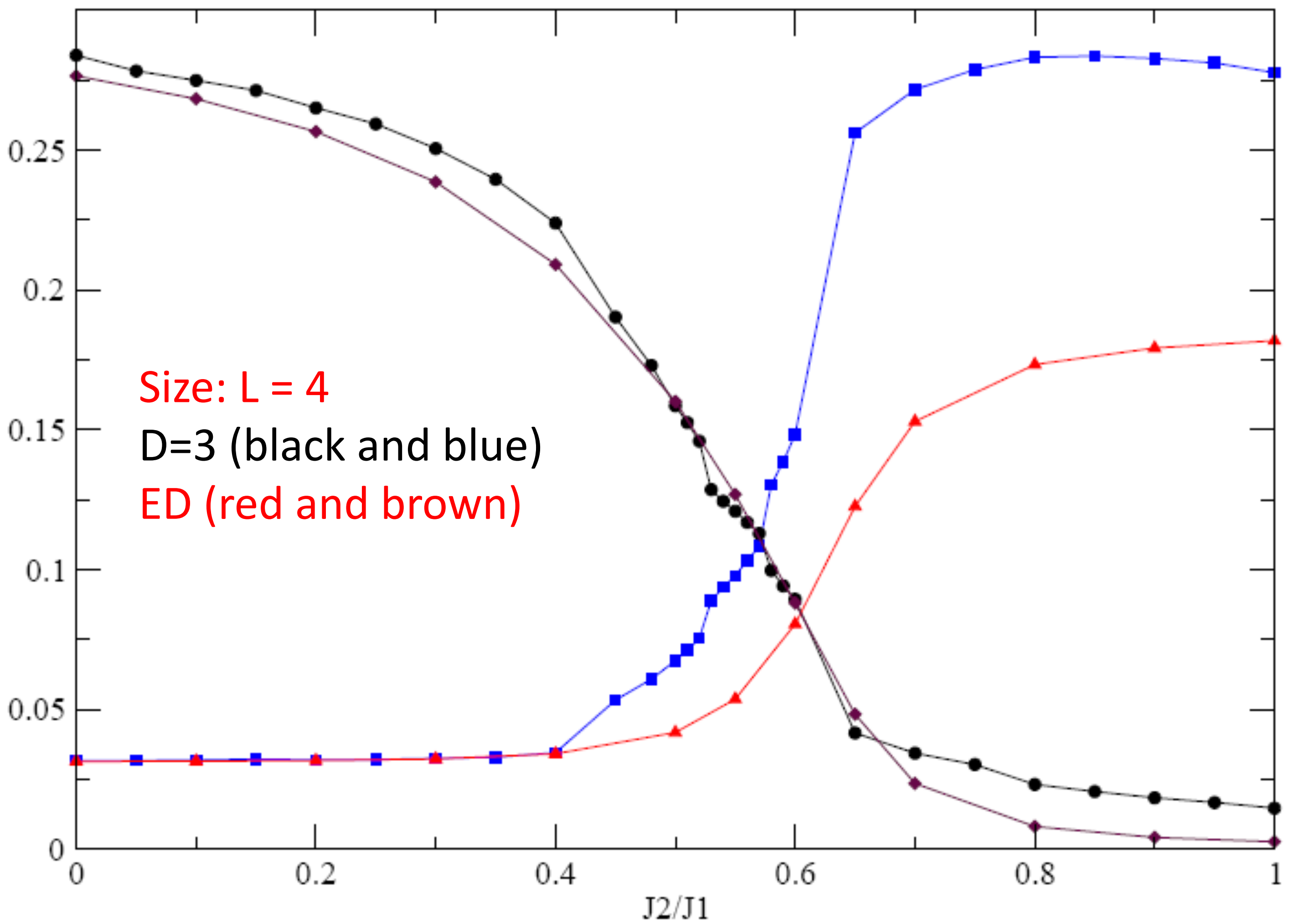
$$M^2 = \langle (\frac{1}{N}\sum_i e^{iQ\cdot R_i} s_i)^2 \rangle,\ Q = (\pi,\pi),(0,\pi)$$

Magnetization square VS. J2/J1



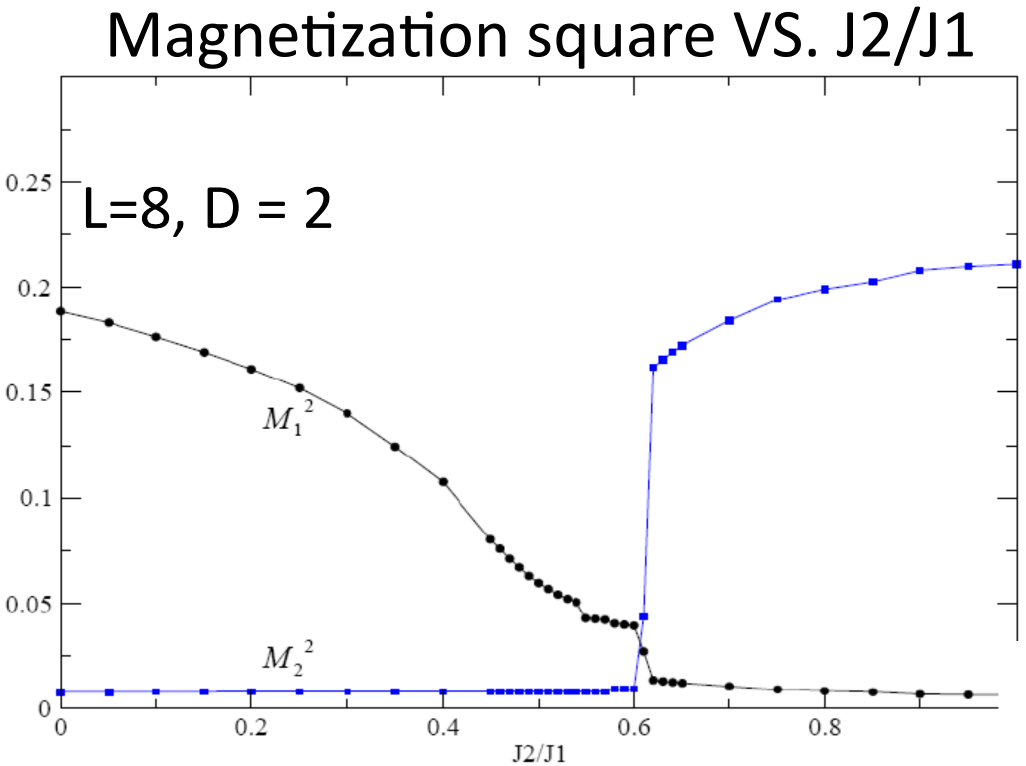
Mr. Hsiao's thesis

Magnetization square VS. J2/J1



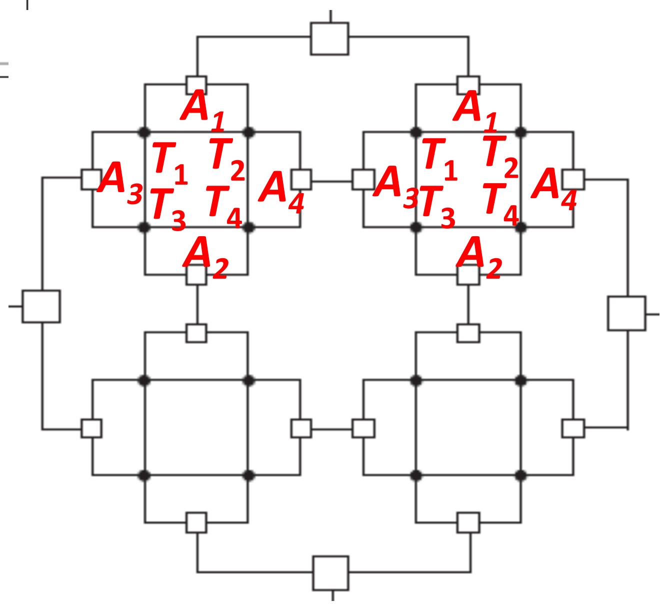
Mr. Hsiao's thesis

Increase system size: L = 8



Two transition points:

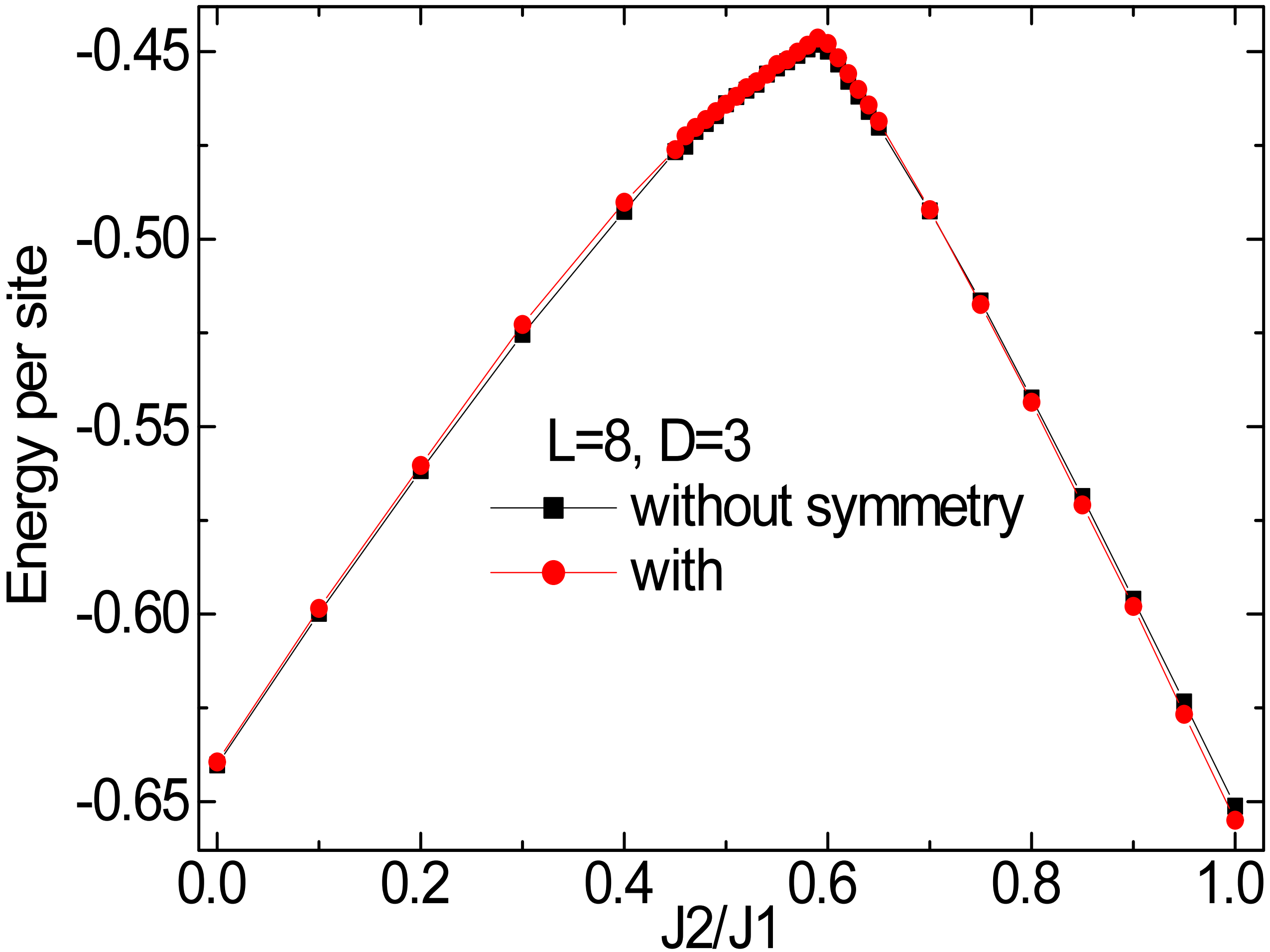
1. ~0.60, first-order
2. unclear, continuous



Increase bond dimension: D = 3

Symmetry applied: one quarter, for big number of parameters

ground state energy VS. J2/J1

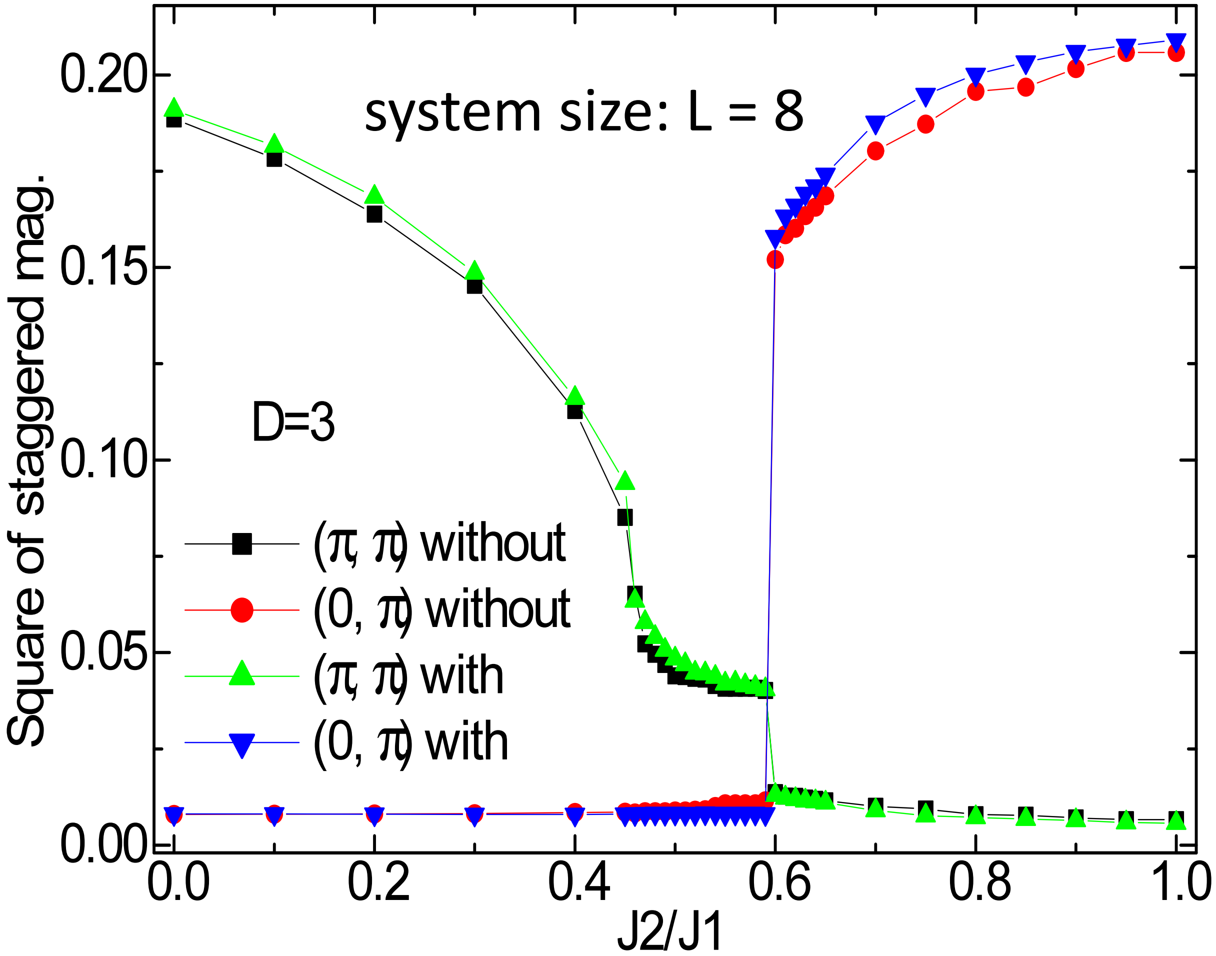


Transition points:

~0.45 continuous

~0.60 First-order

Magnetization square VS. J2/J1

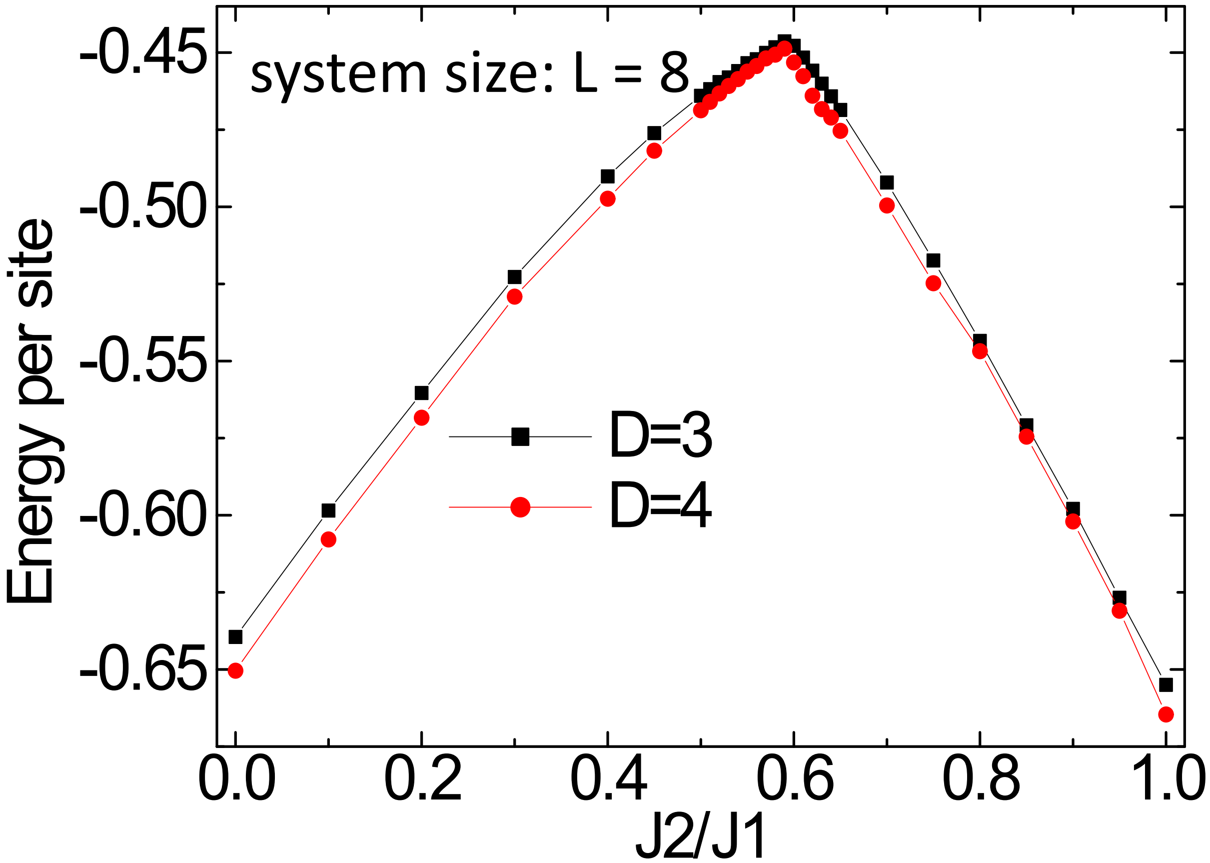


Transition points:

~0.45 continuous

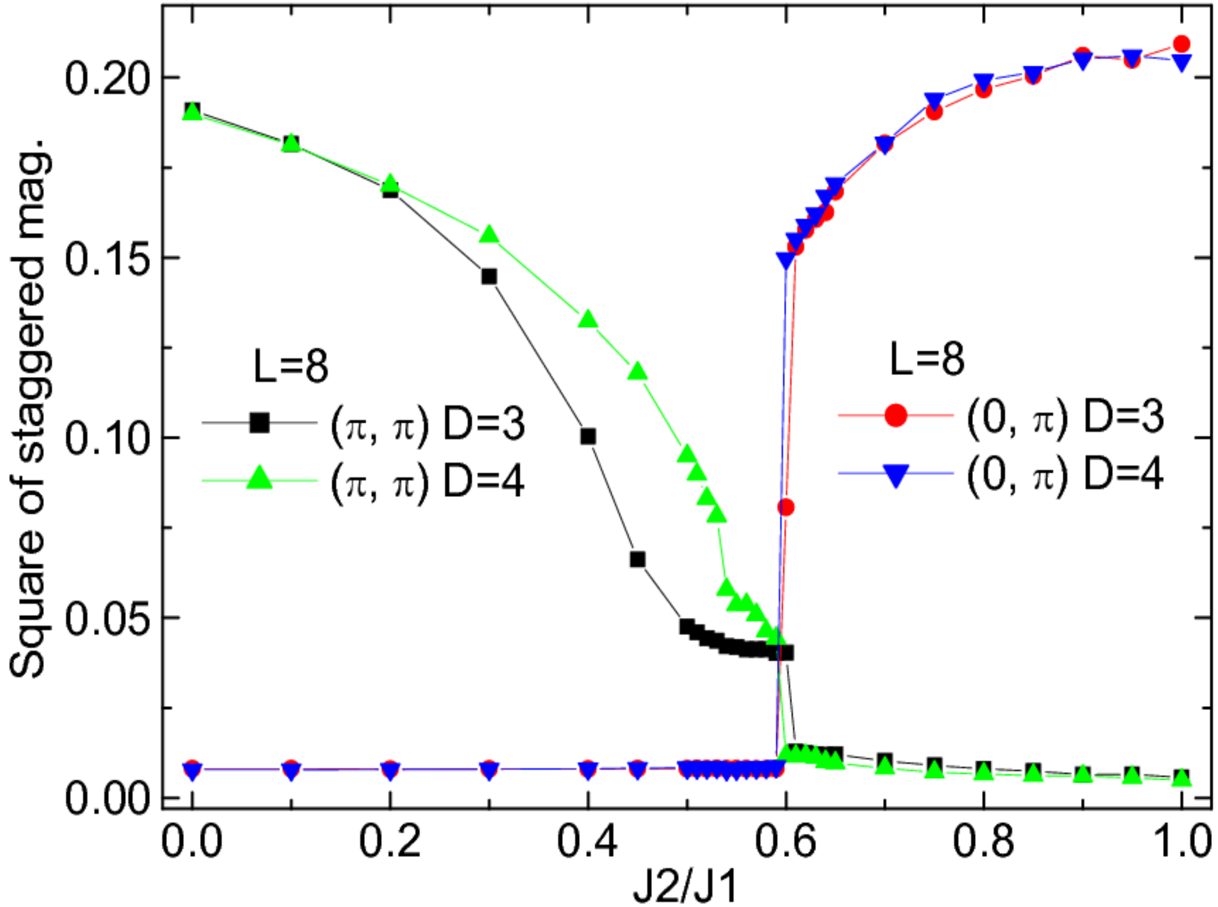
~0.60 First-order

ground state energy VS. J2/J1



Transition points: ~0.60

Magnetization square VS. J2/J1



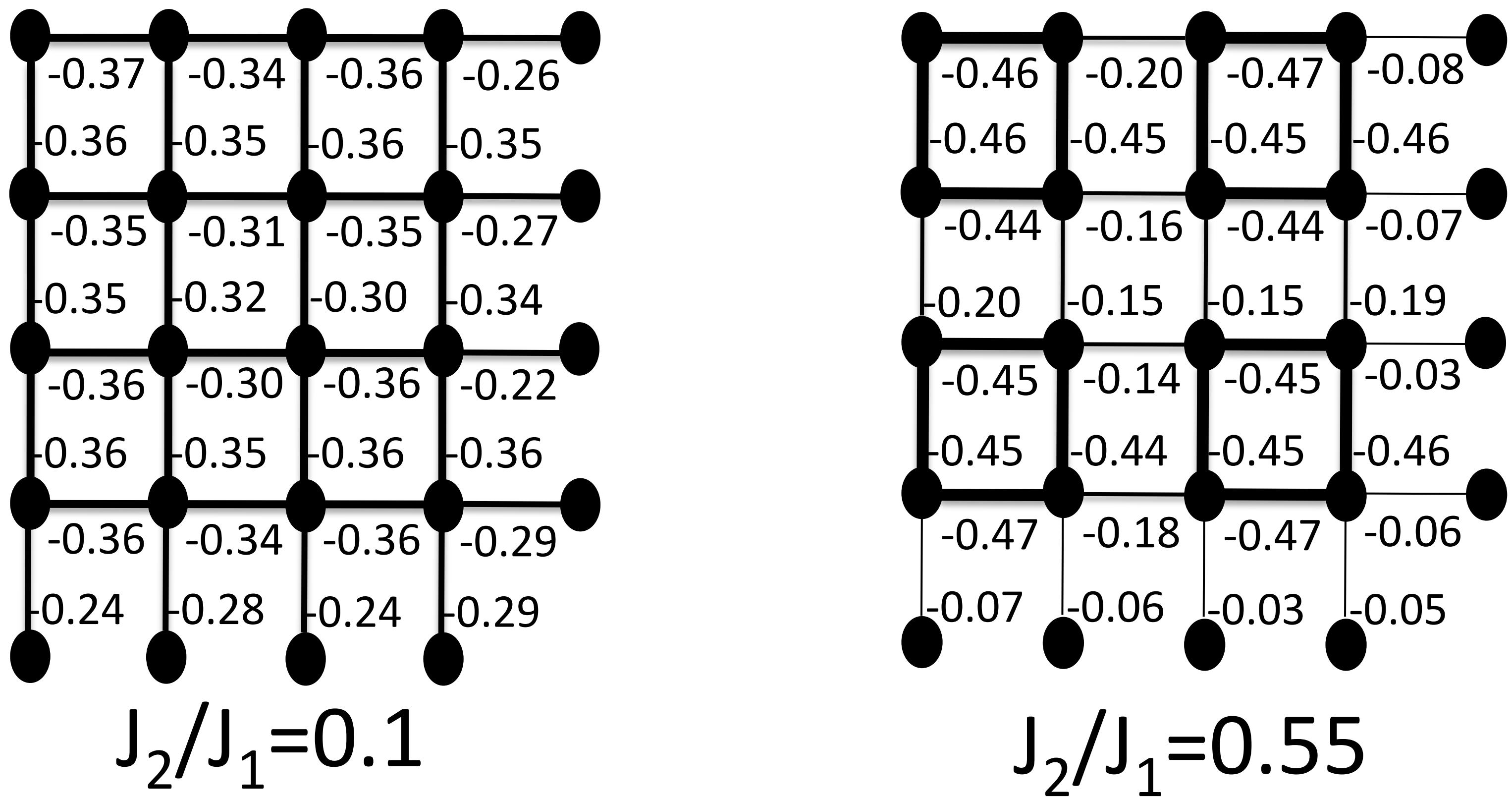
Transition points:

~0.53

~0.60

Other correlation functions

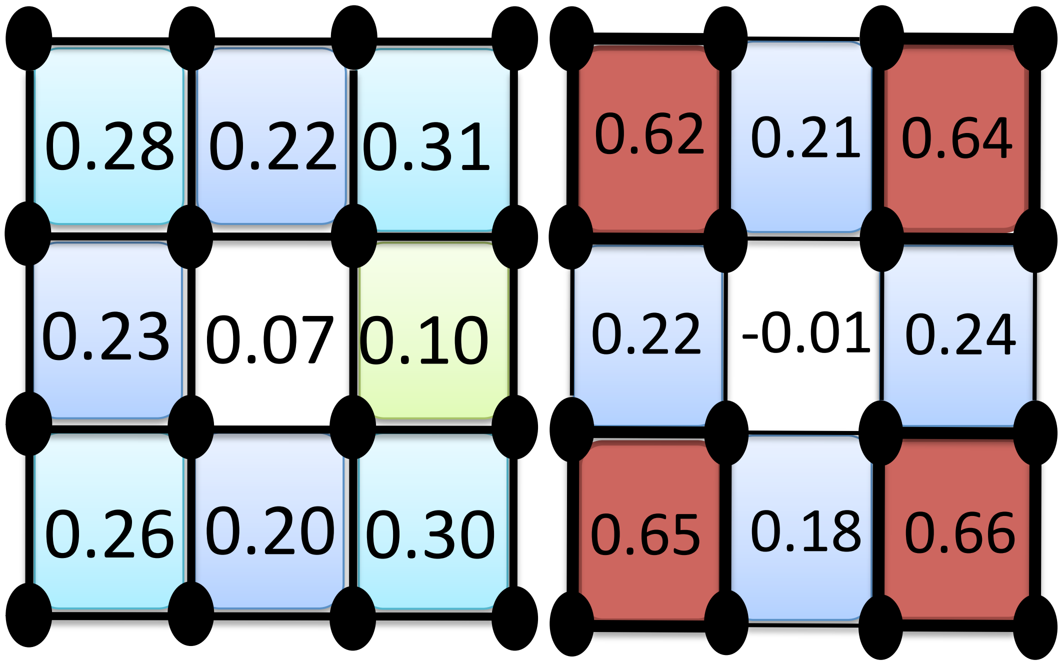
Nearest spin-spin correlation: $\left\langle \vec{S_i} \cdot \vec{S_j} \right\rangle$



system size: L = 8, D=4

Other correlation functions

Plaquette order parameter



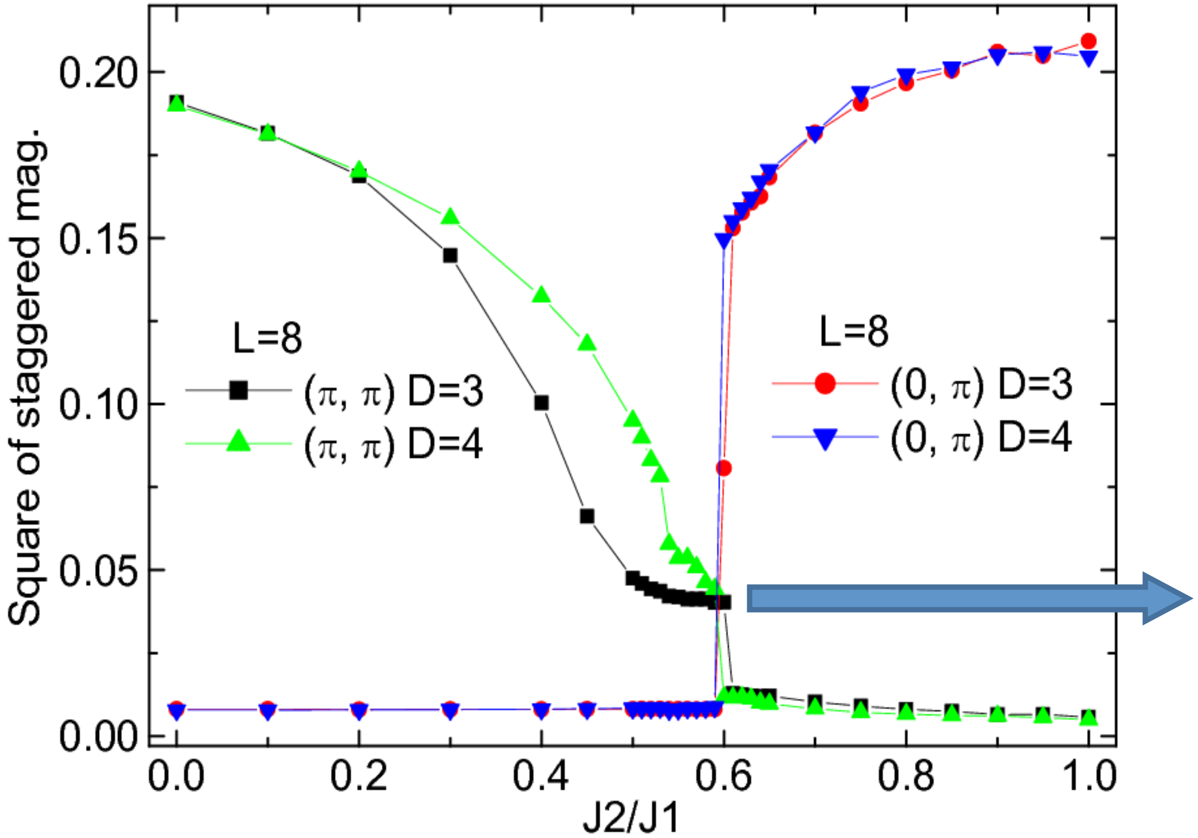
$J_2/J_1=0.1$ $J_2/J_1=0.55$

$$
\begin{aligned}
Q_{\alpha\beta\gamma\delta} &= \frac{1}{2}\left(P_{\alpha\beta\gamma\delta} + P^{-1}_{\alpha\beta\gamma\delta}\right) \\
&= 2\left(\mathbf{S}_\alpha \cdot \mathbf{S}_\beta \mathbf{S}_\gamma \cdot \mathbf{S}_\delta + \mathbf{S}_\alpha \cdot \mathbf{S}_\delta \mathbf{S}_\beta \cdot \mathbf{S}_\gamma - \mathbf{S}_\alpha \cdot \mathbf{S}_\gamma \mathbf{S}_\beta \cdot \mathbf{S}_\delta\right) \\
&\quad + 1/2\left(\mathbf{S}_\alpha \cdot \mathbf{S}_\beta + \mathbf{S}_\gamma \cdot \mathbf{S}_\delta + \mathbf{S}_\alpha \cdot \mathbf{S}_\delta + \mathbf{S}_\beta \cdot \mathbf{S}_\gamma\right) \\
&\quad + 1/2\left(\mathbf{S}_\alpha \cdot \mathbf{S}_\gamma + \mathbf{S}_\beta \cdot \mathbf{S}_\delta + 1/4\right).
\end{aligned}
$$

V. Murg *et al.*, Phys. Rev. B 79, 195119 (2009)

system size: L = 8, D=4

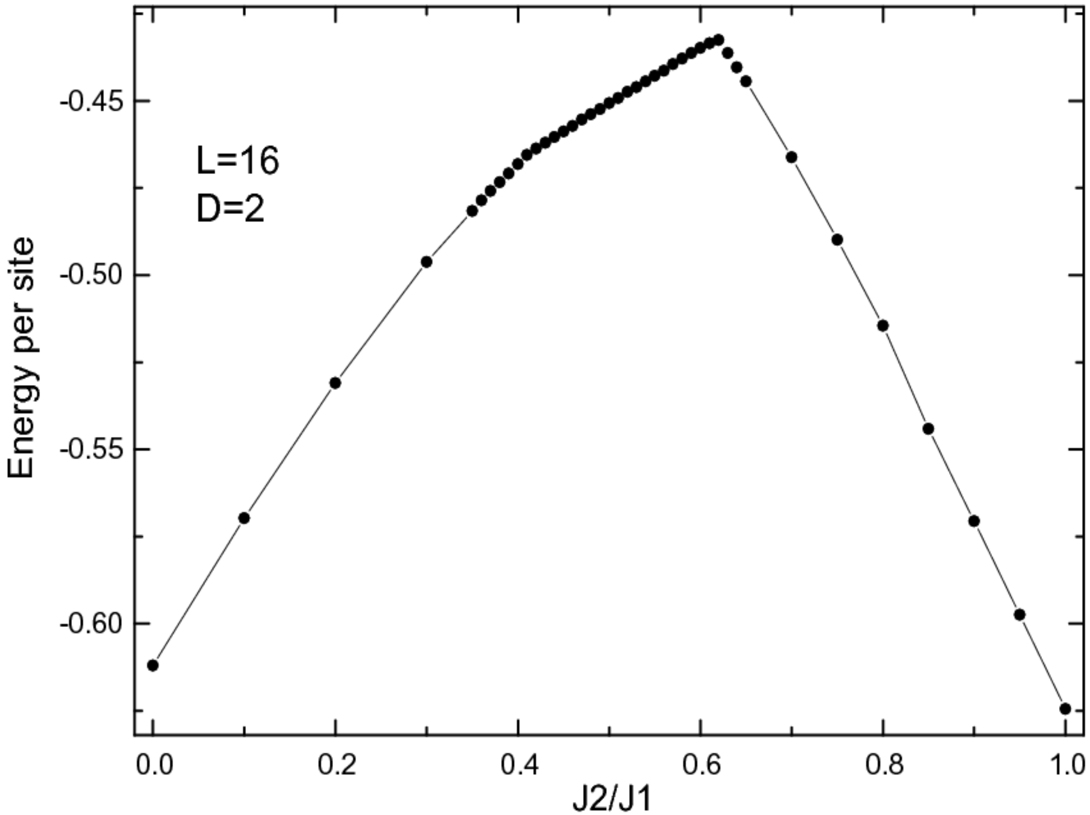
Magnetization square VS. J2/J1



size effect?

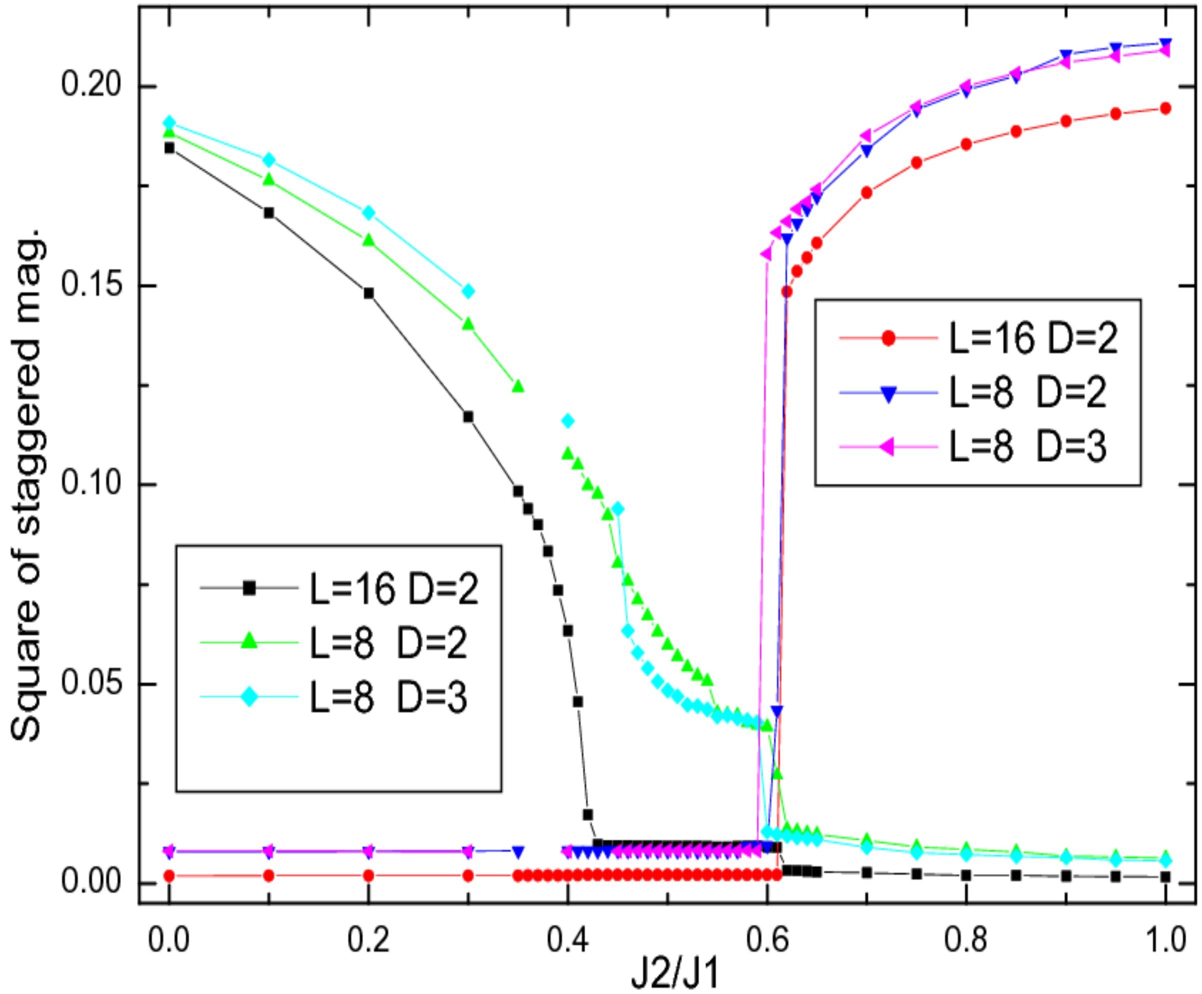
Increase system size: L = 16, but D = 2

ground state energy VS. J2/J1



Transition points:
~0.42
~0.62

Magnetization square VS. J2/J1

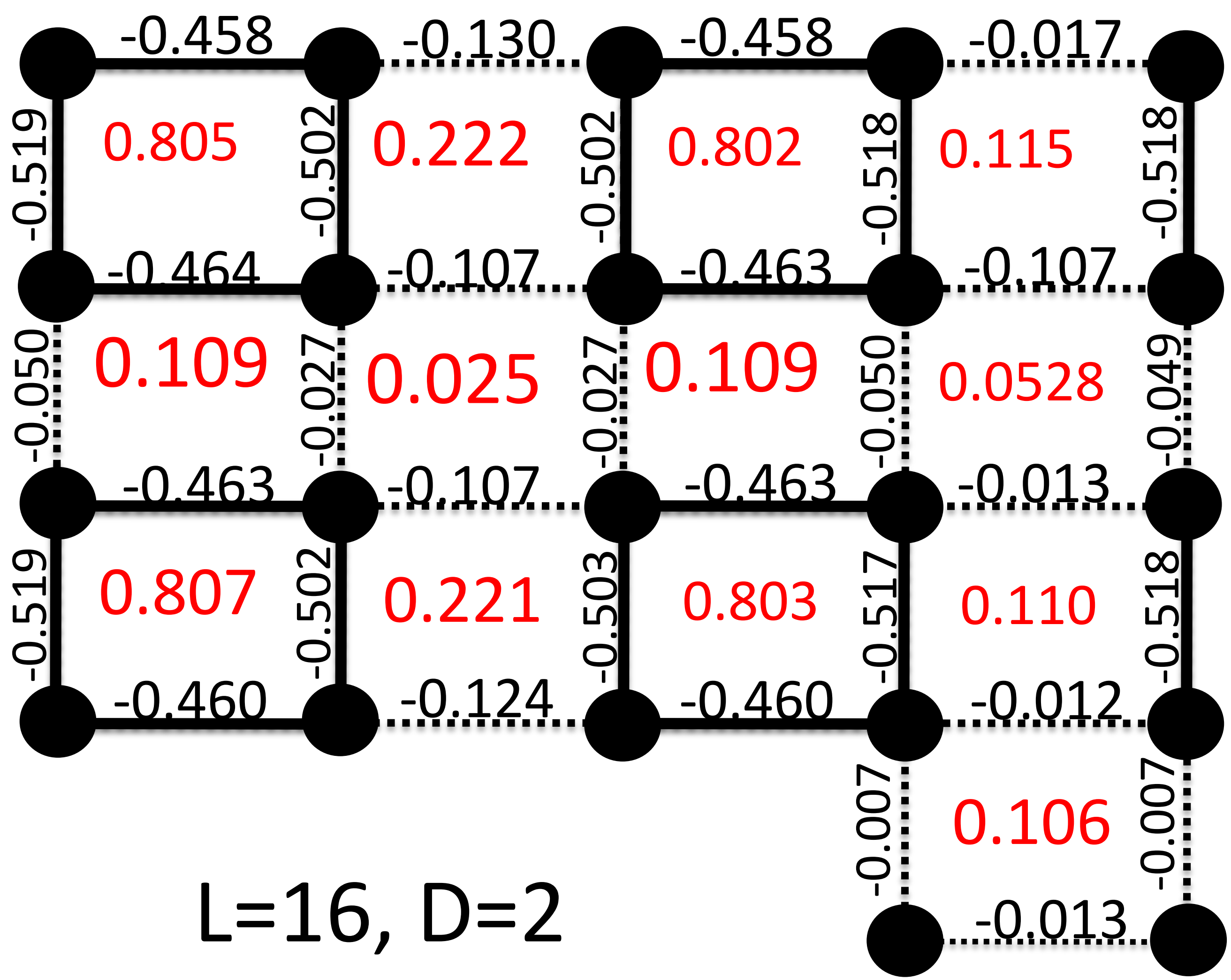


L=16, D=2 Transition points:

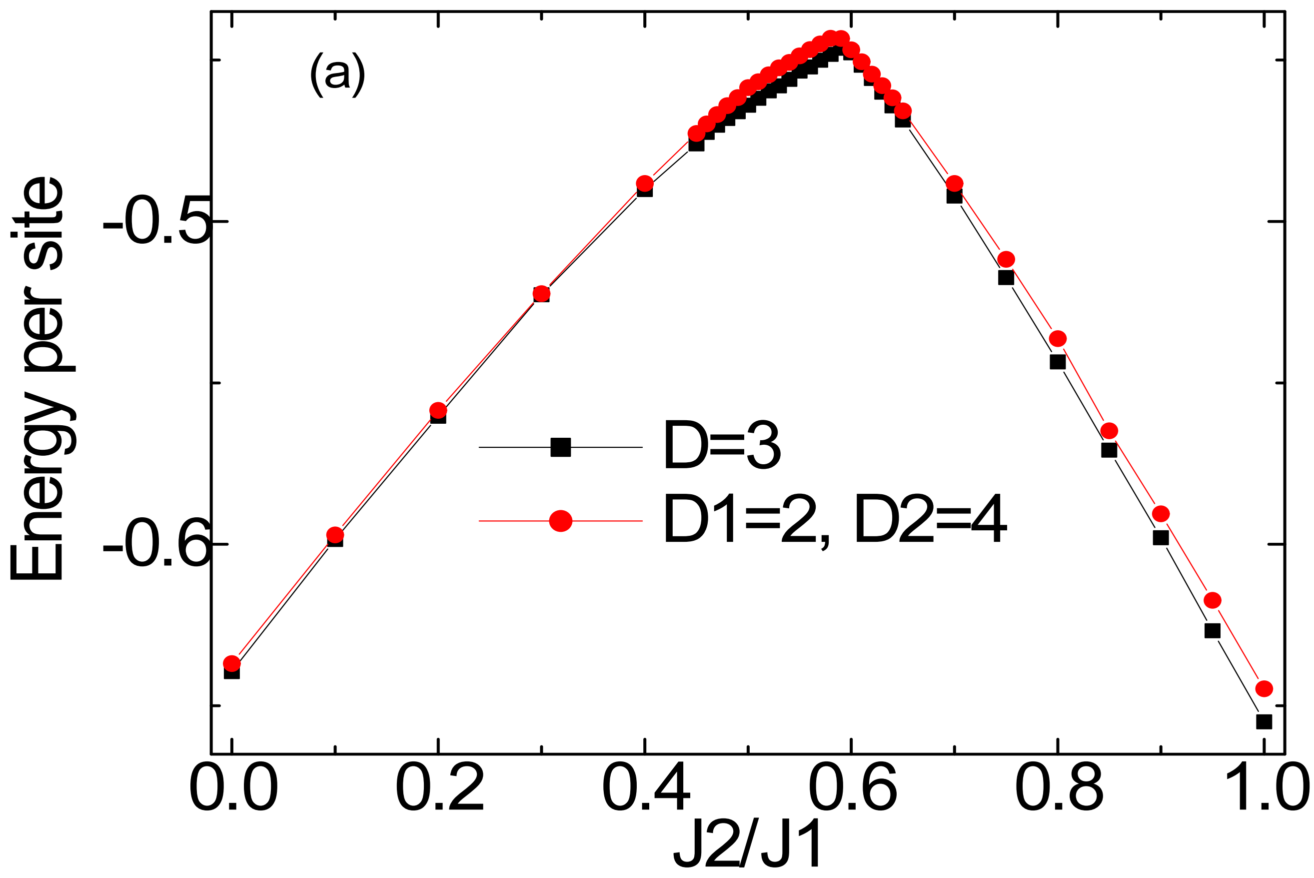
~0.42

~0.61

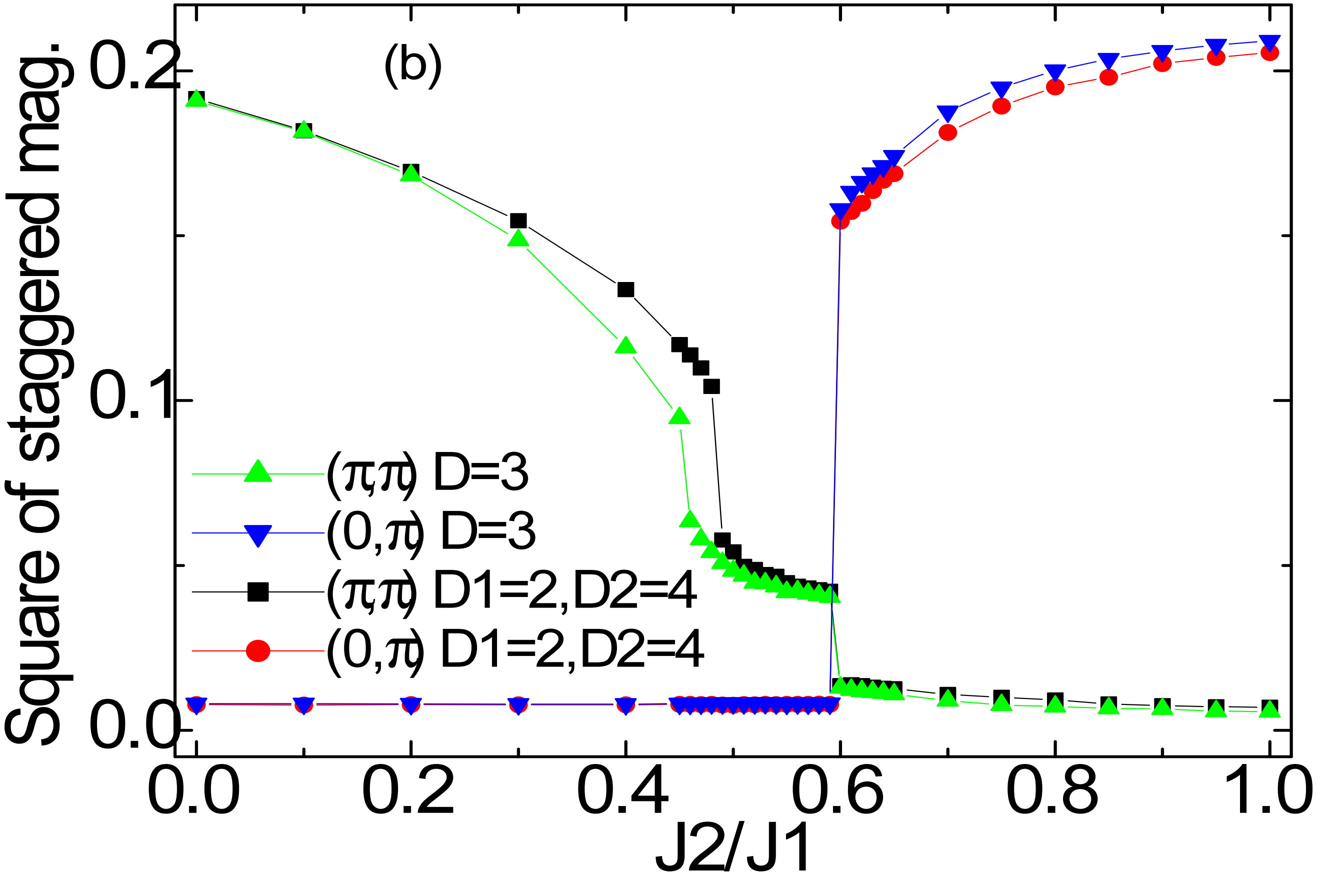
correlation functions:
1. nearest spin-spin interaction (**Black numbers**)
2. plaquette order parameter (**Red numbers**)



system size: L = 8

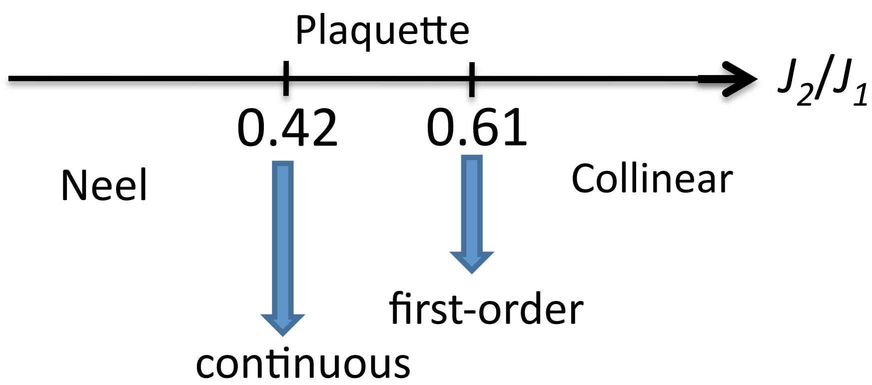


system size: L = 8



D. Summary:

1. Phase transition points:
    - ~0.42 (continuous)
    - ~0.61 (first-order)



2. Phase: plaquette order

3. method:
    - a) variational
    - b) plaquette renormalized TNS:
        for other models.

Thank you
for your attention!