Numerical Study of 2D Spin Models via Tensor Product States

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Acknowledgement & References

- Collaborators:
  - Prof. Ming-Fong Yang, Tunghai University.
  - Ms. Chen-Yen Lai, now at UC Riverside.

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- References:

  - Pochung Chen, Chen-Yen Lai, Ming-Fong Yang, "*Field Induced Spin Supersolidity in Frustrated Spin-1/2 Spin-Dimer Models*", arXiv:0910.5081.
  - Pochung Chen, Chen-Yen Lai, Ming-Fong Yang, "*Numerical study of spin-1/2 XXZ model on square lattice from tensor product states*", JSTAT, **10**, P10001, 2009.

Outline

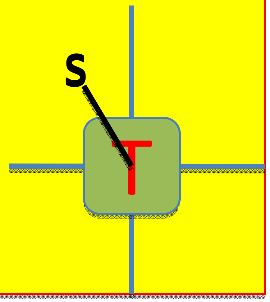
- Introduction of tensor product state
  - Represent tensor product state.
  - Optimize tensor product state.
  - Evaluate expectation values.
- Application to 2D spin models
  - Frustrated spin ½ spin-dimer model. (Supersolidity).
  - Spin ½ XXZ model. (First order phase transition).
- Summary and outlook

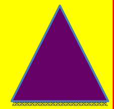
Introduction to our TPS approach

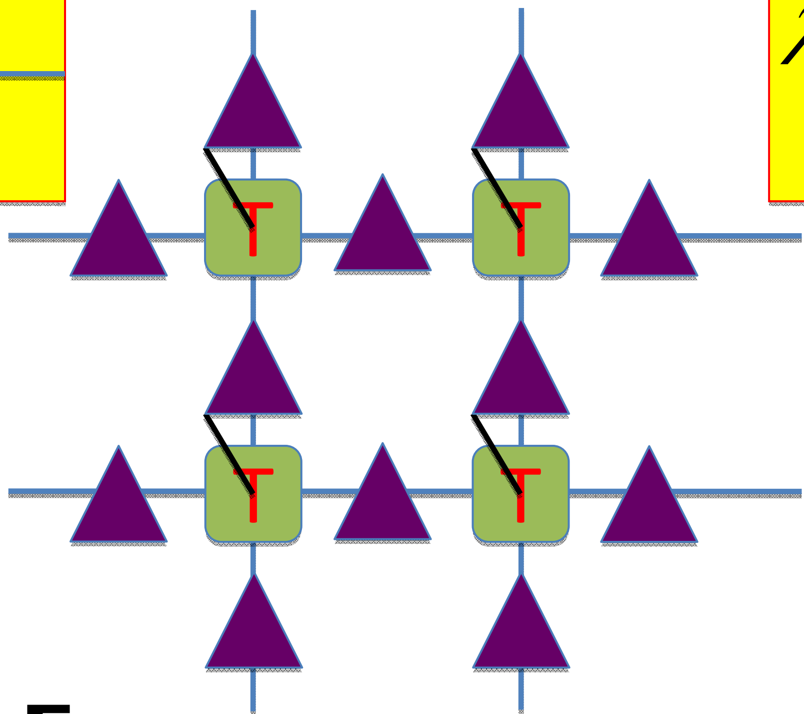
- Wave-function ansatz:
  - 2D Tensor product state (2D-TPS).
- Optimization:
  - Imaginary time evolution.
  - 2D Time-Evolving Block Decimation (2D-TEBD).
- Expectation value:
  - Tensor renormalization group (2D-TRG).
- References:
  - M. Levin, C. P. Nave, PRL 99, 120601 (2007).
  - Z.C. Gu, M. Levin, X.G. Wen, PRB 78, 205116 (2008).
  - H.C. Jiang, Z.Y. Weng, T. Xiang, PRL 101, 090603(2008).

2D Tensor Product State (TPS)

Represent wave-function by a tensor network

$$T^{S}_{uldr} =$$ 

$$\lambda_{ij} = \lambda_i \delta_{ij} =$$ 



$$\left|\Psi\right\rangle = \mathrm{Tr}\left[T^{S_i}_{u_i l_i d_i r_i} \lambda_k T^{S_j}_{u_j l_j d_j r_j} \lambda_q \cdots \right] \left|S_i S_j \cdots \right\rangle$$

Imaginary Time Evolution

- Use imaginary time to reach the ground state
- Assume initial state has some overlap with GS

$$\left|\Psi(0)\right\rangle = A_0\left|G\right\rangle + A_1\left|E_1\right\rangle + A_2\left|E_2\right\rangle + \cdots$$

- Imaginary time evolution single out the GS

$$e^{-HT}\left|\Psi(0)\right\rangle = A_0\left|G\right\rangle + A_1 e^{-E_1 T}\left|E_1\right\rangle + A_2 e^{-E_2 T}\left|E_2\right\rangle + \mathrm{L}$$

- Obtain ground state by

$$\left|G\right\rangle = \lim_{N\to\infty} \frac{\left(e^{-\tau H}\right)^N \left|\Psi(0)\right\rangle}{\left\|\left(e^{-\tau H}\right)^N \left|\Psi(0)\right\rangle\right\|}$$

Suzuki-Trotter Formula

- Consider Hamiltonian with NN terms

$$H = \sum_{\langle ij \rangle} H_{ij} = H_{12} + H_{34} + \cdots + H_{23} + H_{45} + \cdots = H_{even} + H_{odd}$$

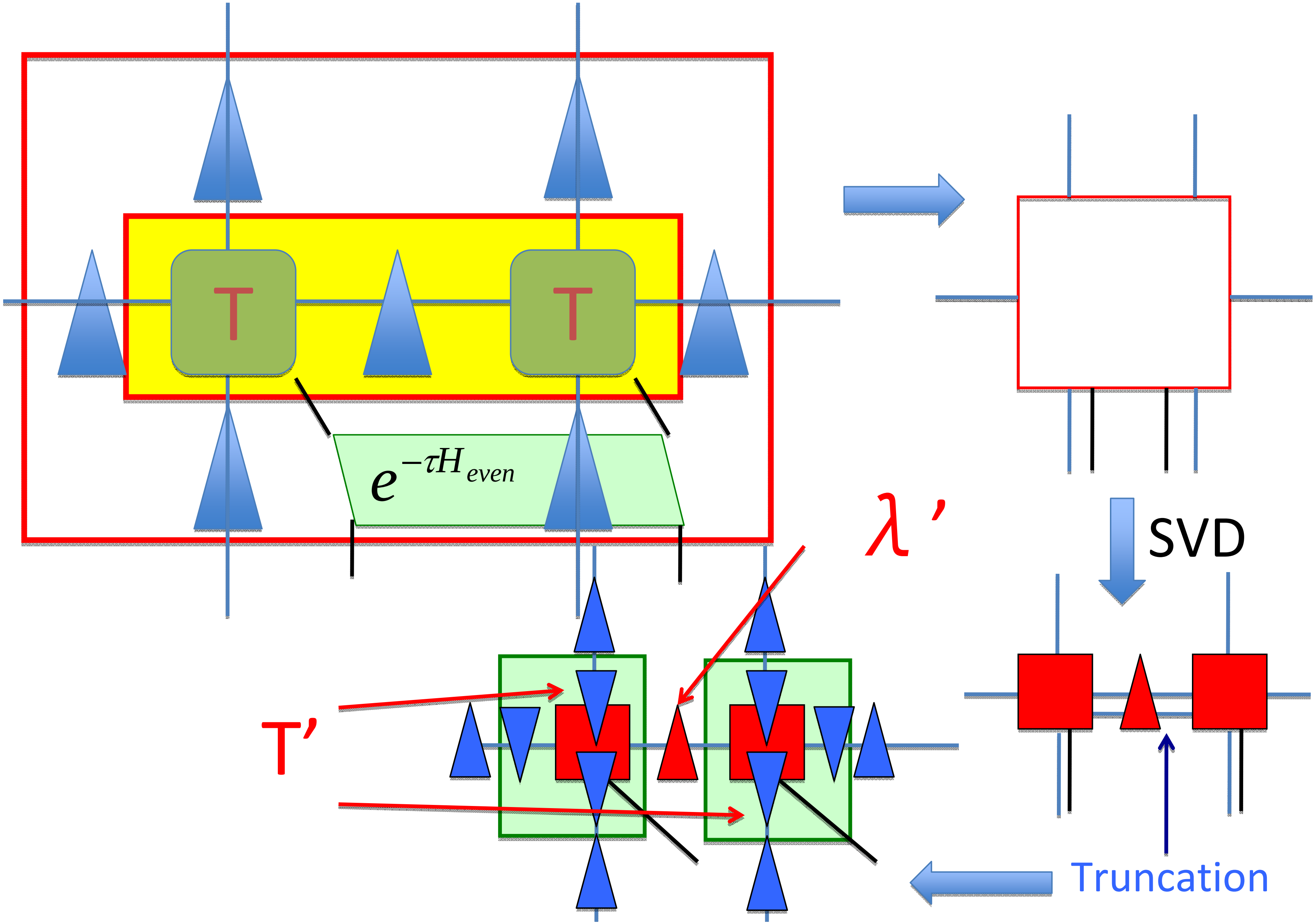
- Suzuki-Trotter Formula $e^{-\tau(A+B)} \approx e^{-\tau A} e^{-\tau B} + O\left(\tau^2\right)$

- Applied to imaginary time evolution

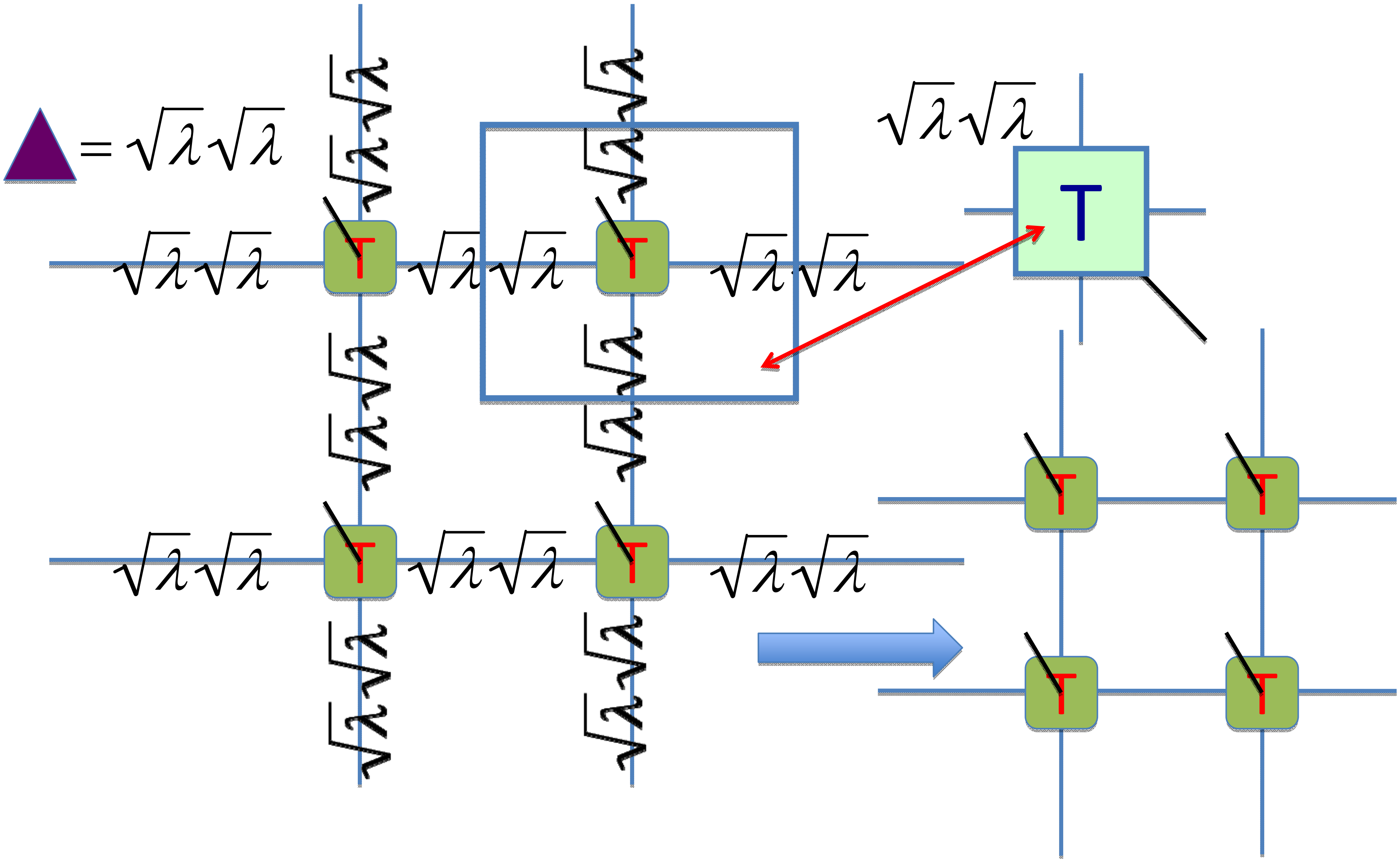
$$e^{-\tau H} \approx e^{-\tau H_{even}} e^{-\tau H_{odd}}$$

- Translational invariant → Simplification

Time-Evolving Block Decimation(TEBD)



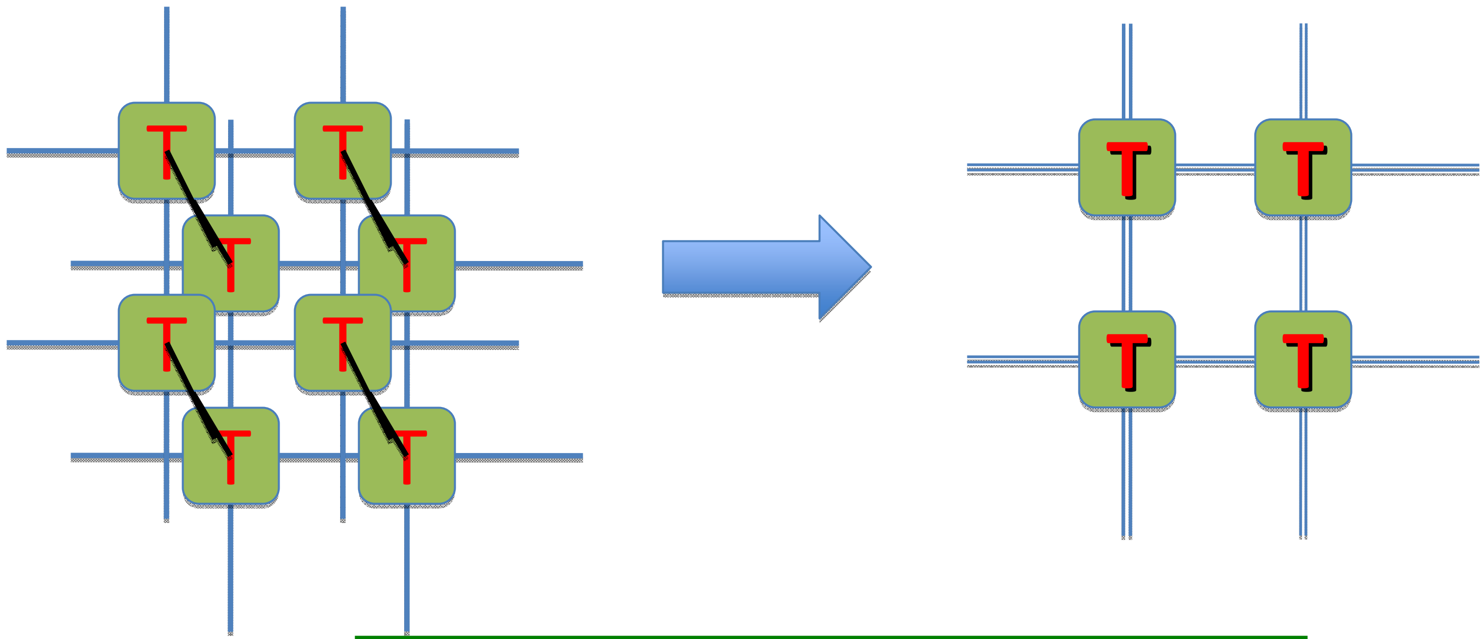
Rearrange the 2D TPS



Expectation Value of 2D TPS

Represent expectation value by the tensor network of **T** tensors

$\langle \Psi | \Psi \rangle =$



Double tensor **T**

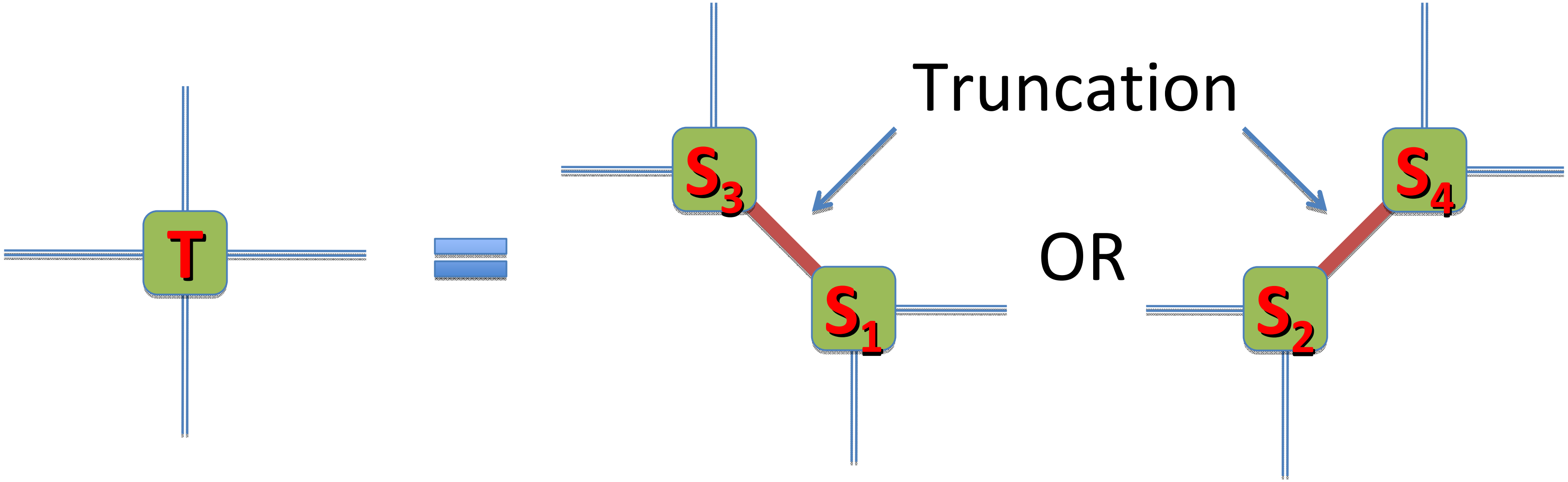
$$\mathbf{T}_{(uu',ll',dd',rr')} = \sum_S T^{*S}_{u'l'd'r'} T^S_{uldr}$$

$$\mathbf{T}^A_{(uu',ll',dd',rr')} = \sum_{S'S} T^{*S'}_{u'l'd'r'} \langle S' | O^A | S \rangle T^S_{uldr}$$

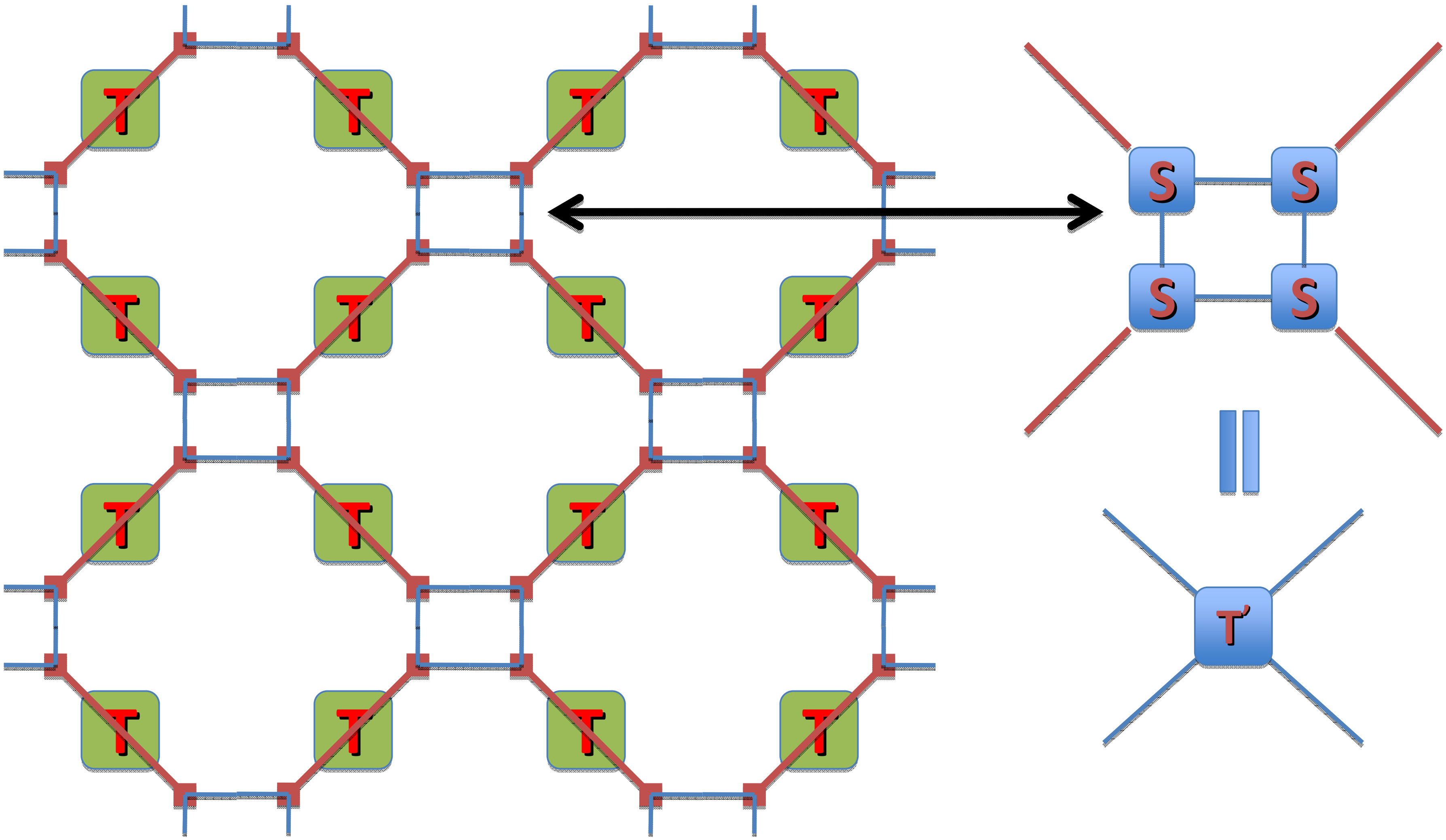
Rewriting the Tensor Network

Rewrite rank 4 tensor **T** into product of two rank 3 tensor **S**

$$\mathbf{T}_{\alpha\beta\mu\nu} \cong \sum_{\gamma=1}^{D_{cut}} S_{3,\alpha\delta\gamma} S_{1,\mu\nu\gamma}$$

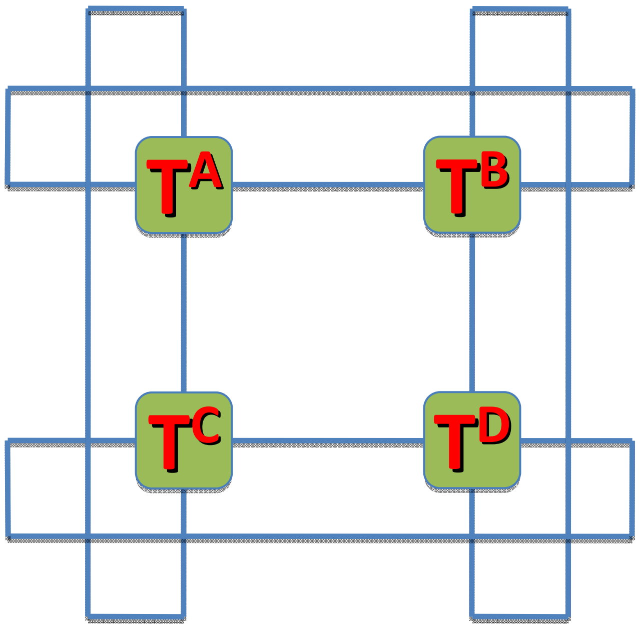


Coarse-Grained Tensor Network



Final 2x2 Plaque

After N iteration of RG, 2x2 plaque effective represent $2^N x 2^N$ lattice
Tensor contract can be done exactly for the 2x2 plaque



Expectation value of TPS can be approximately but efficiently calculated via TERG

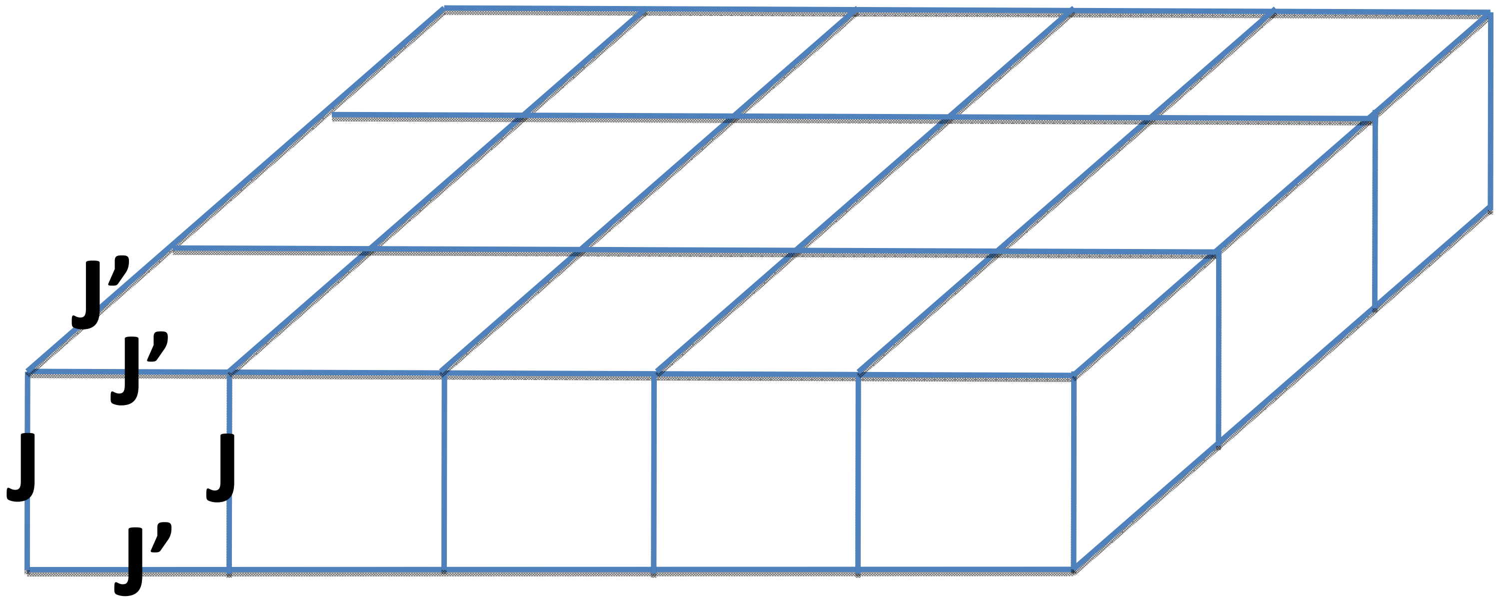
Combined TPS+TEBD+TRG Method

- Applications:
  - 2D Spin ½ Spin-Dimer Model on square lattice.
    - With frustration.
    - Spin supersolid phase.
  - 2D Spin ½ XXZ Model on square lattice.
    - First order transition.

Spin Supersolidity in Spin-1/2 Spin-Dimer Models

Anisotropic Spin-Dimer Model

$$H = J\sum_{i} S_{i1}S_{i2} - h\sum_{i\alpha} S^{z}_{i\alpha} + J'\sum_{<i,j>\alpha} S^{x}_{i\alpha}S^{x}_{j\alpha} + S^{y}_{i\alpha}S^{x}_{j\alpha} + \Delta S^{z}_{i\alpha}S^{z}_{j\alpha}$$

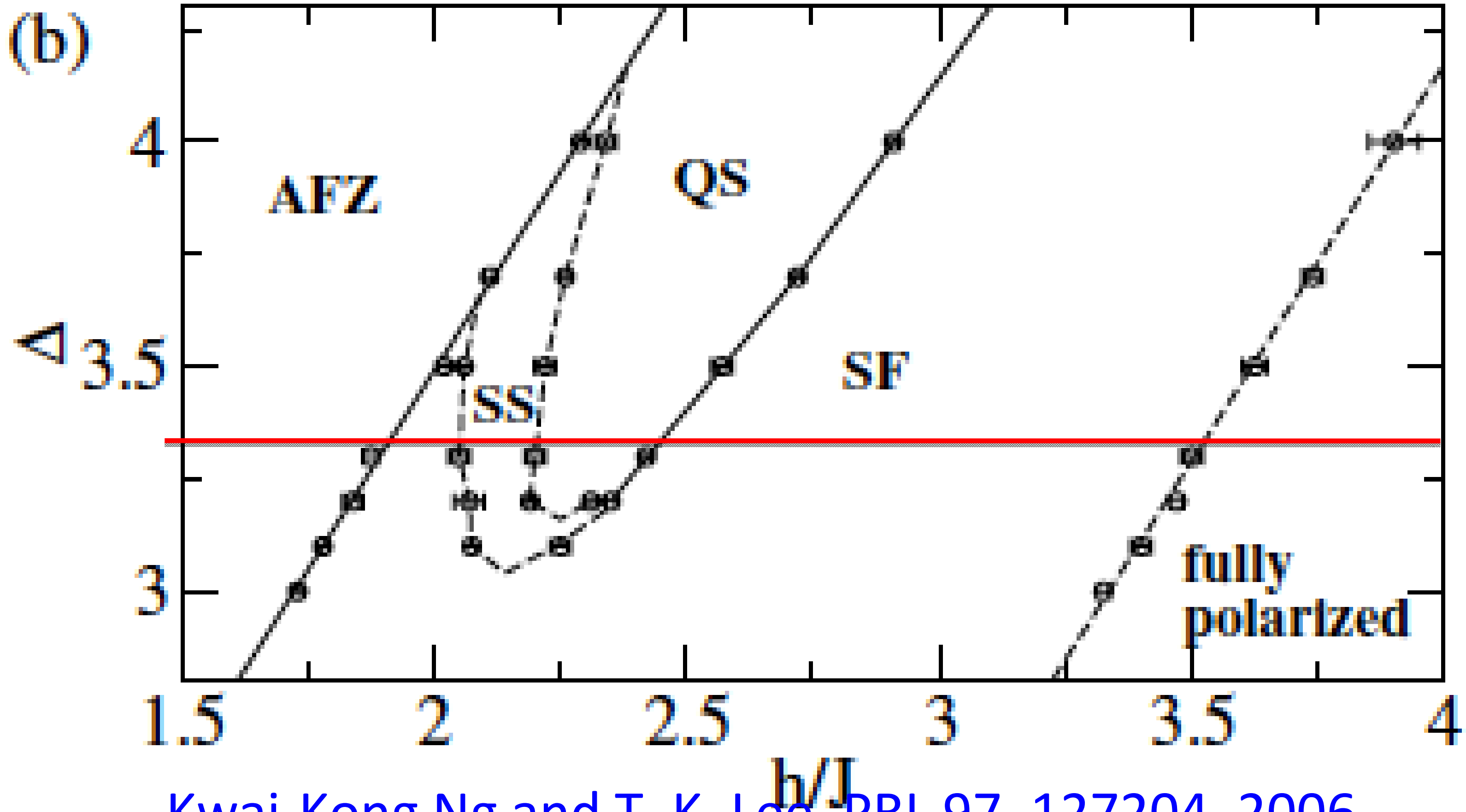


Order Parameters

- $m^z{}_u \rightarrow$ triplet excitation density.
- $m^x{}_s \rightarrow$ triplet condensation density (superfluid density).
- $m^z{}_s \rightarrow$ checkerboard solid order (structure order).
- Supersolid phase $\rightarrow$ $m^x{}_s \neq 0$ and $m^z{}_s \neq 0$.

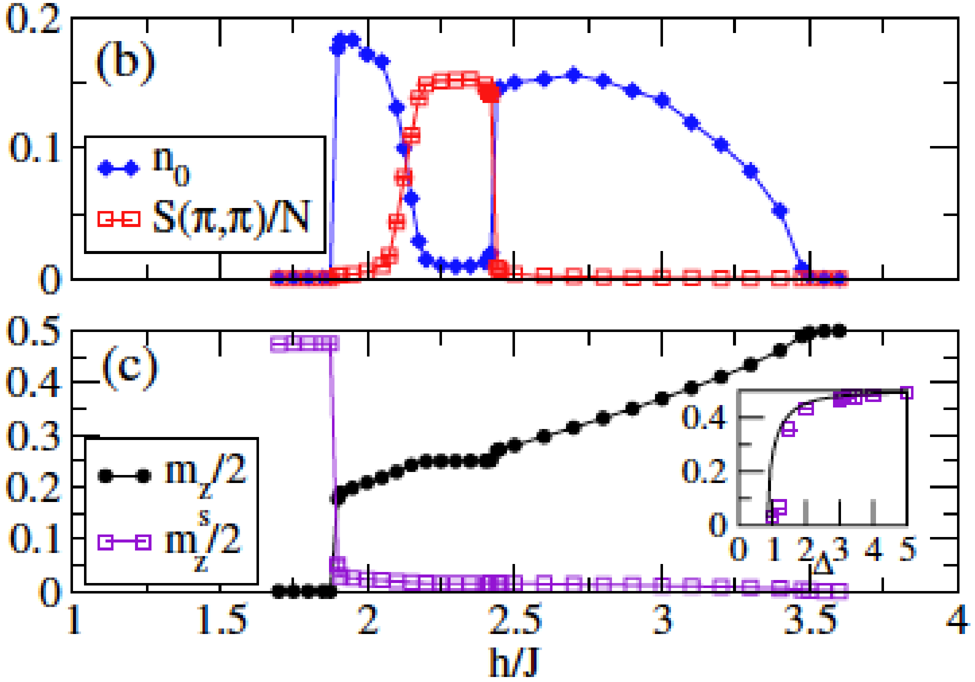
Phase Diagram of Anisotropic Spin-Dimer Model

$$H = J\sum_{i} S_{i1}S_{i2} - h\sum_{i\alpha} S^{z}_{i\alpha} + J' \sum_{<i,j>\alpha} S^{x}_{i\alpha}S^{x}_{j\alpha} + S^{y}_{i\alpha}S^{x}_{j\alpha} + \Delta S^{z}_{i\alpha}S^{z}_{j\alpha}$$



Kwai-Kong Ng and T. K. Lee, PRL 97, 127204, 2006.

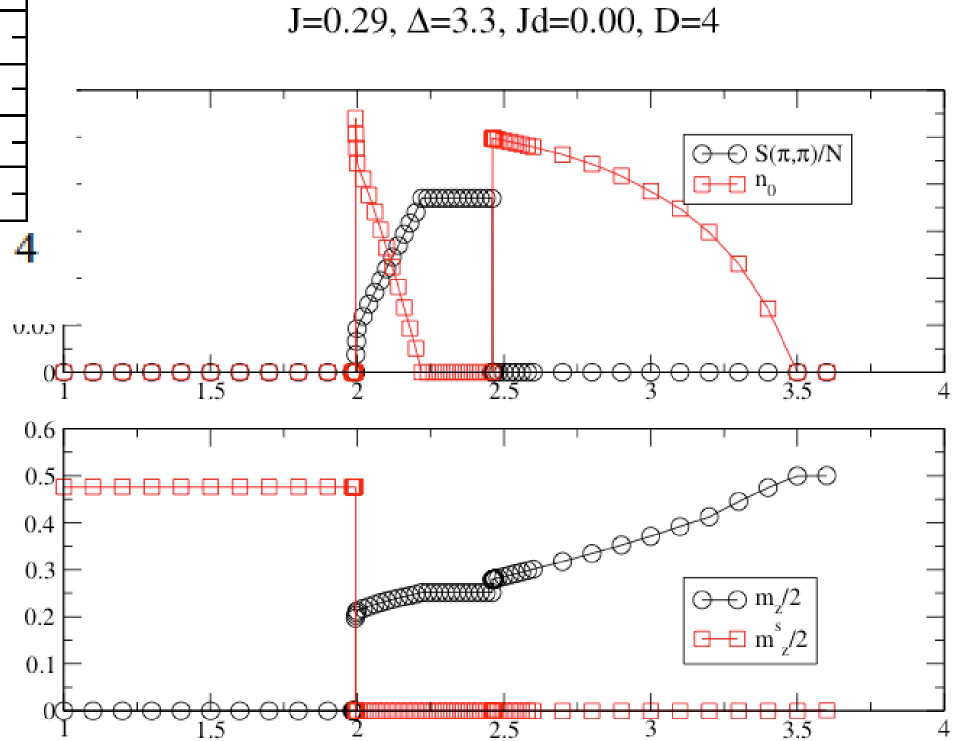
Field-Induced Phase Diagram



J'=0.29, Δ =3.3,

Kwai-Kong Ng and T. K. Lee,
PRL 97, 127204, 2006.

Our result

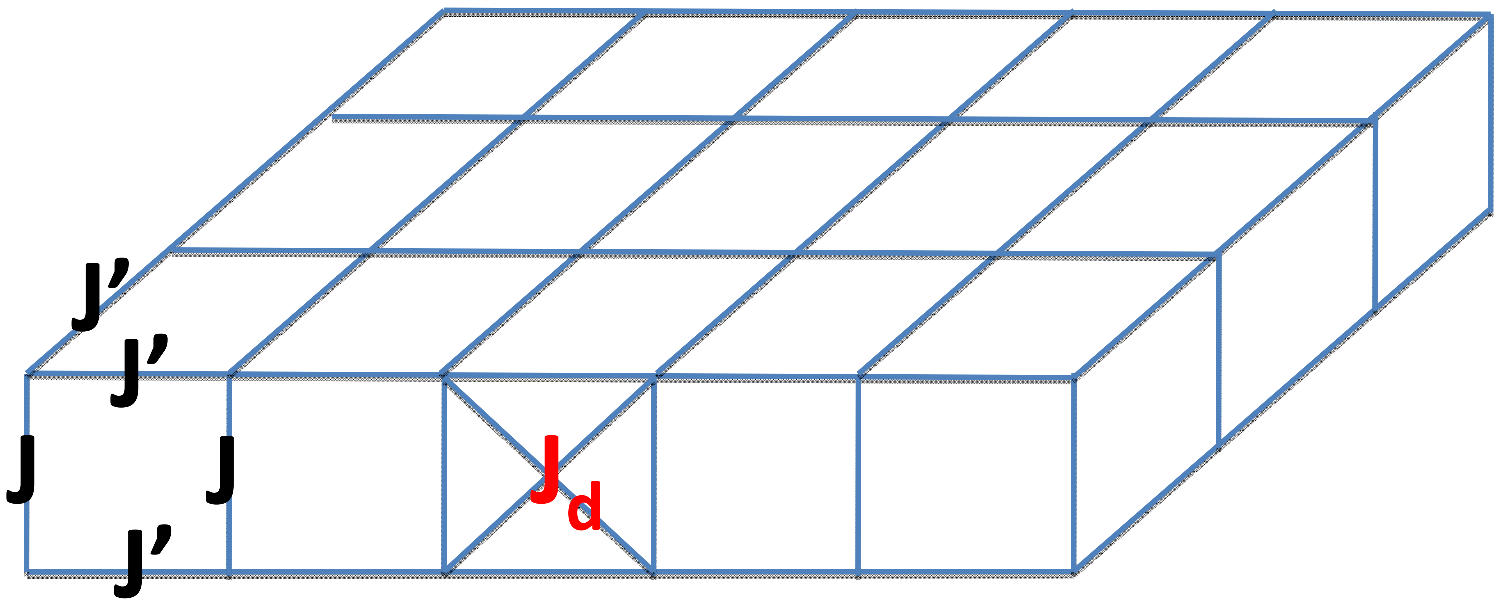


Isotropic Spin-Dimer Model

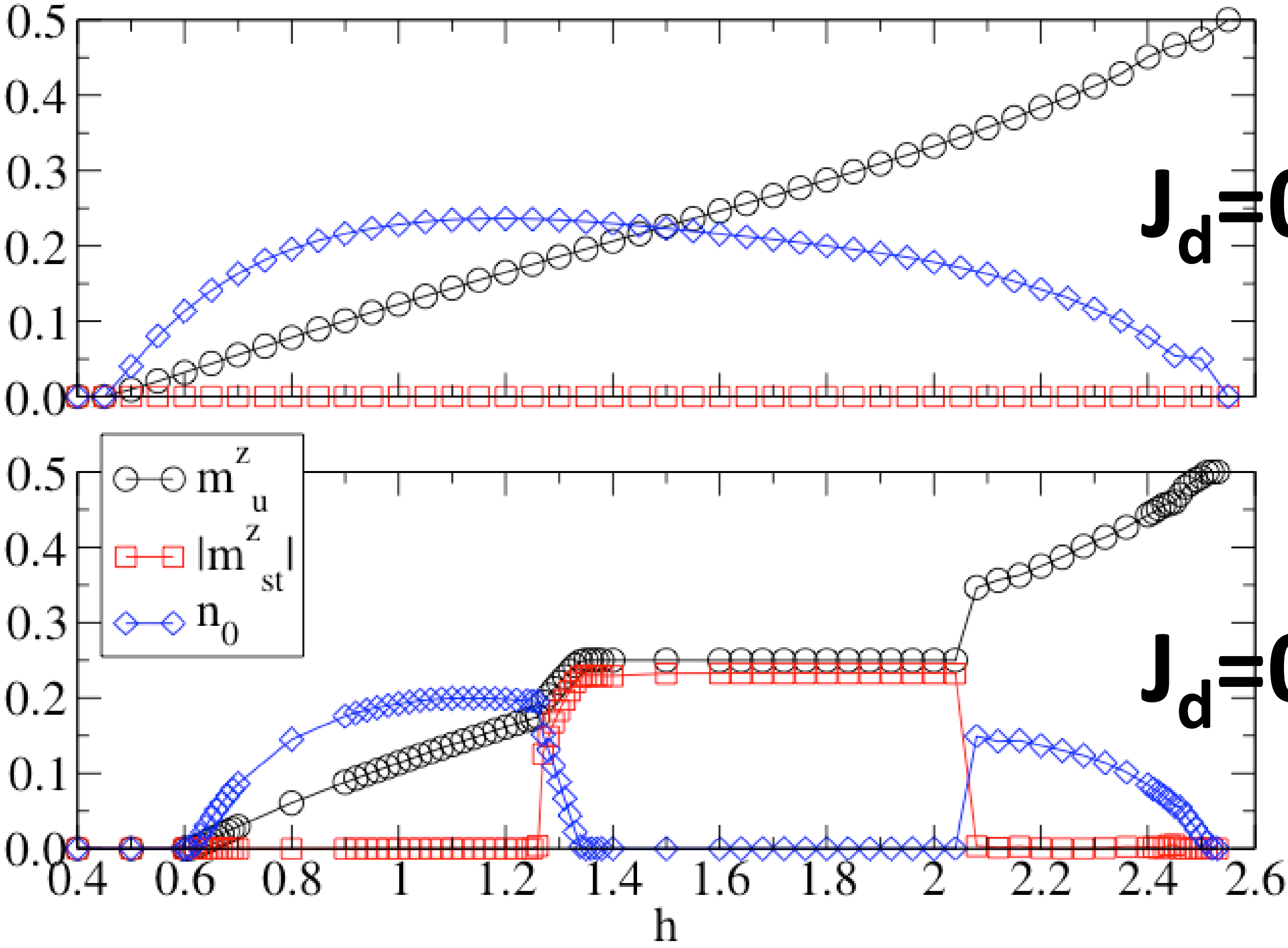
Motovation:

- Hard to realize selective anisotropy.
- Large Δ≈3 is needed.
- Anisotropy as effective Hamiltonian of frustrating interlayer interaction.

$$H = J\sum_{i} S_{i1}S_{i2} - h\sum_{i\alpha} S^{z}_{i\alpha} + J'\sum_{<i,j>\alpha} S_{i\alpha}S_{j\alpha} + J_{d}\sum_{<i,j>\alpha} S_{i\alpha}S_{j\bar{\alpha}}$$



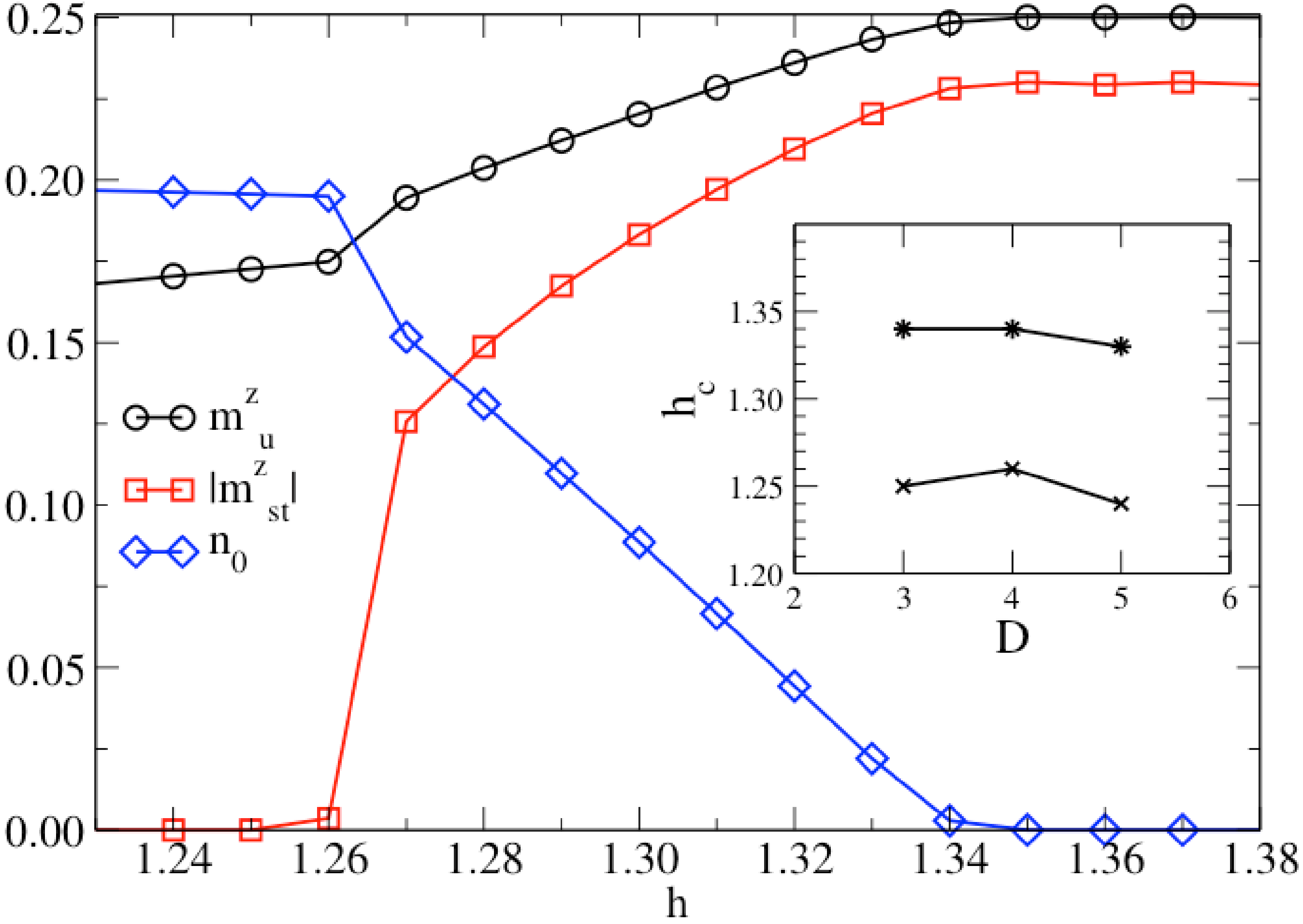
Results (J'=0.38)



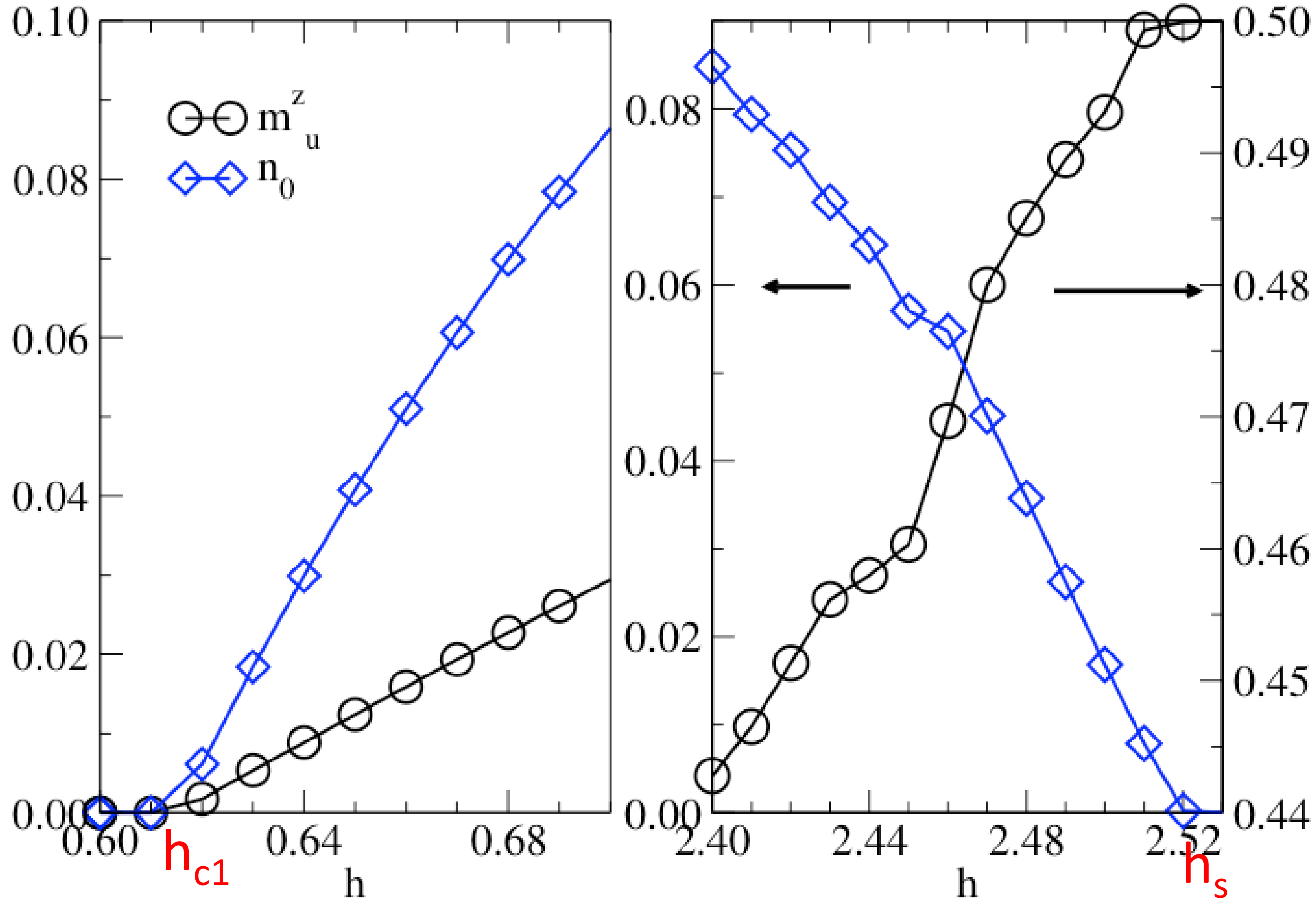
J_d=0.15

J_d=0.21

Results ($J'=0.38$, $J_d=0.21$)



Results (J'=0.38)



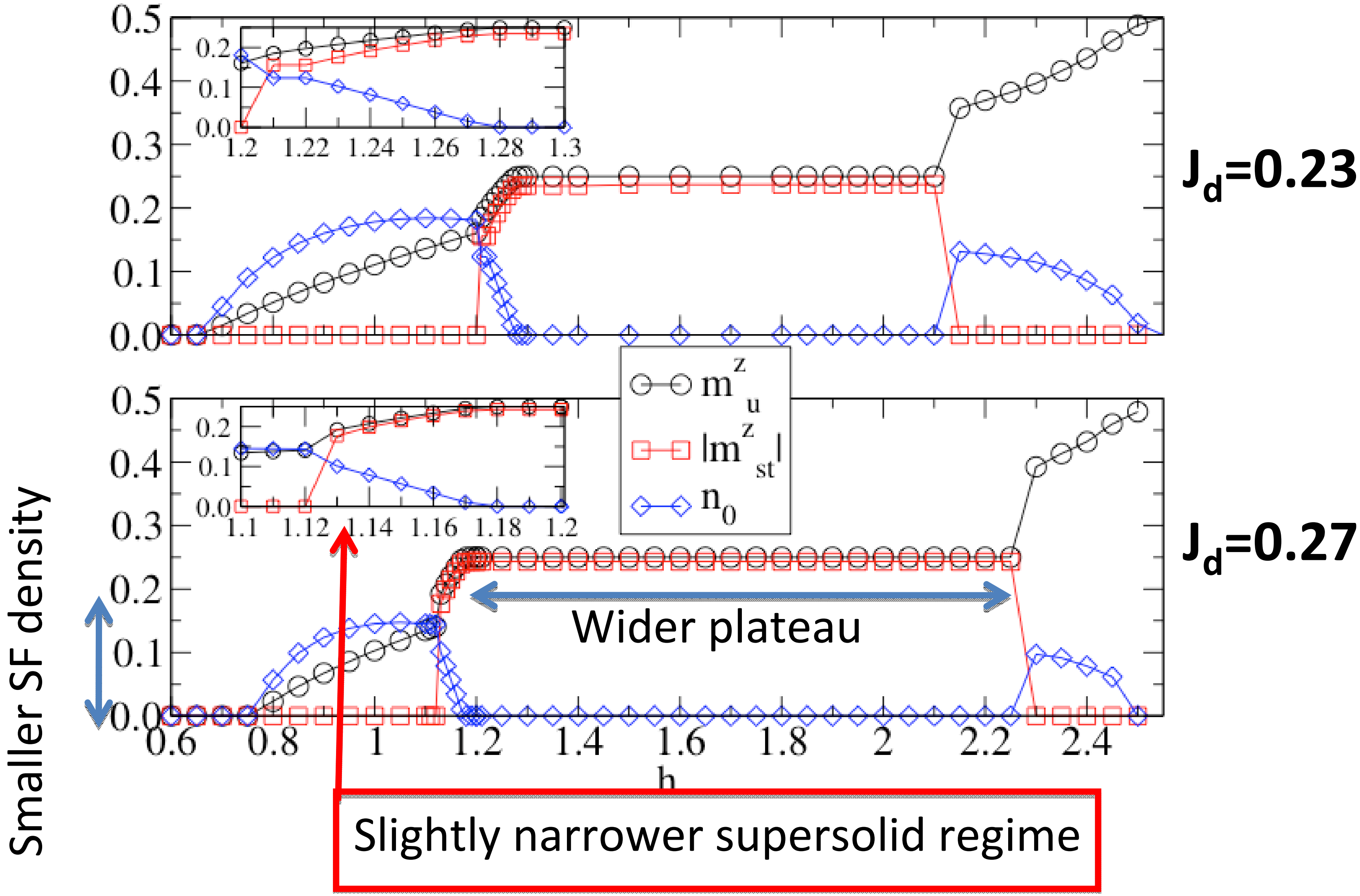
Perturbation expansion

$$h_{c1} \approx 1 - 2(J - J_d) - \frac{3}{2} J (J - J_d)^2$$

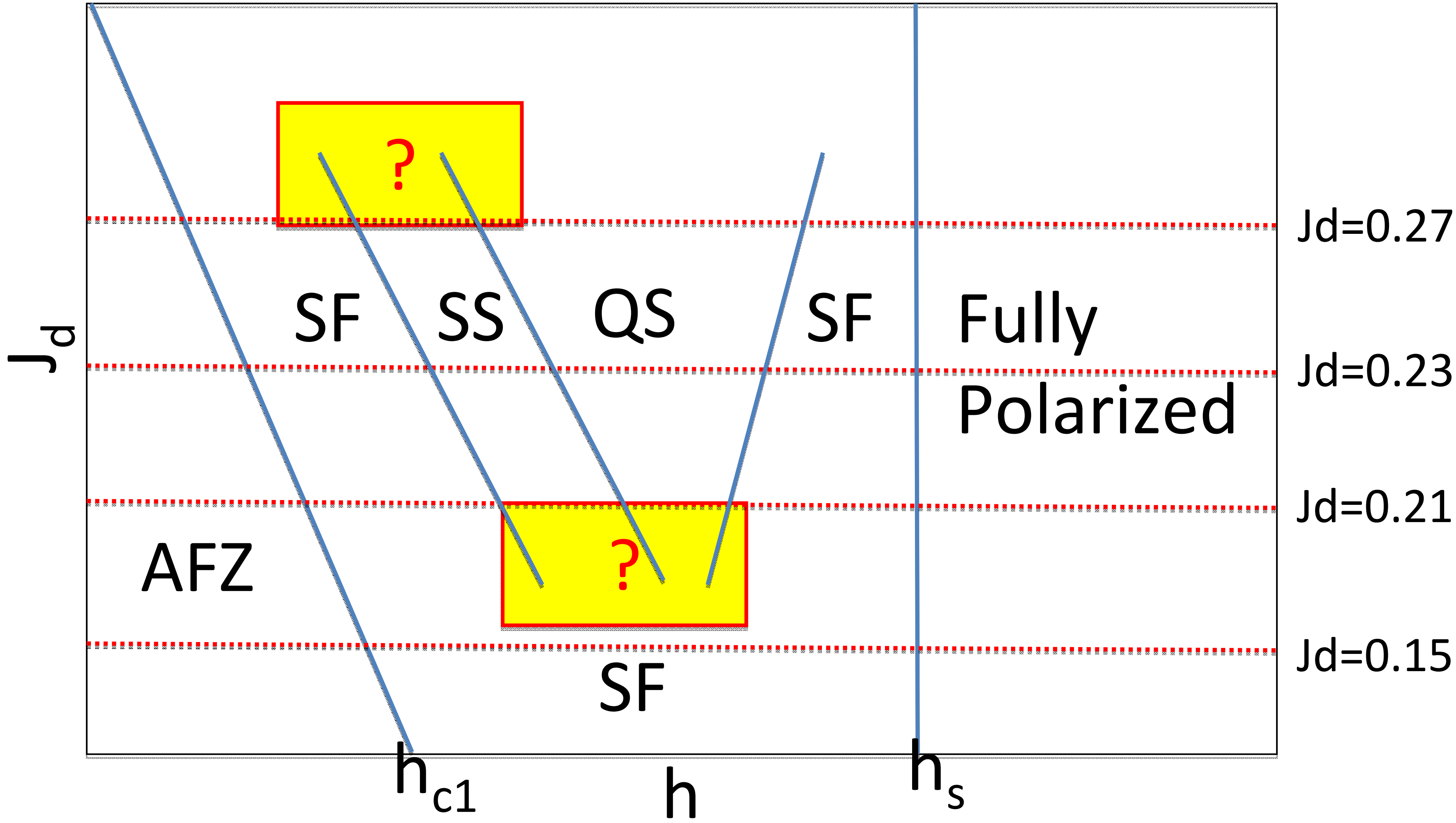
Exact analytical calculation

$$h_s = 1 + 4J$$

Results (J'=0.38, J_d=0.23, 0.27)



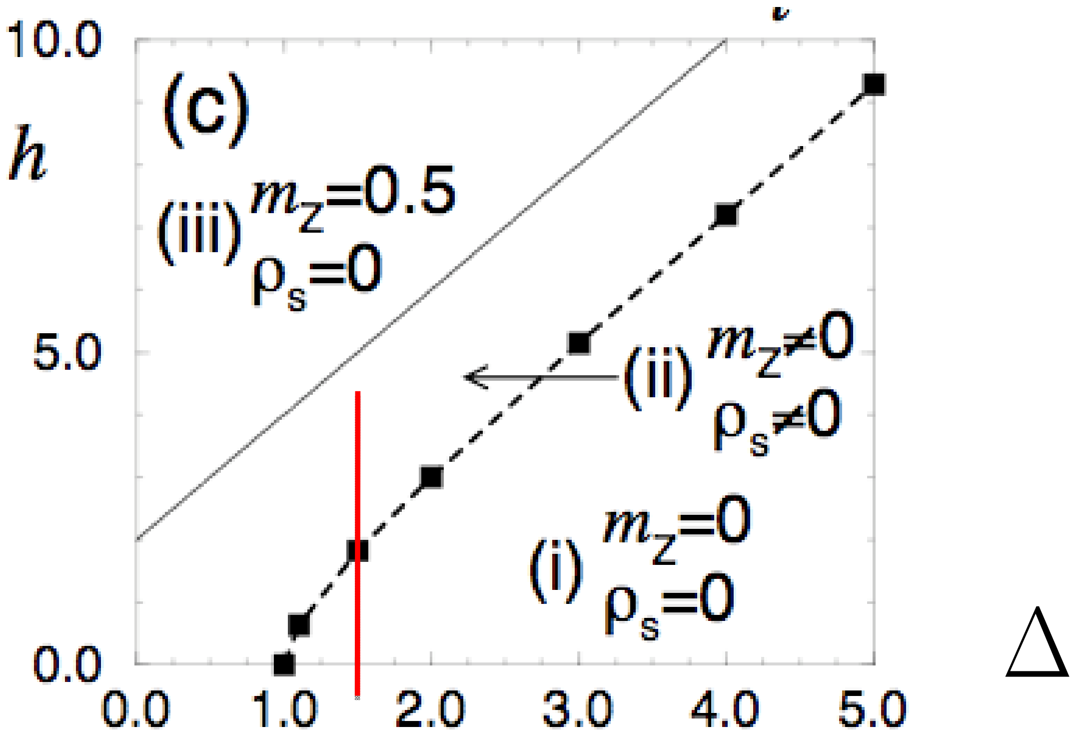
Phase Diagram



•Pochung Chen, Chen-Yen Lai, Ming-Fong Yang, arXiv:0910.5081.

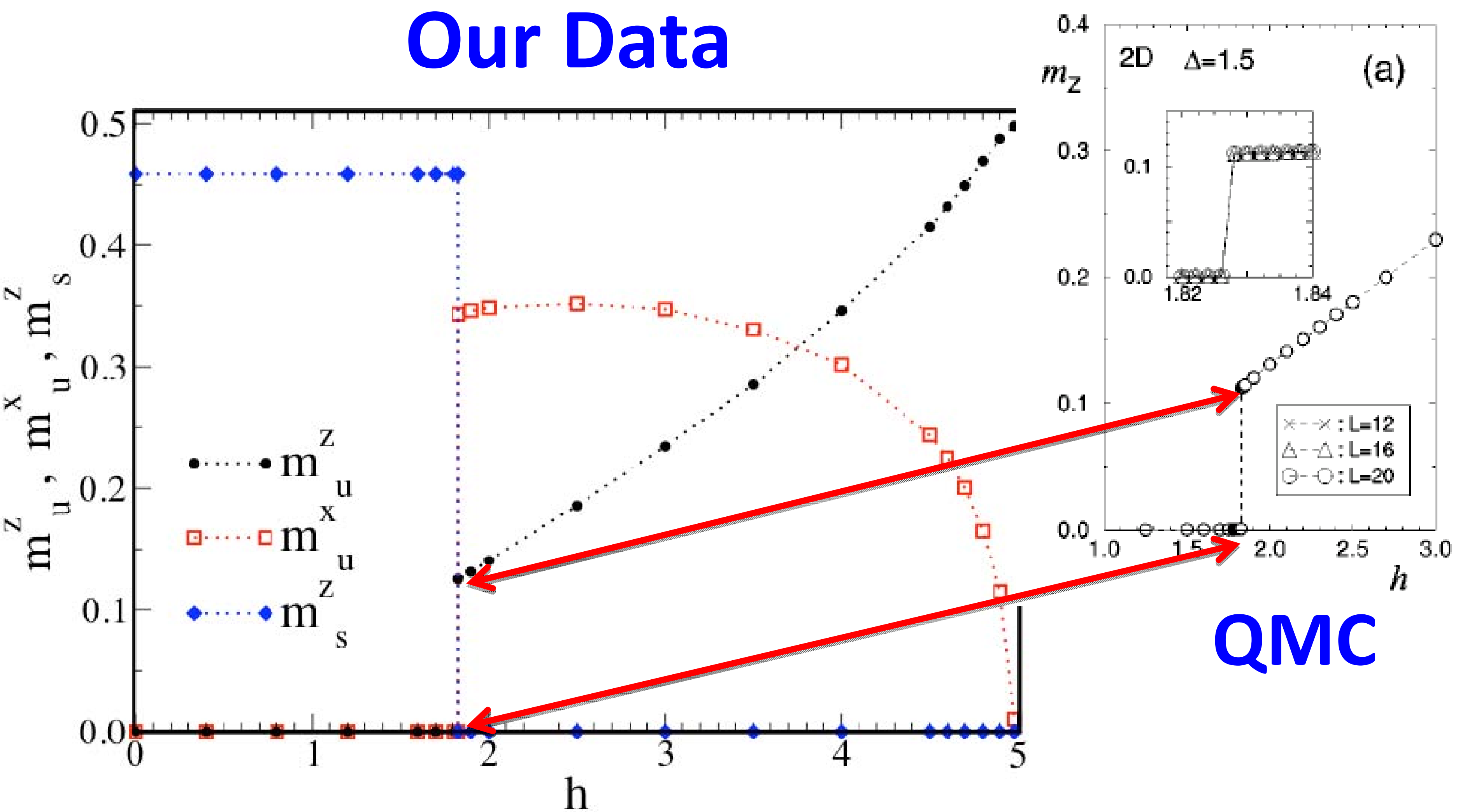
Spin ½ XXZ Model on Square Lattice

$$H = J\sum_{\langle ij\rangle} -S_i^+ S_j^- - S_i^- S_j^+ + \Delta S_i^z S_j^z - h\sum_i S_i^z$$

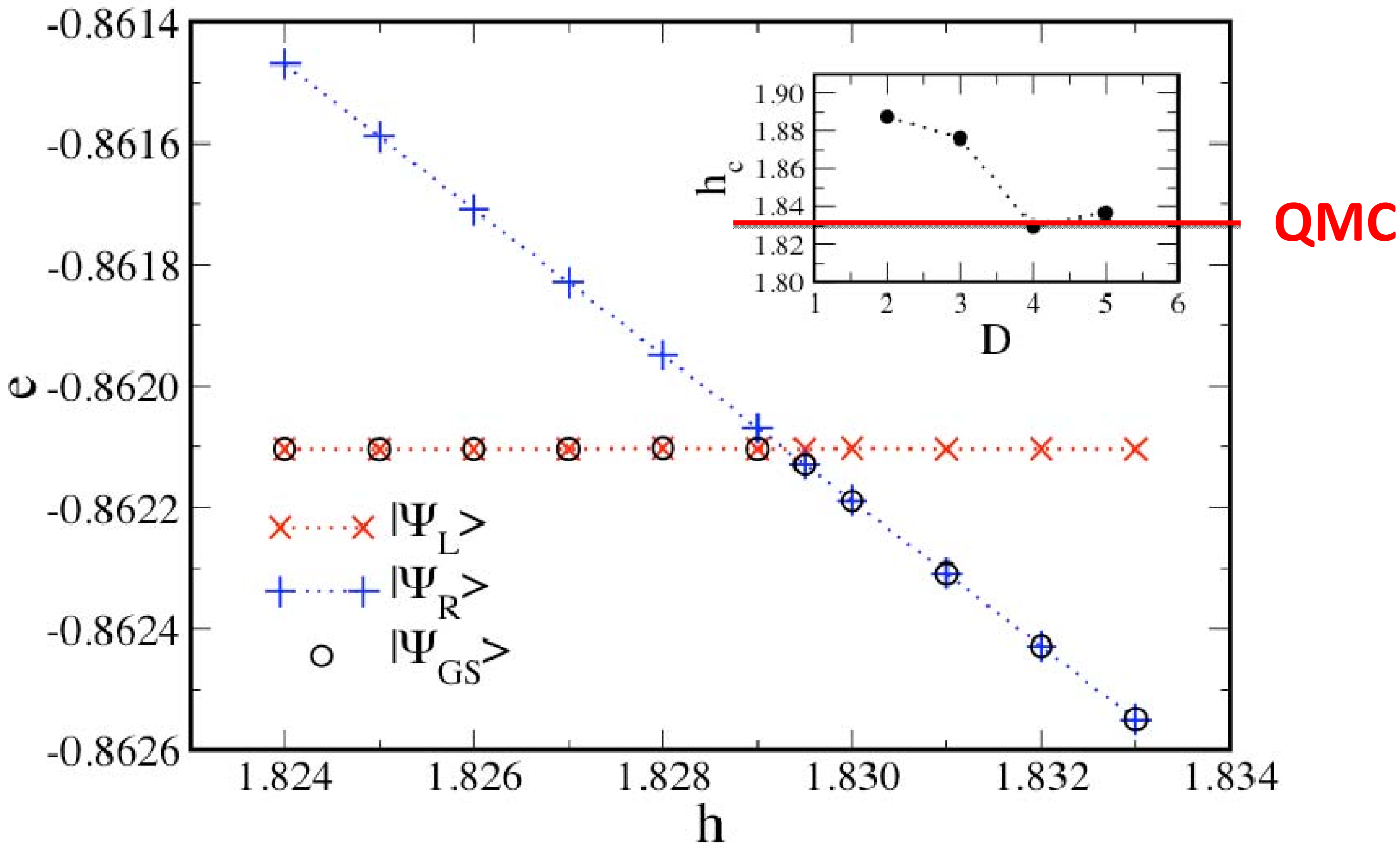


•Pochung Chen, Chen-Yen Lai, Ming-Fong Yang, JSTAT, **10**, P10001, 2009.

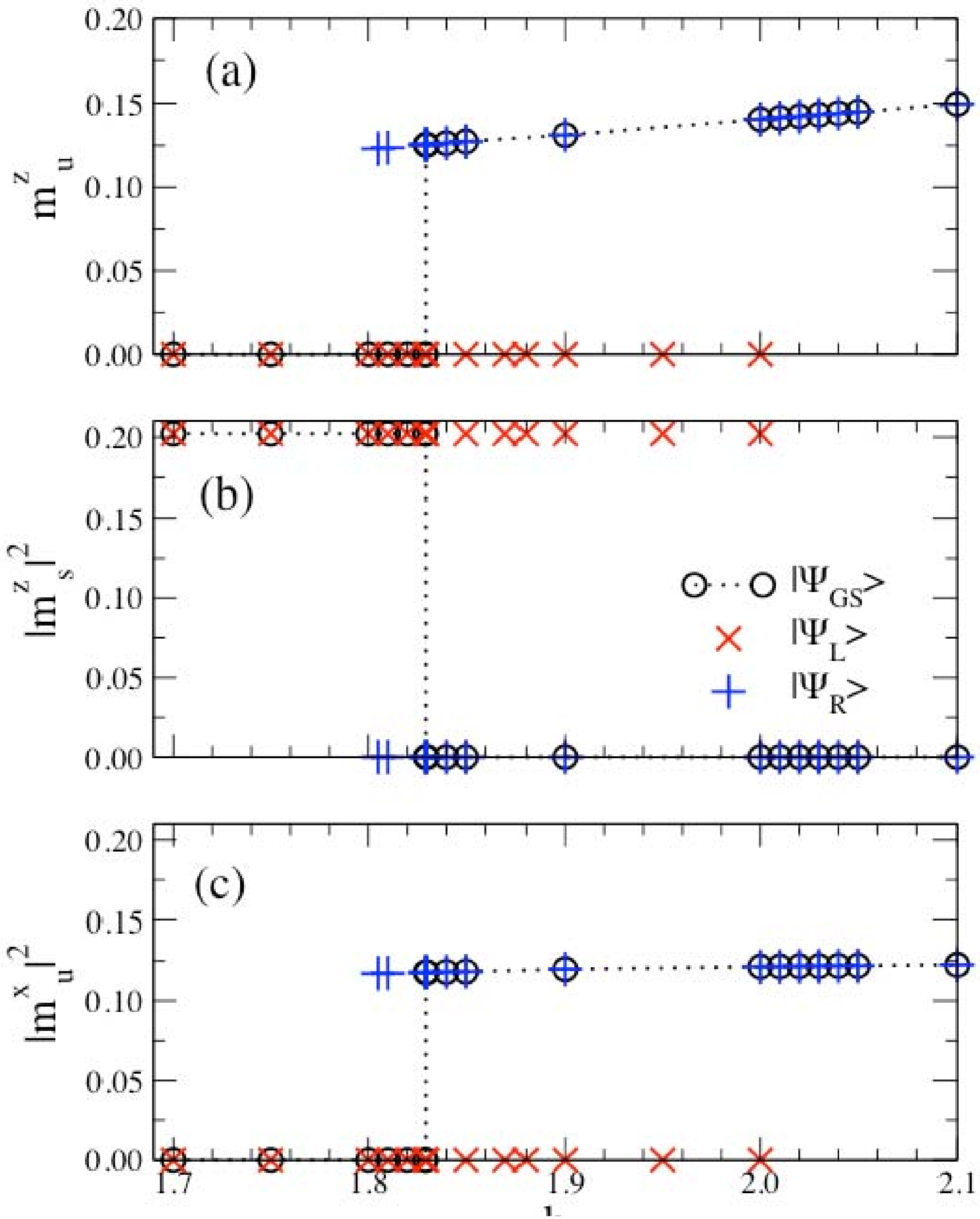
XXZ Model (Δ =1.5)



Level Crossing of 1th Order Transition



Hysteresis



(a)
(b)
(c)
0.20
0.15
0.10
0.05
0.00
1.7
1.8
1.9
2.0
2.1
m^z_u
$|m^z_s|^2$
$|m^x_u|^2$
$|\Psi_{GS}>$
$|\Psi_L>$
$|\Psi_R>$

Summary : It Works!

- Frustrated spin-dimer model.
  - Existence of supersolid phase for a range of J_d.
  - Accurate determination of h_{c2} and h_{c3}.
  - Basic idea of the full phase diagram.

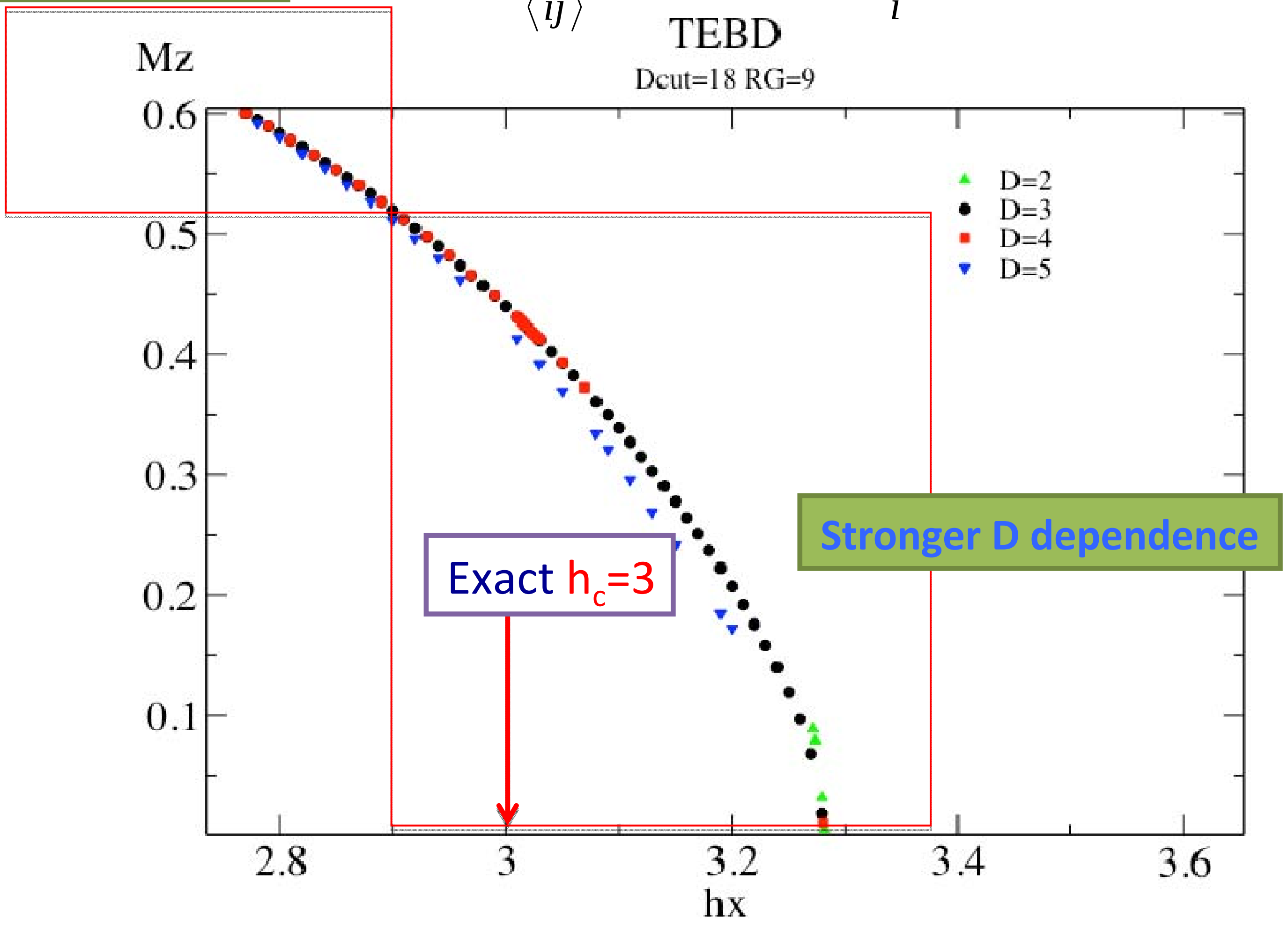
- 2D XXZ model.
  - Accurate determination of first order transition.

Error Analysis

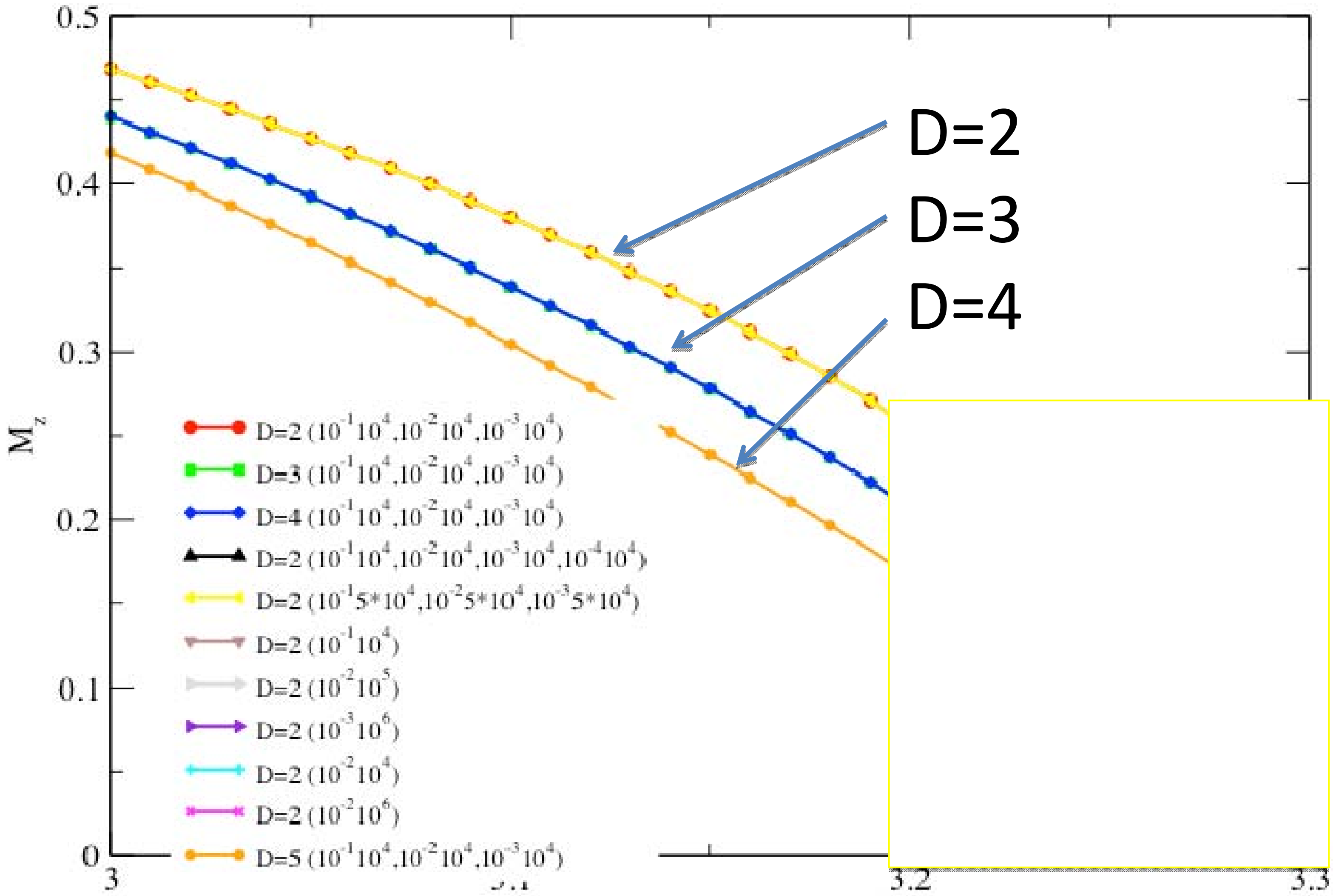
- Possible sources of error
  - Gapless excitation.
  - Trotter error.
  - Inaccurate effective environment.
  - Insufficiently large bond dimension D.
- Comparison with other TNS calculations.
  - Direct optimization of TPS (D=2).
  - iPEPS (iMPS).
  - iPEPS (Corner transfer matrix).

2D Transverse Ising Model

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h_x \sum_i \sigma_i^x$$



Bond dimension *D* dependence



Thank You

以有涯逐無涯

Use the *finiteness* to

capture the *infiniteness*

Tensor network state representation of a many-body state

$$\left|\psi\right\rangle = \sum_{i_1 \cdots i_N} \psi_{i_1 \cdots i_N} \left|i_1 \cdots i_N\right\rangle \Longrightarrow \left|\psi\right\rangle = \sum_{i_1 \cdots i_N} \mathbf{TN}(i_1 \cdots i_N) \left|i_1 \cdots i_N\right\rangle$$

1D MPS $\left|\Psi\right\rangle = \sum_{s_1 s_2 \cdots s_N} \mathrm{Tr}\left[\mathrm{T}_1(s_1) \cdots \mathrm{T}_N(s_N)\right] \left|s_1 s_2 \cdots s_N\right\rangle$