

# Nested Tensor Network Method and its applications

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2018. 07. 11

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## Brief history about tensor network state

Strongly correlated systems is difficult:

- Analytically: non-perturbative, no obvious small parameters
- Numerically: Exponential wall: degree of freedom grows exponentially with system size

*Weak Coupling Approach:* Suitable for weak-coupling systems

- Convert a many-body problem into single-body: mean field theory, density functional theory

*Strong Coupling Approach:*

- keeps only a finite set of many-body basis:
- Configuration interactions(CI), Coupled Cluster Expansion, QMC, Numerical RG.

- ✓ AKLT authors(1987): prototype of matrix product state and honeycomb tensor-network
- ✓ **M. Fannes(1991)**: MPS in name of Finitely Correlated State (FCS), and Tree Tensor Network state (TTN)
- ✓ Niggemann: special TNS for honeycomb Heisenberg model, equivalence between exp. cal. and classical PF
- ✓ Ostlund and Rommer (1995): DMRG (1992)'s wavefunction is a MPS, area law
- ✓ Sierra and Martin-Delgado: general wavefunction ansatz to study a quantum lattice model
- ✓ Nishino: in name of Tensor Product State (TPS), general variational ansatz to study 3D classical model

## Why do we need **tensor** renormalization?

- Projected Entangled Pair State (PEPS, 2004)
- Multi-scale Entanglement Renormalization Ansatz (MERA, 2007)
- Correlator Product State (CPS, 2009)
- Projected Entangled Pair State (PEPS, 2014)

### ✓ Density Matrix Renormalization Group

- Best method for 1D quantum model
- Violet area law
- 2D->1D, artificial long-range interaction
- Hope: extrapolation, even gapped case

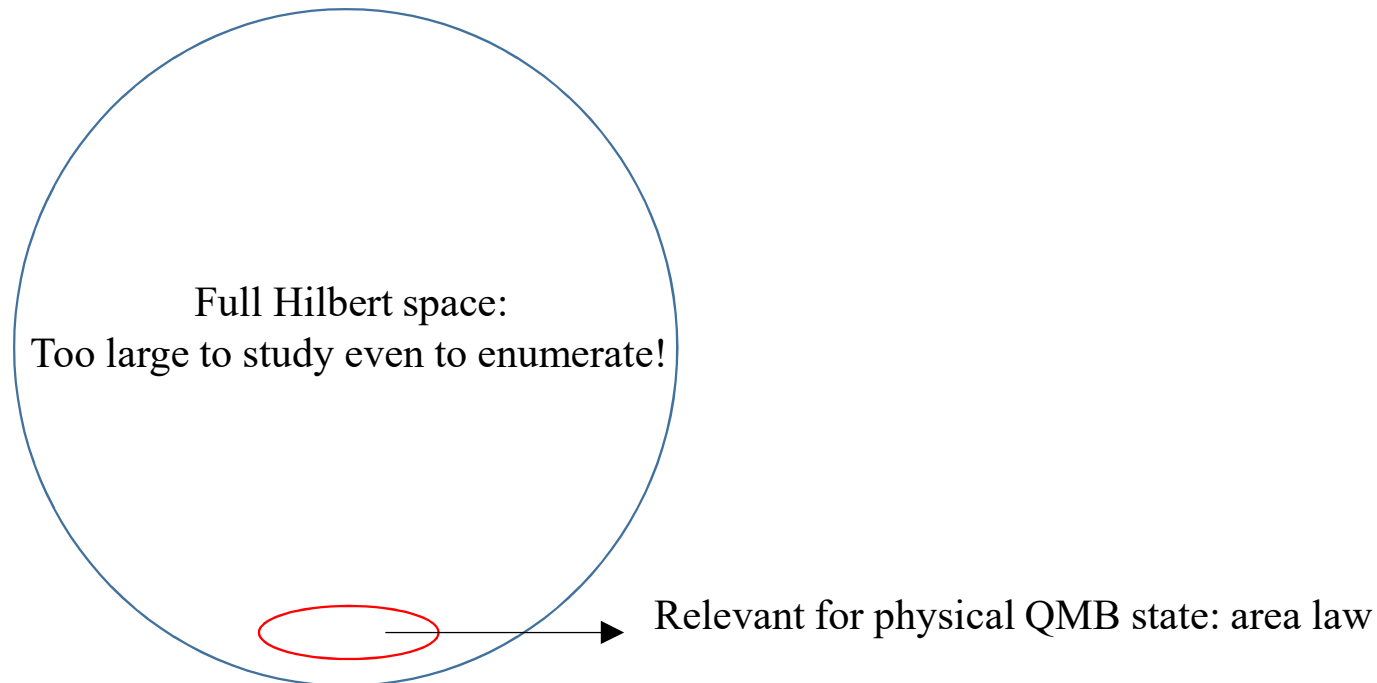
### ✓ Quantum Monte Carlo

- No dimension consideration
- Suffer from the “**minus-sign**” problem for fermion and frustrated spin system

**A possible direction:** Tensor Renormalization (TNS, TNM)

## Why renormalization is possible?

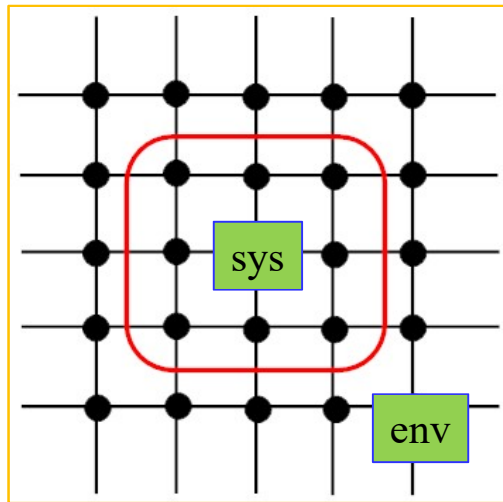
- Hilbert space is compressible:



*Ref:* D. Poulin, A. Qarry, R. Somma, F. Verstraete, Phys. Rev. Lett. 106, 170501 (2011)

## About the corner: Area law of Entanglement Entropy

- (Boundary) Area Law in quantum information: for a gapped system with local H



$$S \sim L^{d-1} \sim \log D_{min}$$

$D_{min}$ :  $N_{min}$  of basis needed to describe the grdst (entanglement entropy) faithfully.

$$\begin{aligned} d = 1: D_{min} &\sim const \\ d = 2: D_{min} &\sim e^L \end{aligned}$$

- 1D: local gapped Hamiltonian with only constant degeneracy of ground state
- Quasi-free (i.e., quadratic int) boson and fermion gapped Hamiltonian: in any D
- Known violation: 1D critical fermion has log correction, 2D critical fermion suggests log correction  
1D critical XY chain (i.e.,  $h \leq 2$  in isotropic case,  $h=2$  in anisotropic case)
- **General belief:** ground state of local gapped Hamiltonian obeys.

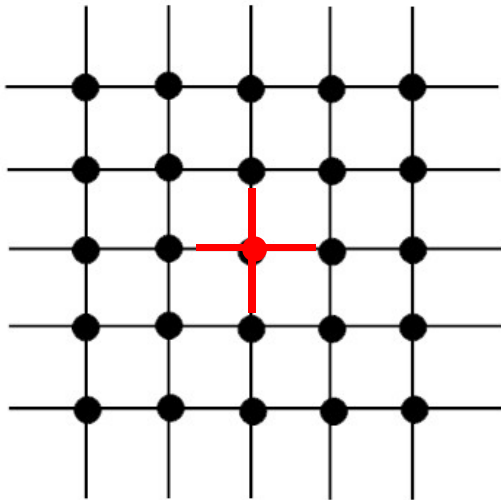
Ref: J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. 82, 277 (2010).

## Classical system: Tensor Network Model

- all statistical models with only local interactions can be represented as *tensor-network models* and effectively evaluated, defined on *real lattice or dual lattice*.

$$Z = \text{Tr} \prod_i T_{x_i y_i z_i w_i}$$

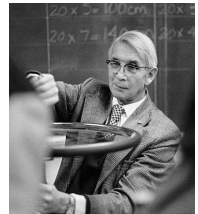
Tensor-network model in real lattice



$$H = -J \sum_{\langle ij \rangle} S_i S_j$$

$$\begin{aligned} Z &= \sum_{S_1 \dots S_N} \exp\left(\beta \sum_i S_i S_{i+1}\right) \\ &= \text{Tr}(A \cdots A) \\ &= \lambda_{\max}^N \quad N \rightarrow \infty \end{aligned}$$

$$A = \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix}$$

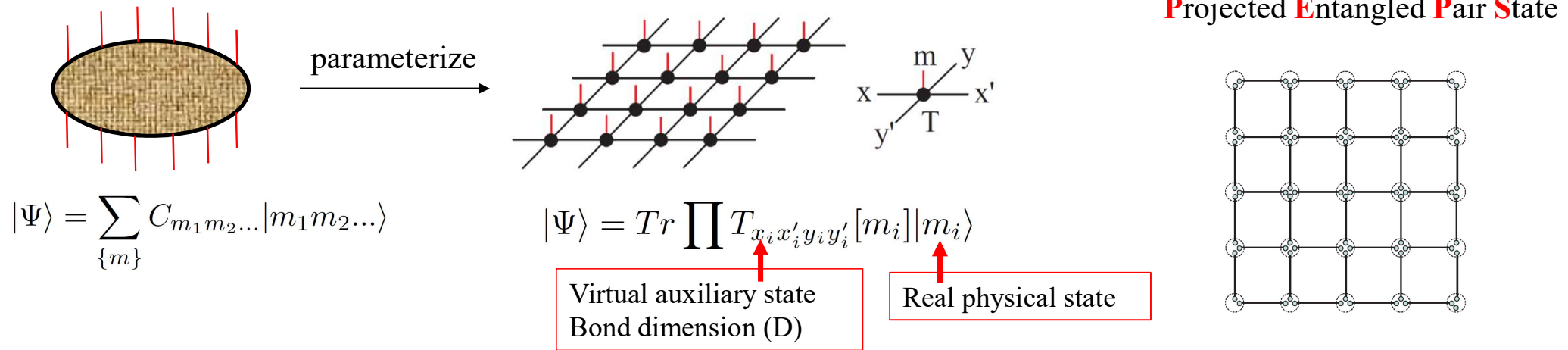


Ernst Ising

## Quantum lattice system: Tensor Network State (TNS)

- *Tensor network state* provides a faithful representation of the ground state wavefunction of a quantum lattice model that satisfies the area law of the entanglement entropy.

- A kind of construction, e.g., PEPS:  $d^N \rightarrow ND^4d$



- 1D case: Matrix Product State (MPS), or Tensor Train, DMRG wavefunction

- ✓ Area law: is believed to be a faithful representation of grdst of *local gapped* H.
- ✓ Formally has no sign problem, can encode fermion sign
- ✓ Can show power-law correlation function, at finite D

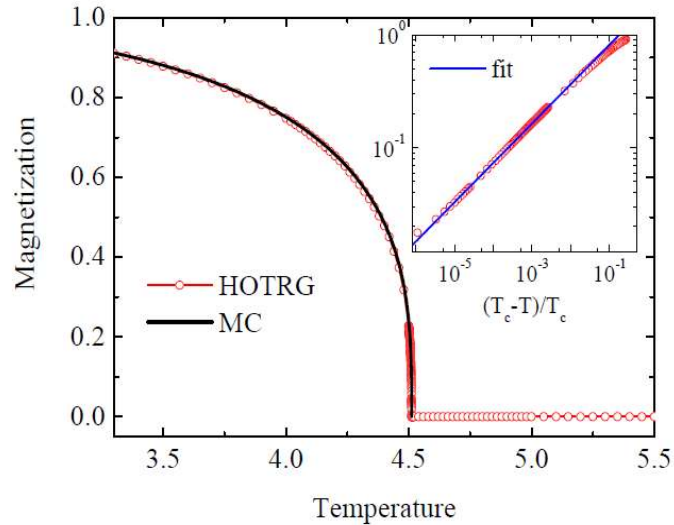
# Successful examples: Ising model on cubic lattice

ZYXie, PRB 86, 045139 (2012)

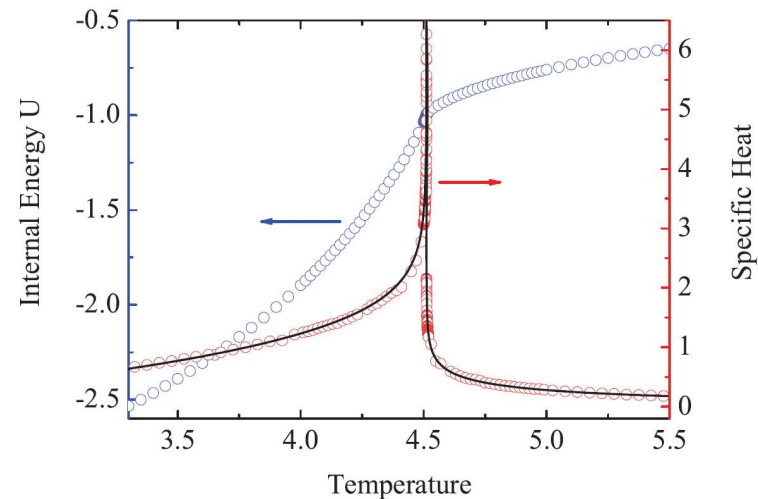
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SWang, et al, CPL 31, 070503 (2014)

## ● Critical point accuracy:



alpha(+): 0.1023  
 alpha(-): 0.1137  
 gamma: 0.3295



| method                   | $T_c$    |
|--------------------------|----------|
| Monte Carlo [33]         | 4.511523 |
| Monte Carlo [25]         | 4.511528 |
| Monte Carlo [35]         | 4.511525 |
| Monte Carlo [36]         | 4.511516 |
| Series Expansion [34]    | 4.511536 |
| KWA [41]                 | 4.5788   |
| CTMRG [13]               | 4.5704   |
| CTMRG [40]               | 4.5392   |
| TPVA [14]                | 4.554    |
| Algebraic variation [37] | 4.547    |
| HOTRG(D=16, from U)      | 4.511544 |
| HOTRG(D=16, from M)      | 4.511546 |

→ former NRG

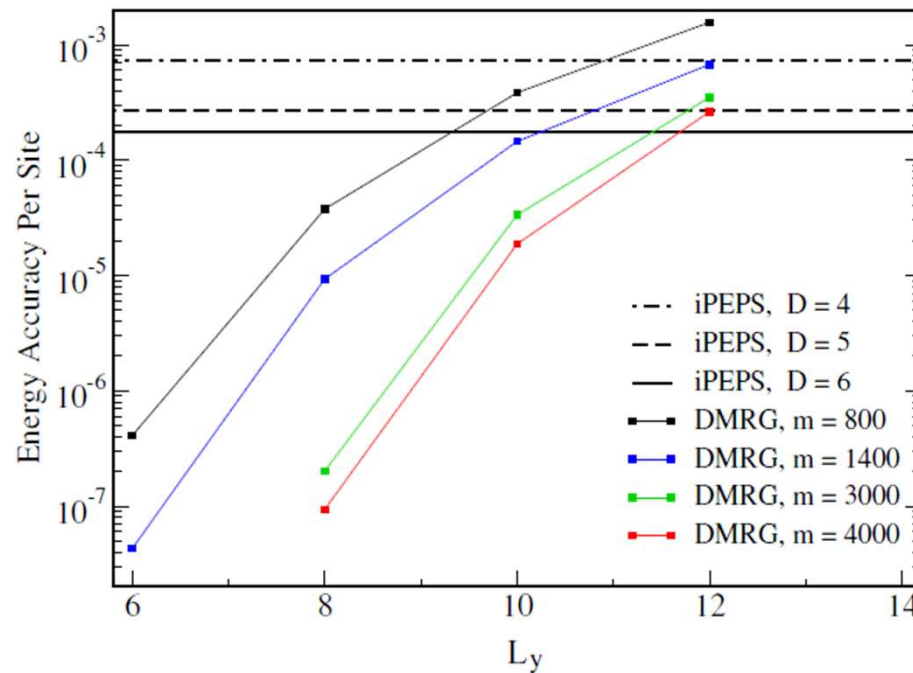
|   |               |
|---|---------------|
| Monte Carlo (2003) <sup>[43]</sup>        | 4.5115248(6)  |
| Monte Carlo (2010) <sup>[44]</sup>        | 4.5115232(17) |
| HOTRG ( $D = 16$ ) (2012) <sup>[24]</sup> | 4.511544      |
| HOTRG ( $D = 23$ , this work)             | 4.51152469(1) |



## Successful examples: Heisenberg model on square lattice

S.R.White, et al, Annu. Rev. CMP 3, 111(2012)

### ➤ spin-1/2 AF Heisenberg model on square lattice: PEPS



Energy accuracy  
VS  
Cylinder width

**DMRG:**

jumps fast as width( $L_y$ ) grows

**PEPS:**

improves as D grows

**6 > 4000**

Note:

iPEPS reference: VMC extrapolation in Sandvik PRB 56, 11678(1997)

DMRG reference: DMRG extrapolation in truncation error at given size.

## Edward-Anderson model on square (with PBC)

$$H(\underline{\sigma}) = - \sum_{(ij) \in E} J_{ij} \sigma_i \sigma_j - \sum_{i \in V} h_i \sigma_i$$

$$P(J) = p\delta_1 + (1-p)\delta_{-1}$$

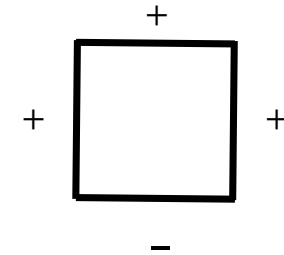
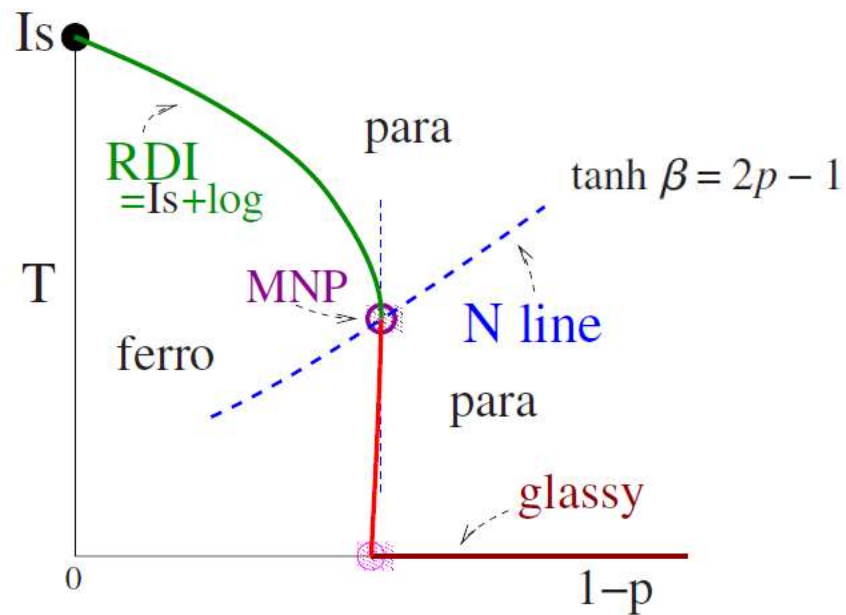


TABLE I. Location of the MNP.

| Methods               | $p^*$         |
|-----------------------|---------------|
| BP [28]               | 0.79          |
| GBP [27,28]           | 0.85          |
| Duality analysis [32] | 0.889 972     |
| Duality analysis [33] | 0.890 813     |
| pTRG                  | 0.890 830(22) |
| Monte Carlo [29]      | 0.890 81(7)   |
| Monte Carlo [43]      | 0.890 83(3)   |



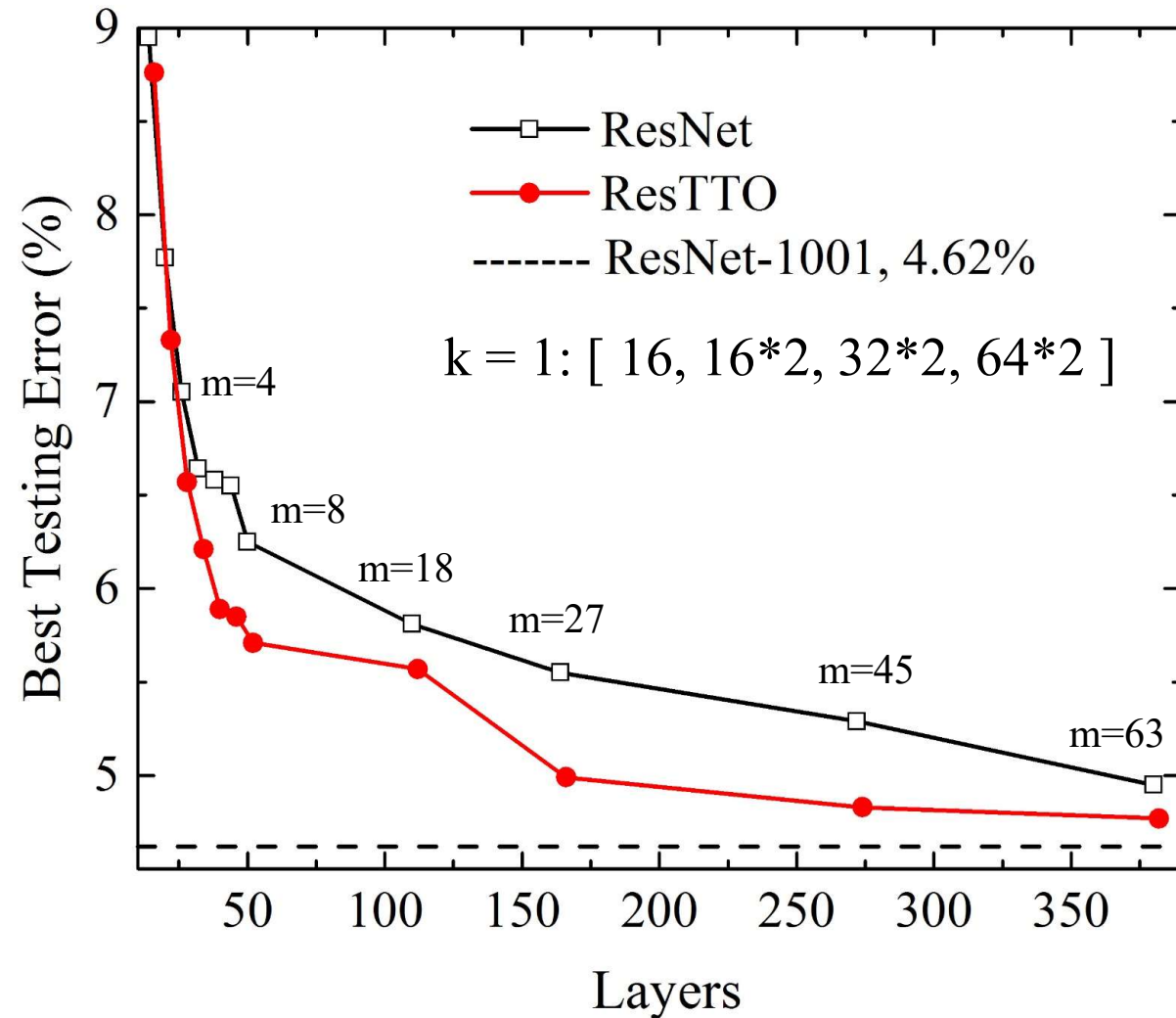
PRB 90, 174201 (2014)

# Deep Learning: ResNet

Our group, *to appear soon*

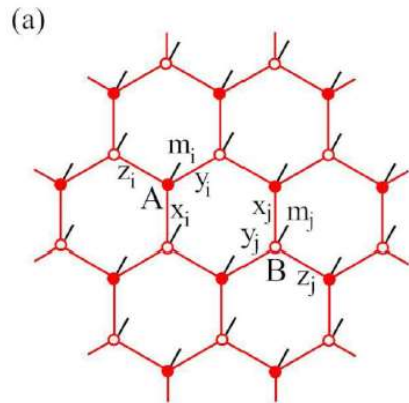
- Additional parameters:  
 $k=1$ ,  $N_a \sim 2300$   
 $k>1$ ,  $N_a \sim 2700 + 8k^2$
- ResNet parameters:  
 $N \sim 400 + 2950*k$   
 $+ (9.6*m-2.5)*10^4 *k^2$

| m  | Layers | $N_a / N$ | Best testing error |
|----|--------|-----------|--------------------|
| 4  | 28     | 0.63%     | 7.05% -> 6.57%     |
| 8  | 52     | 0.31%     | 6.25% -> 5.71%     |
| 18 | 112    | 0.13%     | 5.81% -> 5.57%     |
| 27 | 166    | 0.09%     | 5.55% -> 4.99%     |
| 45 | 274    | 0.05%     | 5.25% -> 4.83%     |
| 63 | 382    | 0.04%     | 4.95% -> 4.77%     |

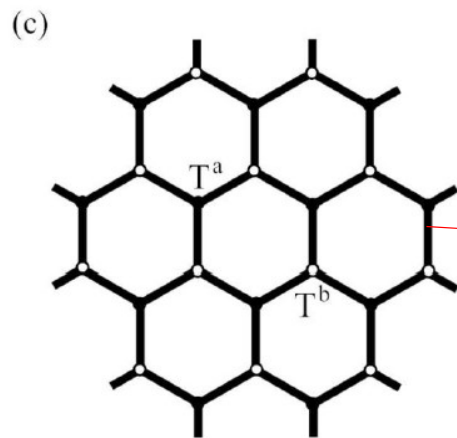


➤ Quantum lattice model:

1. determine the tensor-network representation of targeted wave-function: time-evolution, energy minimization



$$|\Psi\rangle = \text{Tr} \prod_{i \in A, j \in B} A_{x_i y_i z_i}[m_i] B_{x_j y_j z_j}[m_j] |m_i m_j\rangle$$



• Time evolution: 
$$e^{-\beta H} |\Psi\rangle = \sum_i e^{-\beta E_i} |\phi_i\rangle \xrightarrow{\beta \rightarrow \text{inf}} e^{-\beta E_0} |\phi_0\rangle$$

how to update/renormalize after a small evolution step

$$||\Psi_f\rangle - e^{-\tau H} |\Psi_i\rangle|$$

(1). Simple update (entanglement mean field approximation)

✓ Use the local entanglement spectra as effective environment

✓ local tree approximation which can be solved by SVD/HOSVD

(2). Full update (Global variation)

Solve the linear equation iteratively  $NX = M^e$

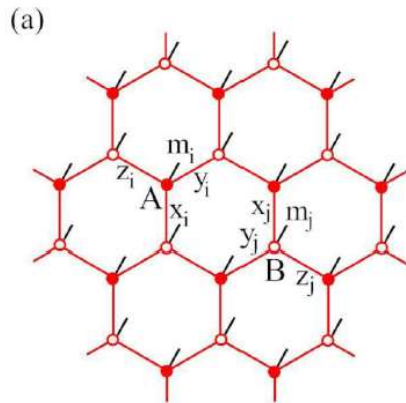
(3). Cluster update:

Use small cluster and its mean field as effective environment

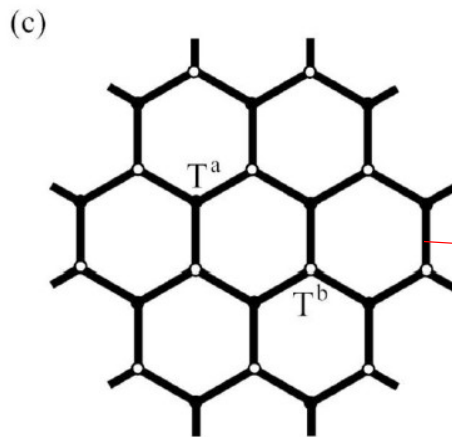
## Bottleneck

➤ Quantum lattice model:

1. determine the tensor-network representation of targeted wave-function:



$$|\Psi\rangle = \text{Tr} \prod_{i \in A, j \in B} A_{x_i y_i z_i}[m_i] B_{x_j y_j z_j}[m_j] |m_i m_j\rangle$$



Bond dimension:  $D^2$

● Energy minimization (global extremum problem):

find a PEPS  $|\Psi\rangle$  which minimize the energy:

$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

This can be done equivalently as an optimization problem

$$\min_{|\Psi\rangle \in \text{family}} (\langle \Psi | H | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle)$$

which can be reduced to generalized eigenvalue problem

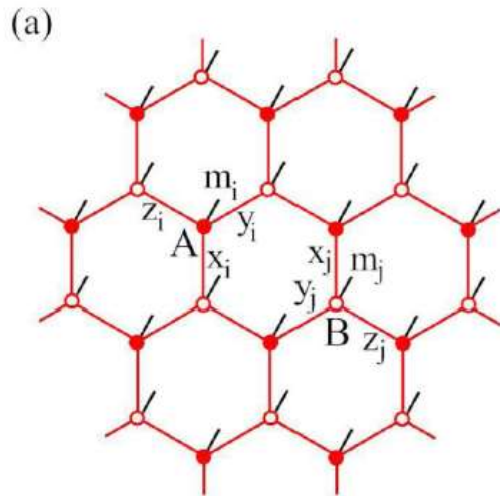
$$H^e X = \lambda N X$$

## Bottleneck

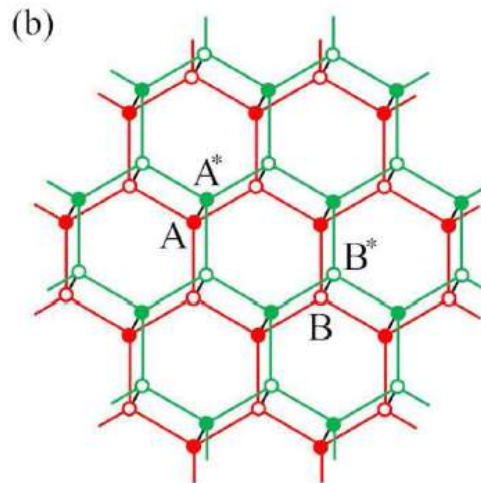
2. contract the network to get the expectation value

Green:  $\langle \Psi |$   
Red:  $|\Psi \rangle$

$$\langle O \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

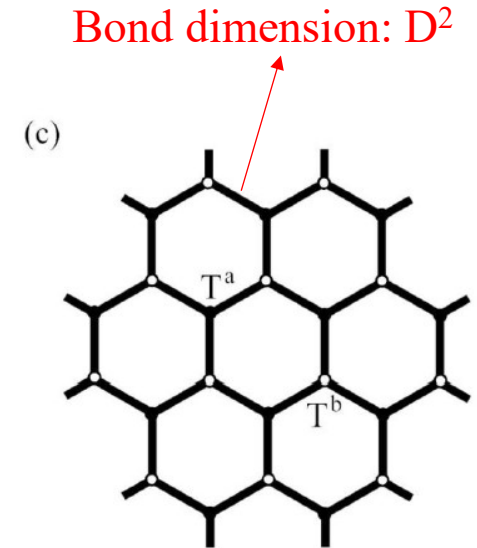


$$|\Psi\rangle = \text{Tr} \prod_{i \in A, j \in B} A_{x_i y_i z_i}[m_i] B_{x_j y_j z_j}[m_j] |m_i m_j\rangle$$



$$T_{xx',yy',zz'}^a = \sum_m A_{xyz}[m] A_{x'y'z'}^*[m],$$

$$T_{xx',yy',zz'}^b = \sum_m B_{xyz}[m] B_{x'y'z'}^*[m].$$



Reduced Tensor Network

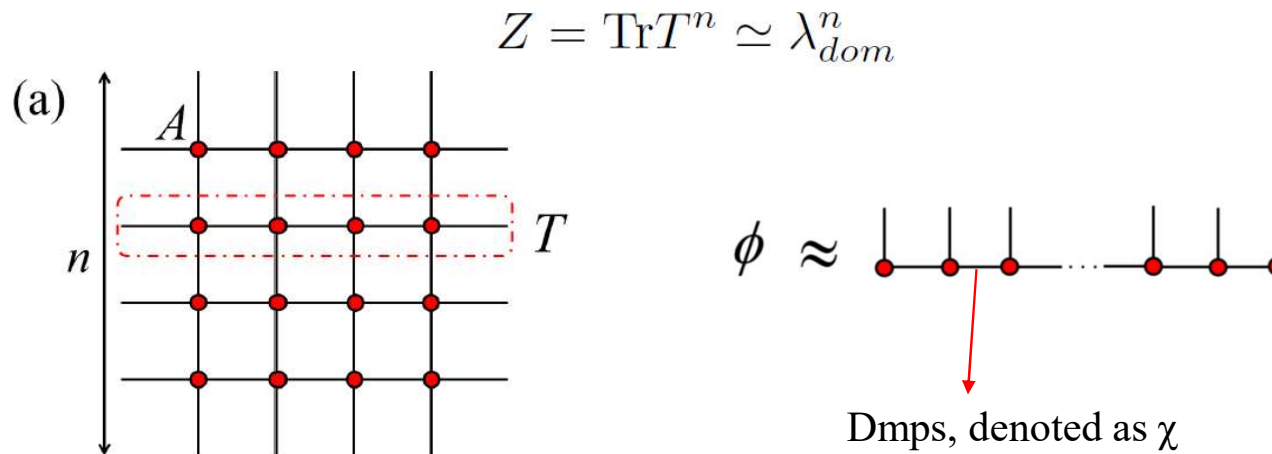
- Renormalization: Compression of DOF (real Hilbert space, or virtual space) by discarding the irrelevant
- Contraction of **RTN** with  $D^2$ : seems unavoidable, the main bottleneck of all TRG methods!

## Why do we need large $D$ and large $\chi$

✓ Time Evolving Block Decimation (TEBD) / Boundary MPS

Target: effective MPS representation of the **dominant eigenvector**

✓ Power method with truncation: not variational!



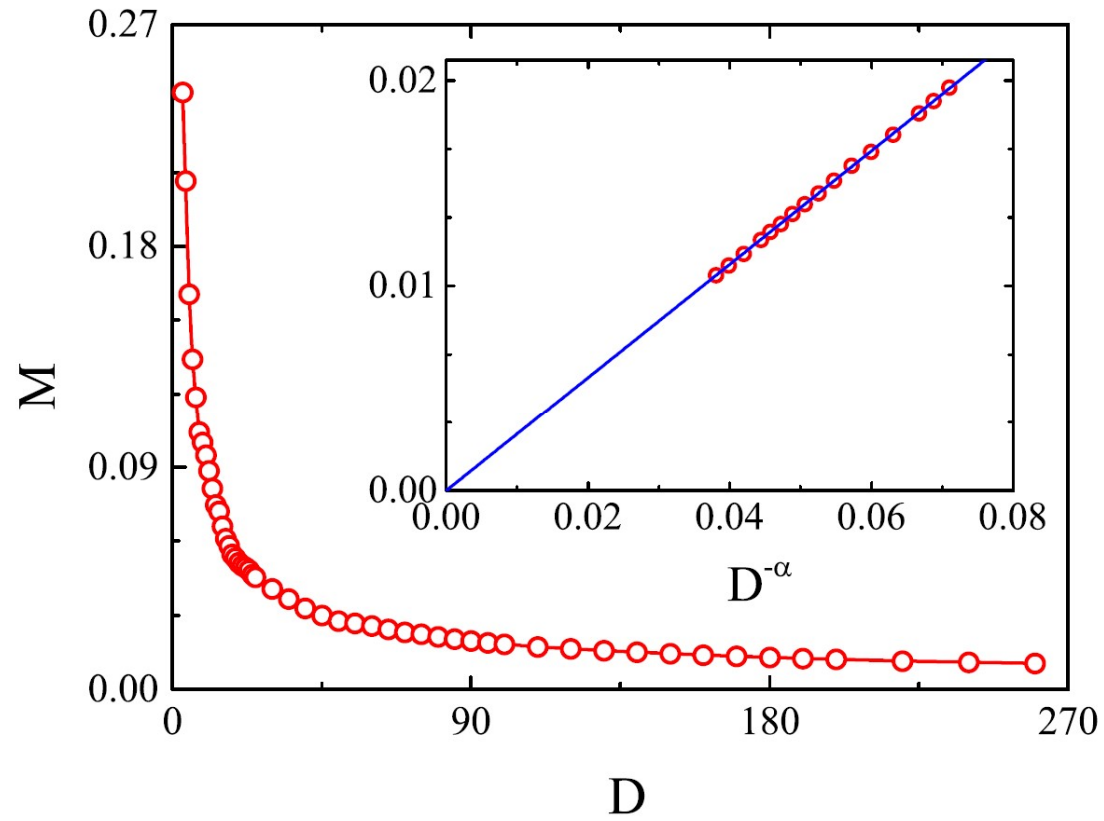
A huge and terrible task!

Memory:  $D^4 \chi^2$   
CPU:  $D^6 \chi^3$

D=10: 750M  
D=13: 6G  
D=20: 190G  
D=25: 1.1T

✓ In principle: We always need a curve of  $O(D)$ , in which each point is obtained by  $\chi$ -scaling ( $\chi \sim D^2$ ).

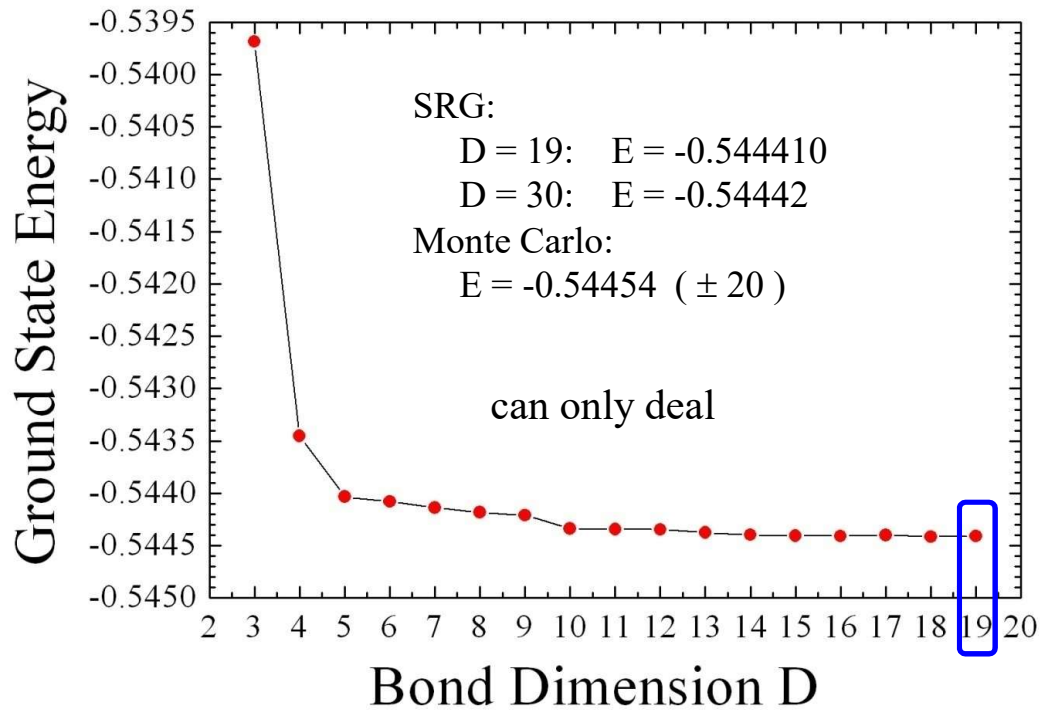
Even though we can obtain wavefunction with very larger  $D$





We can only deal with small D when doing expectation value calculation

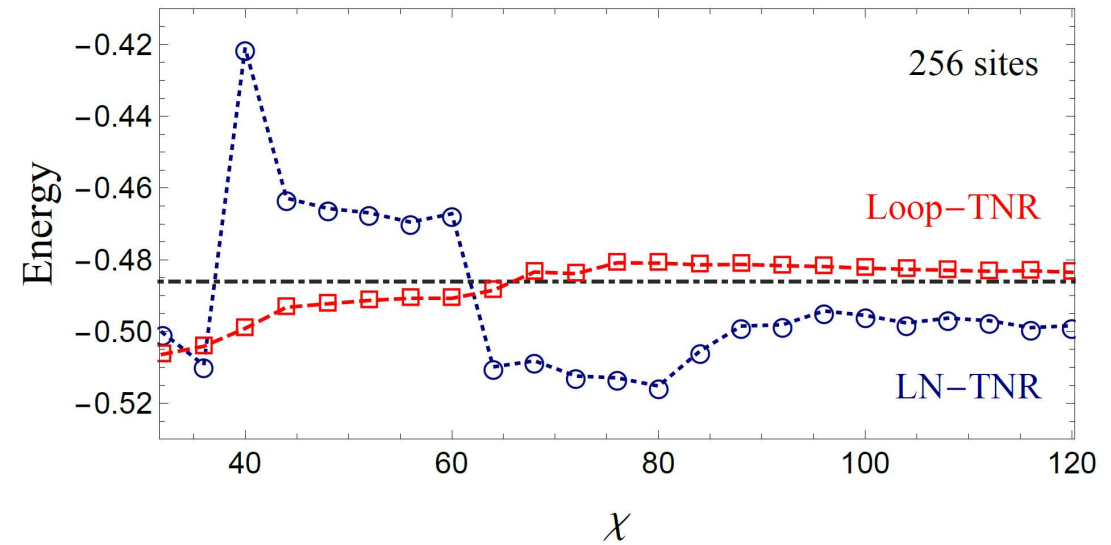
HHZhao, *et al*, PRB 81, 174411 (2010)



AF Heisenberg model on honeycomb lattice  
 With U(1) symmetry

$$S[x_i] + S[y_i] + S[z_i] = m_i$$

Shuo Yang, *et al*, PRL 118, 110504 (2017)



3-state RVB wavefunction

( $J_1$ - $J_2$  AF Heisenberg model on square lattice): N = 256

## Especially for Fermion: Larger D

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### Fermions with 2D tensor networks

**Simulate fermions in 2D?**

Before April 2009: **NO!**

Since April 2009: **YES!**

Short-range correlation in momentum space,  
long-range correlation in real space,  
more entanglement entropy  
Fermi surface, BEC(Bose metal)

P. Corboz's contribution:

PRL 113, 046402 (2014): t-J,  $D^*=7$

PRB 93, 045116 (2016): Hubbard,  $D^*=8$

Science 358, 1155 (2017): Hubbard,  $D^*=8\sim 9$

#### Different formulations:

P. Corboz and G. Vidal, Phys. Rev. B 80, 165129 (2009)

T. Barthel, C. Pineda, and J. Eisert, Phys. Rev. A 80, 042333 (2009)

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, Phys. Rev. A 81, 052338 (2010)

Q.-Q. Shi, S.-H. Li, J.-H. Zhao, and H.-Q. Zhou, arXiv:0907.5520

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, Phys. Rev. A 81, 010303(R) (2010)

C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A 81, 050303(R) (2010)

P. Corboz, R. Orus, B. Bauer, G. Vidal, PRB 81, 165104 (2010)

I. Pizorn, F. Verstraete, Phys. Rev. B 81, 245110 (2010)

Z.-C. Gu, F. Verstraete, X.-G. Wen. arXiv:1004.2563

Even very strong misunderstanding, e.g.,

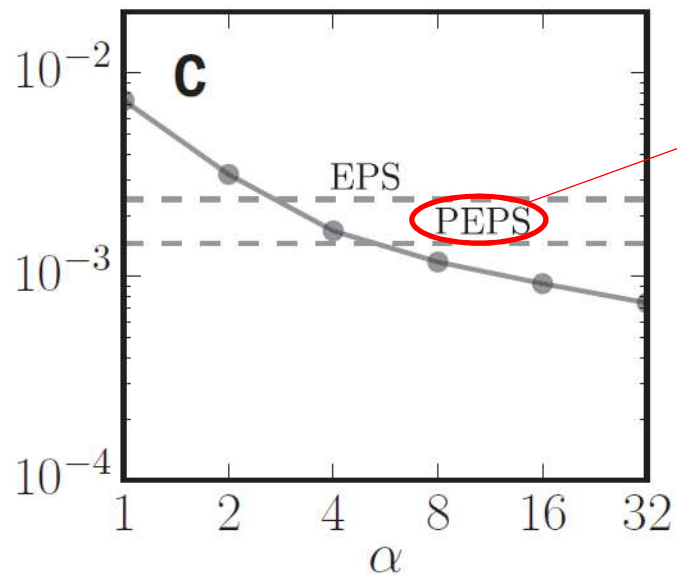


Editor's Summary

### Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo and Matthias Troyer (February 9, 2017)

*Science* **355** (6325), 602-606. [doi: 10.1126/science.aag2302]



$D \leq 6$ , in PRB 90, 064425 (2014)

dashed line). **(c)** Accuracy for the AFH model on a 10-by-10 square lattice with PBCs, compared with the precision obtained by EPS [upper dashed line (35)] and PEPS [lower dashed line (36)]. For all cases considered here, the NQS approach reaches MPS-grade accuracies in one dimension and systematically improves the best known variational states for 2D finite lattice systems.

## For Monte Carlo: Larger Size is important!

Y. Iqbal, et al, arXiv: 1606.02255

T. Li, arXiv: 1601.02165

Finite size vs Thermodynamic limit  
**qualitatively different**

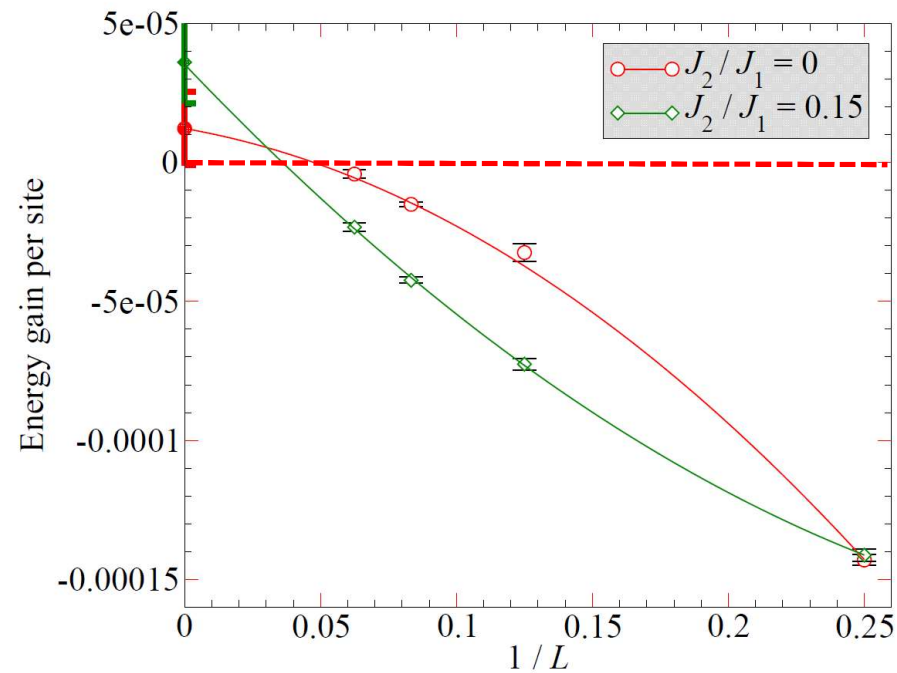
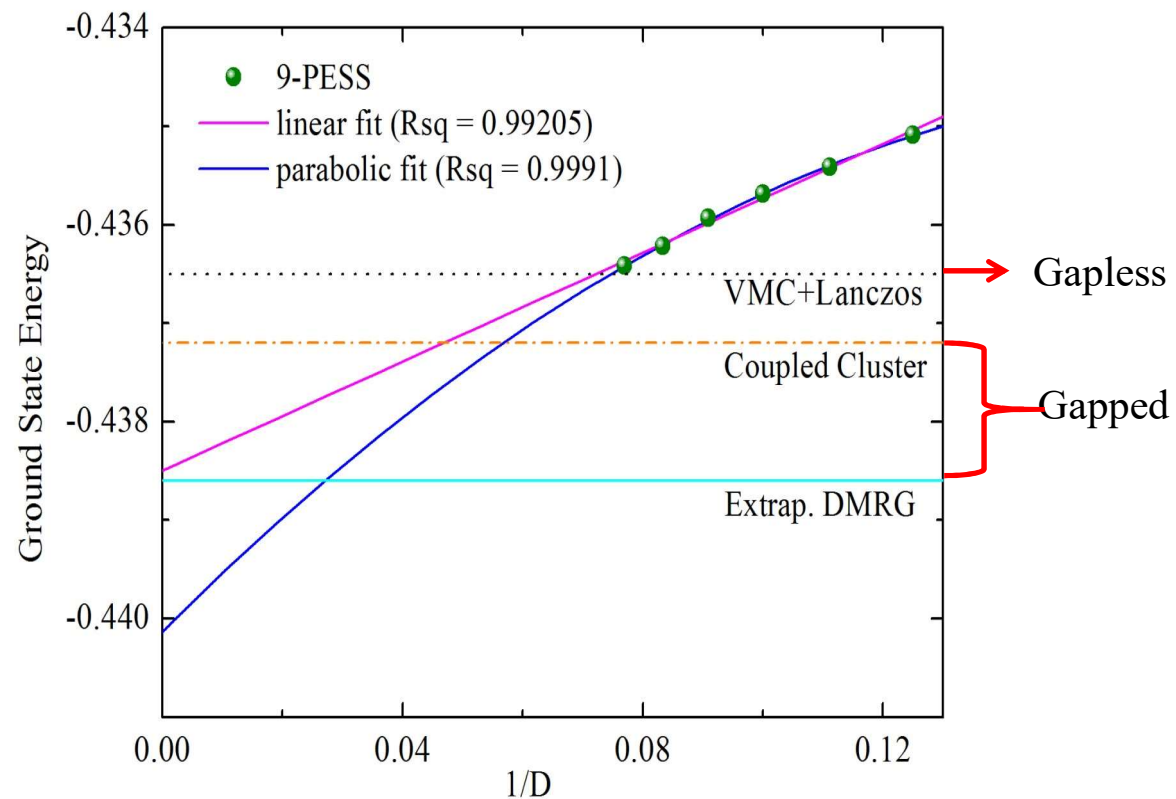
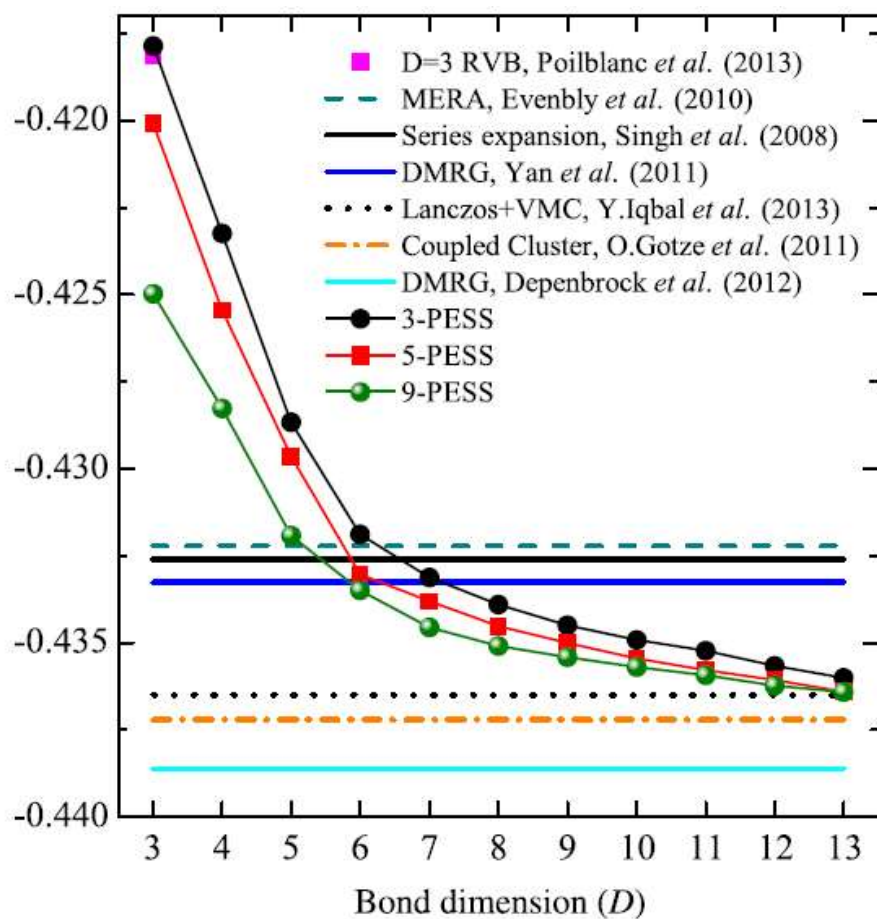


FIG. 1. The size scaling of the energy gain per site  $\Delta E = E_{Z_2} - E_{U(1)}$  is shown for  $J_2 = 0$  and  $J_2/J_1 = 0.15$ , for  $L = 4, 8, 12$  and  $16$  clusters. The results for  $L = 4$  and  $8$  are from Ref. [4].

For TNS: Larger  $D$  is important!



Which extrapolation is the correct one!  
Gapped or gapless?

# Accept ? No! Some former efforts

Green:  $\langle \Psi |$   
Red:  $|\Psi \rangle$

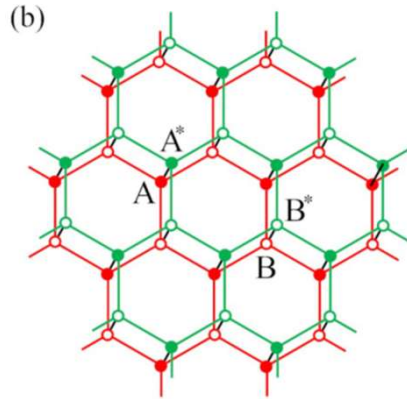
- ◆ Partial summation of the physical indices: Monte Carlo sampling

[33] L. Wang, I. Pizorn, and F. Verstraete, *Phys. Rev. B* **83**, 134421 (2011).

[34] W.-Y. Liu, S.-J. Dong, Y.-J. Han, G.-C. Guo, and L. X. He, *Phys. Rev. B* **95**, 195154 (2017).

[35] H.-H. Zhao, K. Ido, S. Morita, and M. Imada, [arXiv:1703.03537](https://arxiv.org/abs/1703.03537).

[Phys. Rev. B 96, 85103 \(2017\)](#)



Does not change the scaling  
Accuracy is lost due to the sampling

System size is limited

- ◆ Single-layer contraction: use only **bra** or **ket**, not their product.

Iztok Pizorn, et al, *Phys. Rev. A* **83**, 052321 (2011)

$$\langle O \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Change the target  
Accuracy is greatly lost

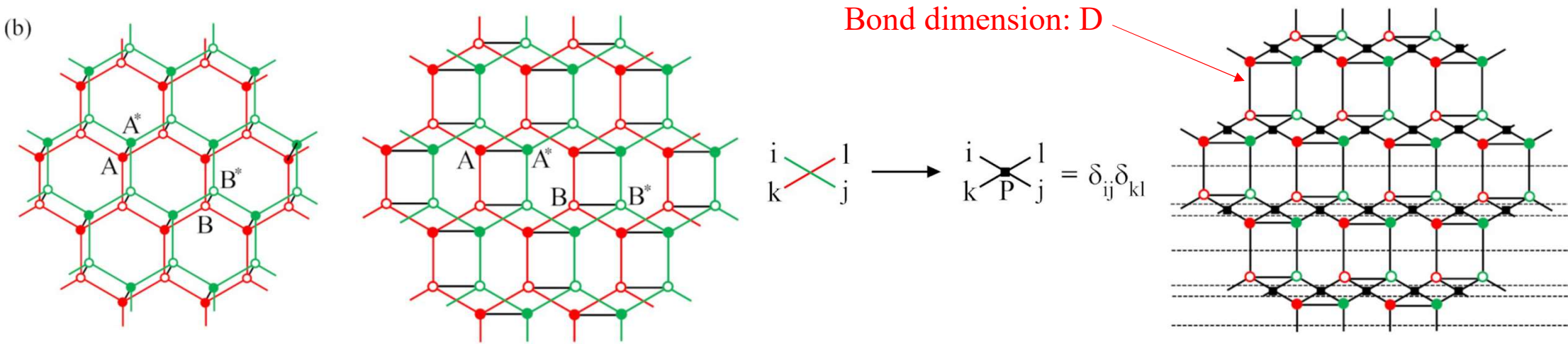
Accuracy is lost

# Nested Tensor Network: Dimension Reduction Technique

Idea: physical indices are not summed over first, but remained and projected to the virtual plane

Green:  $\langle \Psi |$   
Red:  $|\Psi \rangle$

ZYXie, *et al*, PRB 96, 045128 (2017)

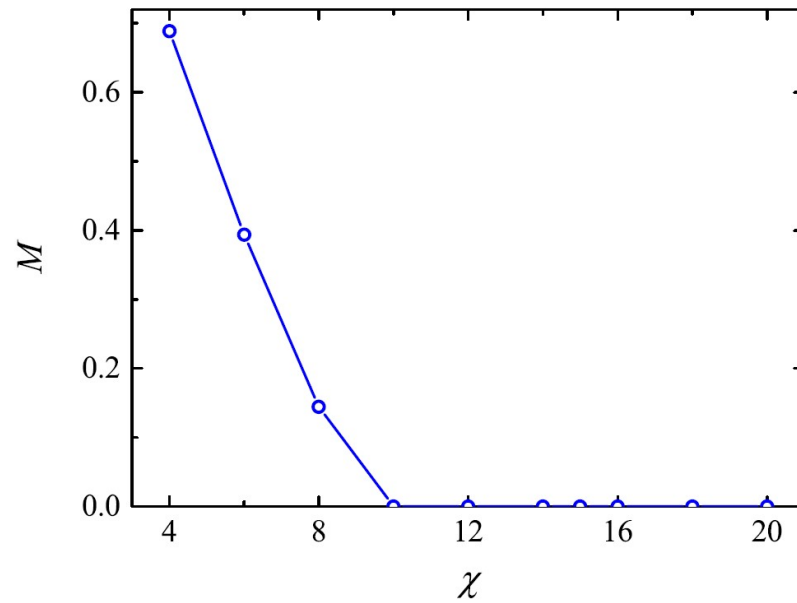


Seems trivial, but the consequence is non-trivial:

Memory:  $D^4 \chi^2 \rightarrow D^2 \chi^2$   
 CPU:  $D^6 \chi^3 \rightarrow D^3 \chi^3$   
 D: **10~13**  $\rightarrow$  **25~30**

Does not change the target  
 Change the scaling essentially  
 Accuracy is actually improved by keeping larger  $\chi$

## Validity Test: Some known state



spin-2 SSS on Kagome:  $D=3$   
 $E = 0, M = 0$

RVB state on KAFH:  $D=3$   
 $E = -0.393124(1)$  finite-size-scaling  
 $E = -0.393123$



## Application 1: Spin-1/2 Kagome anti-ferromagnetic Heisenberg (AFHK) model

$$H = J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

### Valence bond crystal

Singh & Huse, PRB 2008 **series expansion**  
 Evenbly & Vidal, PRL 2010 **MERA**  
 Iqbal, Becca & Poilblanc, PRB 2011 **VMC**

### Gapped spin liquid (Topological)

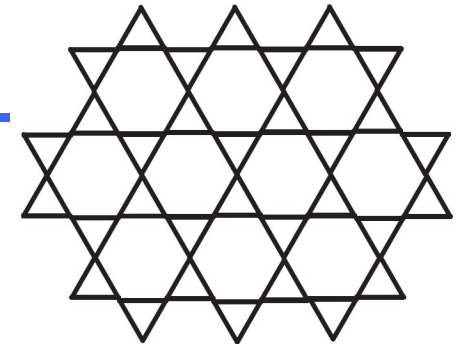
Jiang, Weng & Sheng, PRL 2008 **DMRG**  
 Yan, Huse & White, Science 2011 **DMRG**  
 Depenbrock, McCulloch & Schollwock, PRL 2012 **DMRG**  
 Jiang, Wang & Balents, Nature Physics 2012 **DMRG**  
 Gong, Zhu & Sheng, Scientific Reports 2014 **DMRG**  
 Li, arXiv:1601.02165 **VMC**  
 Mei, Chen, He & Wen, arXiv:1606.09639 **SU(2)-PESS**

### Gapless spin liquid (Algebra)

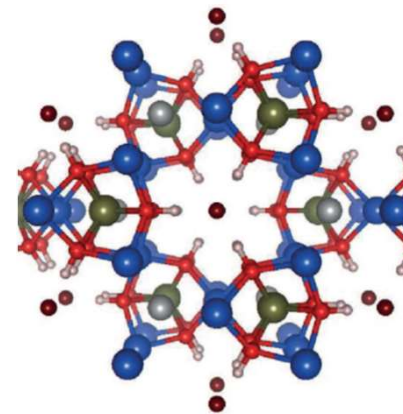
Hastings, PRB 2000  
 Ran, Hermele, Lee & Wen, PRL 2007 **VMC**  
 Iqbal, Becca, Sorella & Poilblanc, PRB 2013 **VMC+Lanczos**  
 Hu, Gong, Becca & Sheng, PRB 2015 **VMC**  
 Jiang, Kim, Han & Ran, arXiv:1610.02024 **SU(2)-PEPS**  
 He, Zaletel, Oshikawa & Pollmann, arXiv:1611.06238 **DMRG**

### Experiment:

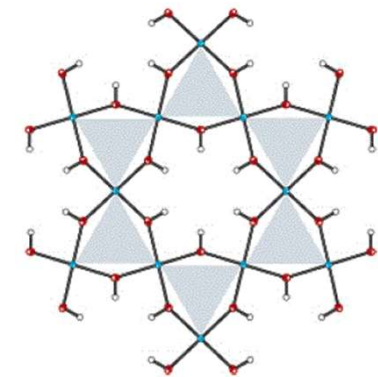
**Nutron Scattering:** tends gapless  
 T. H. Han, *et al*, Nature(2012).  
**NMR:** gapped  $\sim [0.03, 0.07]$   
 M.X.Fu, *et al*, Science(2016)



Kaomge lattice



$\text{Cu}_3\text{Zn}(\text{OH})_6\text{FBr}$



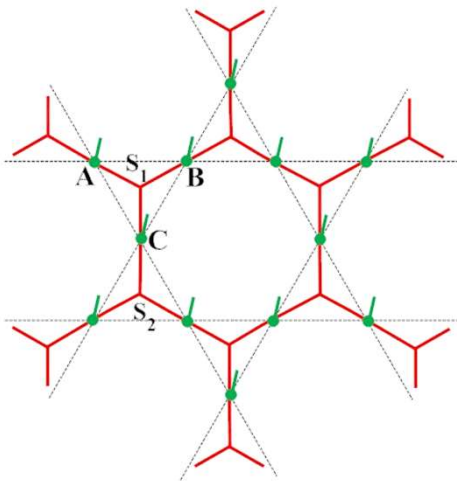
Herbertsmithite  
 $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$

# Generalization pair entanglement to simplex entanglement

## Projected entangled *simplex* states (PESS) ansatz

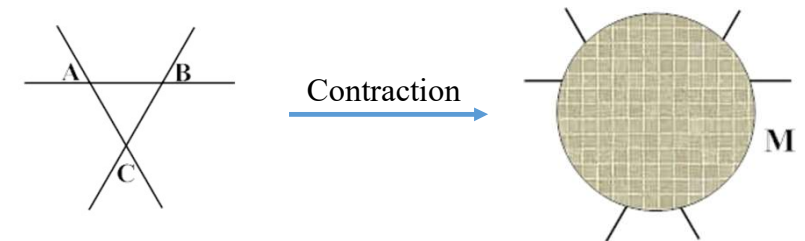
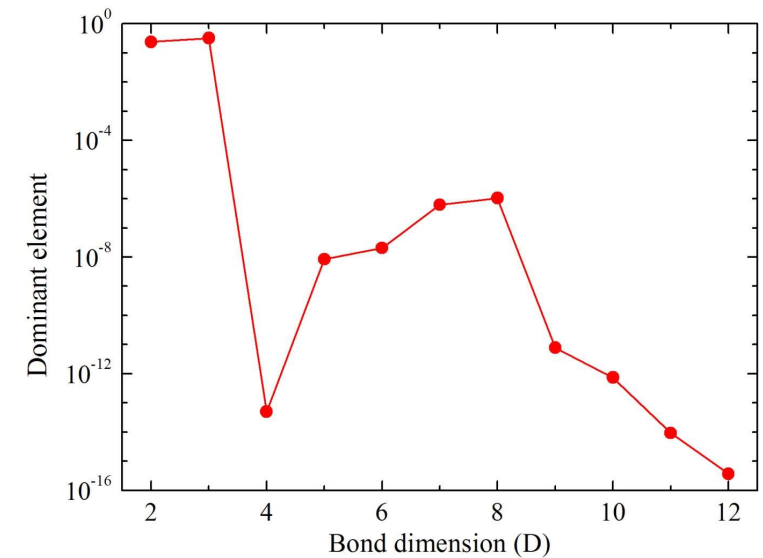
ZYXie, *et al*, PRX 4, 011025 (2014).

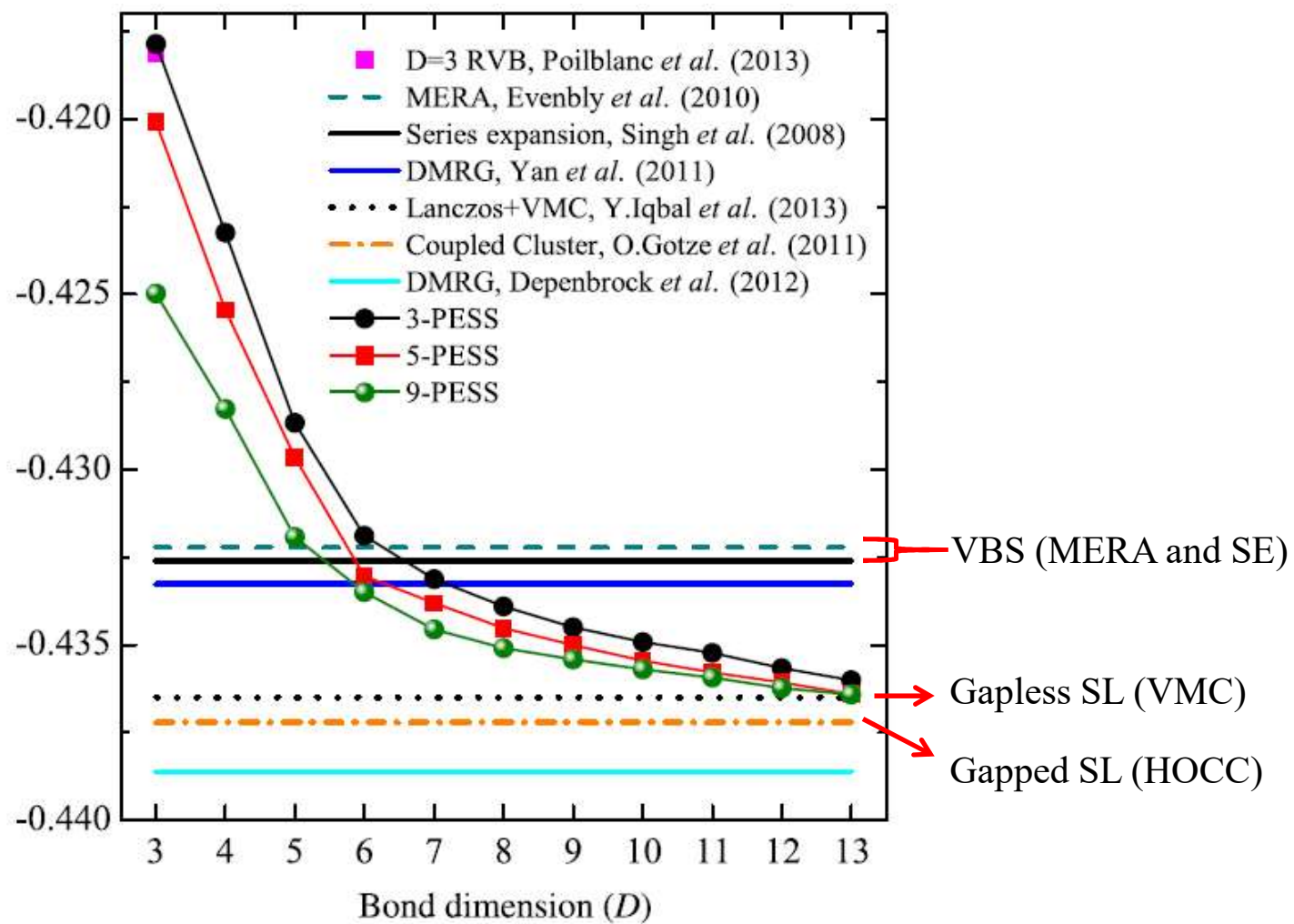
Simplex ~ possible building block, such as triangle for Kagome



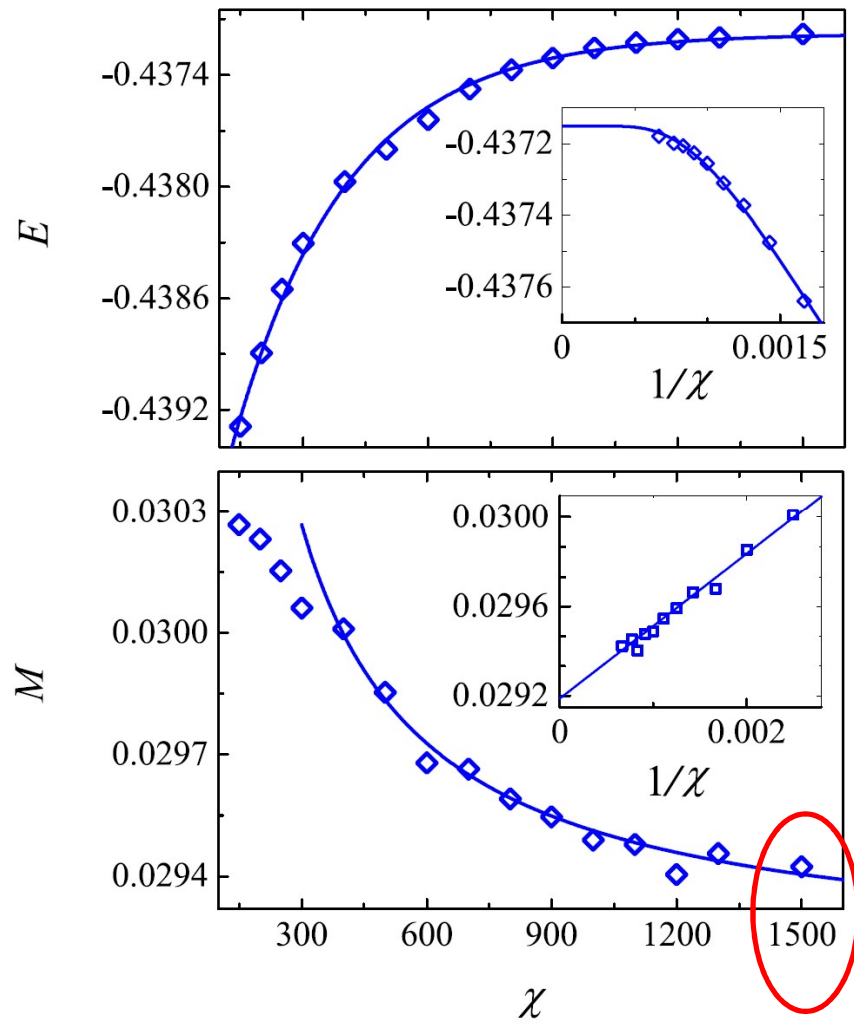
- Introduce a simplex tensor  $S$ :  
triangle/simplex entanglement, instead of pair
- defined on unfrustrated lattice:  
honeycomb, no hidden frustration here!
- A better representation for frustrated systems

$$|\Psi\rangle = \sum_{\{m\}} \sum_{ijkl\dots} A_{ia}[m_1] B_{jb}[m_2] C_{kc}[m_3] S_{1,abc} S_{2,ij'k'} \dots |m_1 m_2 m_3 \dots\rangle$$



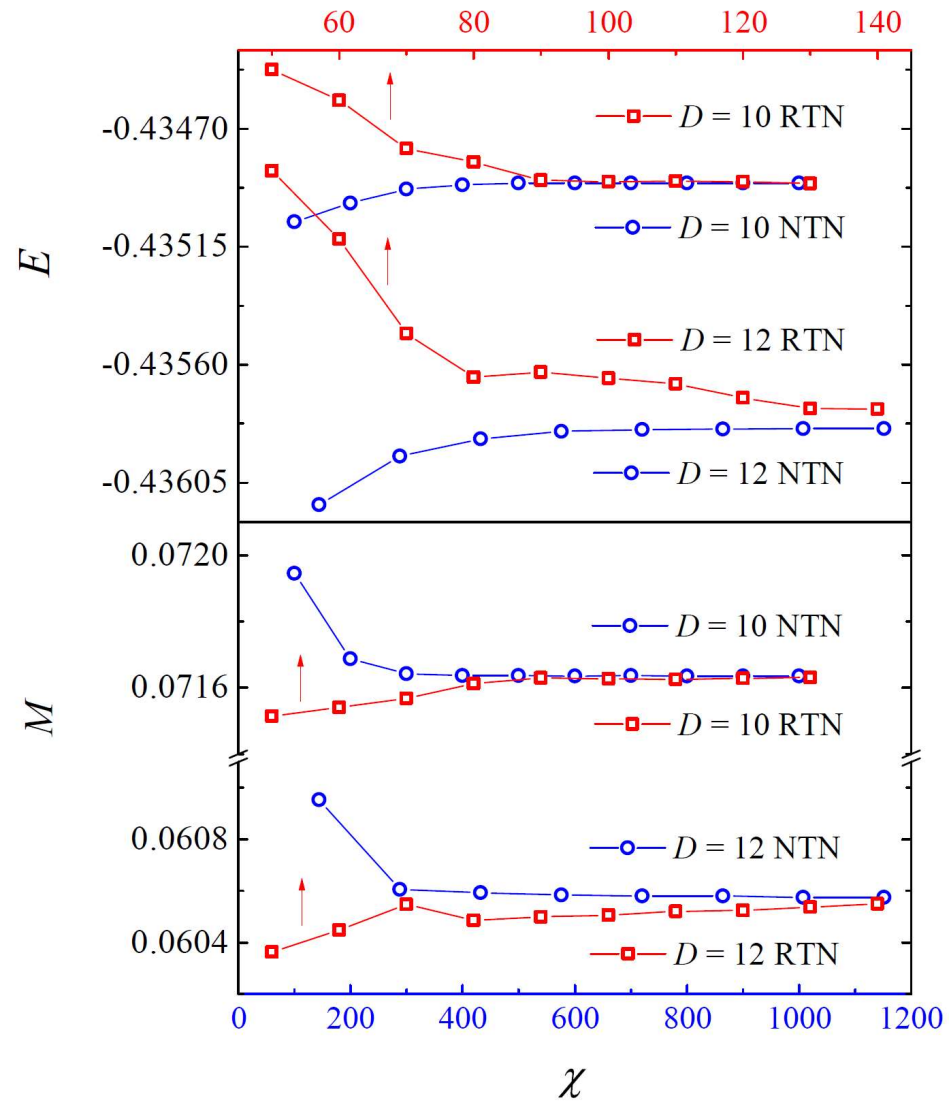
Published Result: with  $D$  up to 13

When RTN can not work:  $D = 24$  e.g.



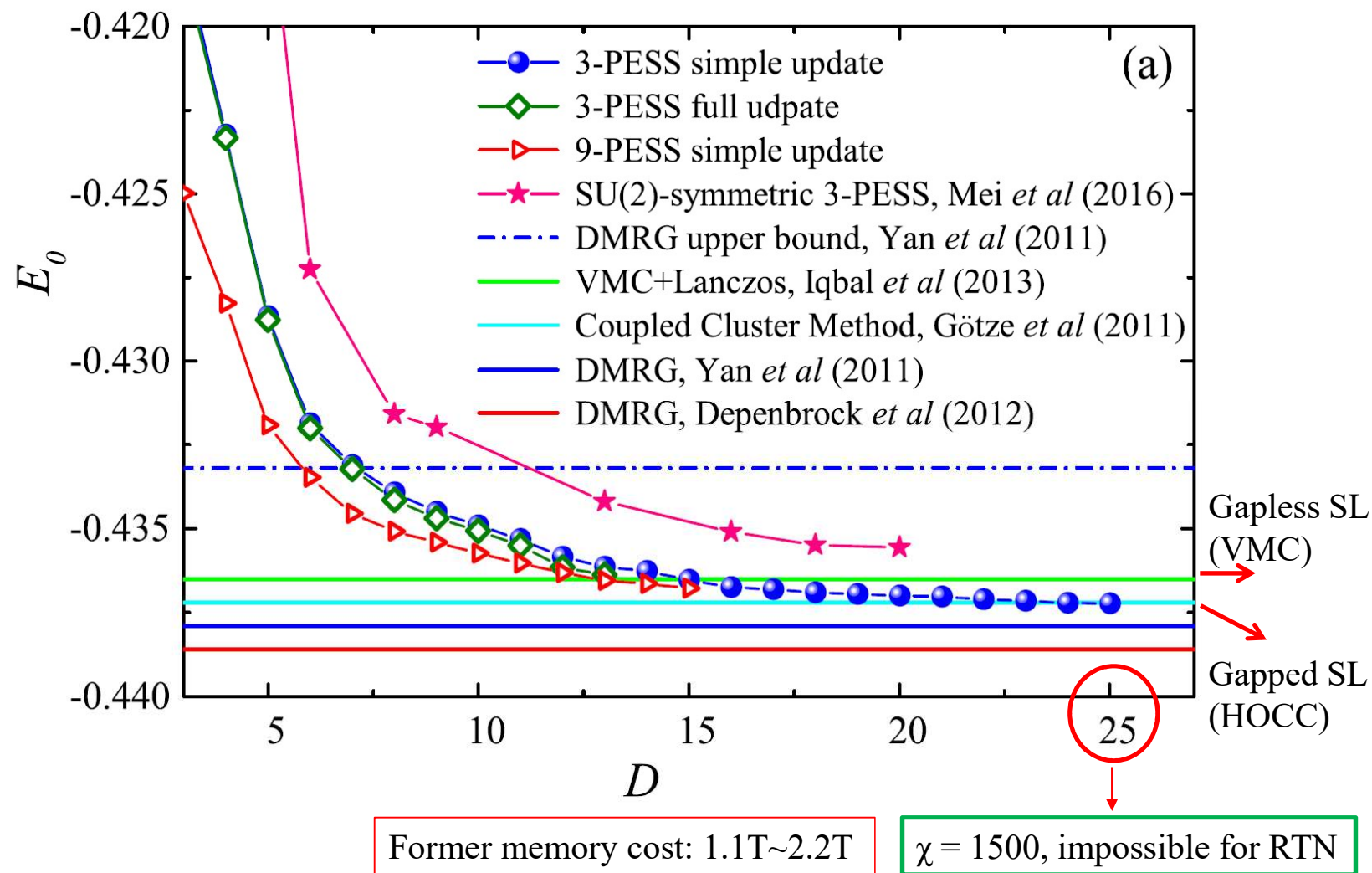
Energy: already exp. converged  
 Mag: only pow. converged, need to increase  $\chi$

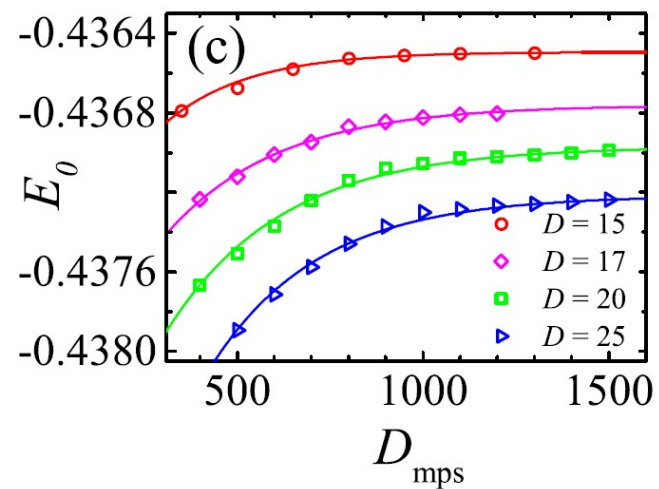
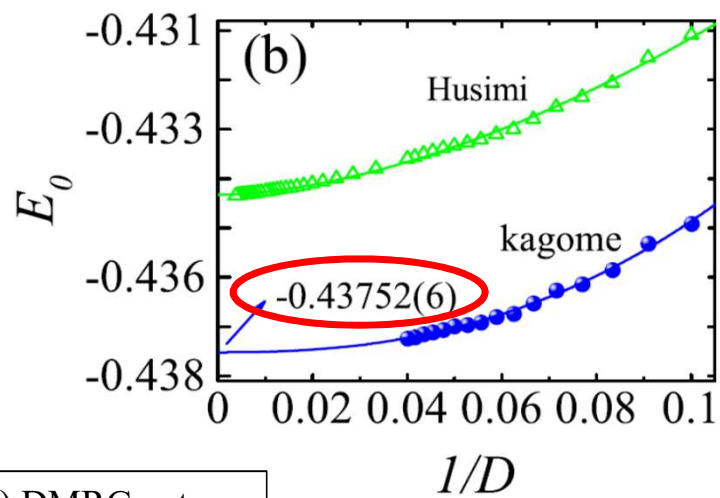
## Convergence Test: when RTN can be applied



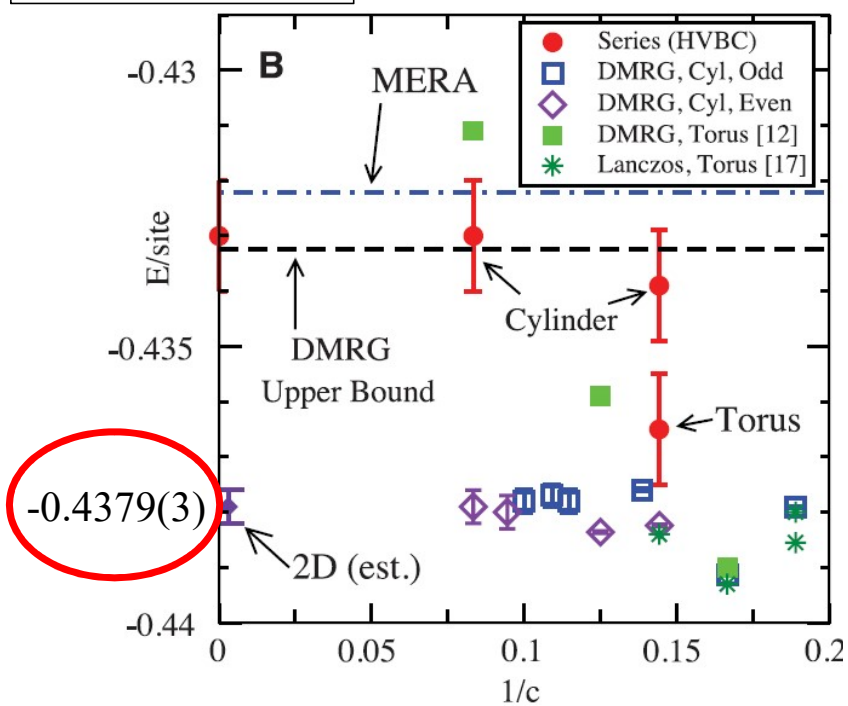
This is important to ensure the convergence:  $X \sim D^2$   
 RTN:  $X \sim 100$   
 NTN:  $X \sim 1000$

## With the help of Nested Tensor Network

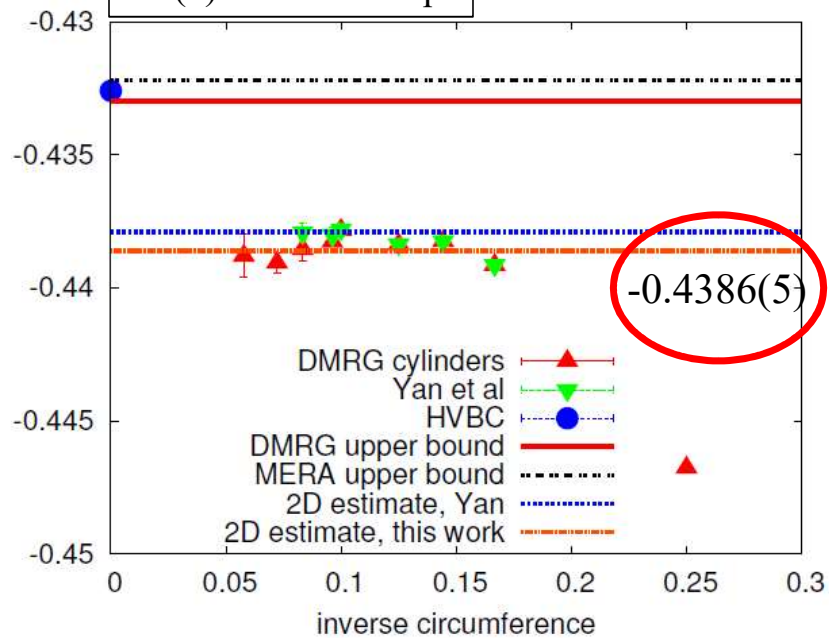
HJLiao, *et al*, PRL 118, 137202 (2017)



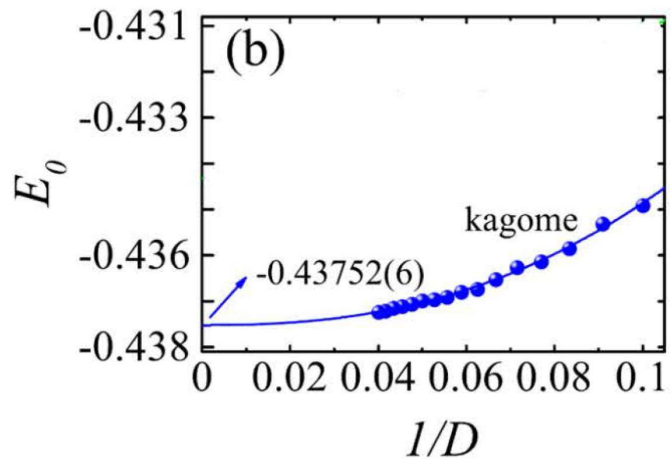
U(1) DMRG extrap:



SU(2) DMRG extrap:

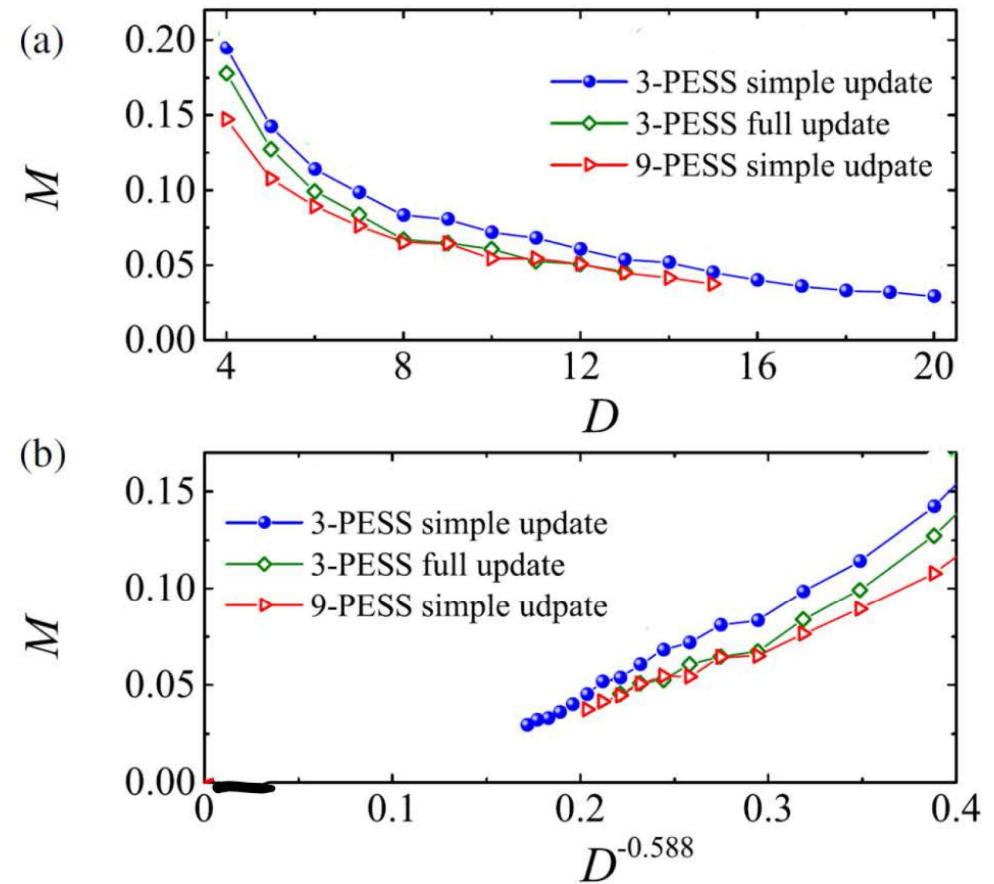


## Large D tells more: probably to be gapless



Scaling-Gap relation: (general belief)

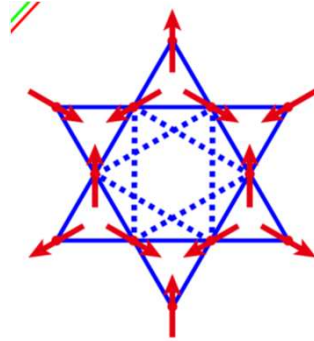
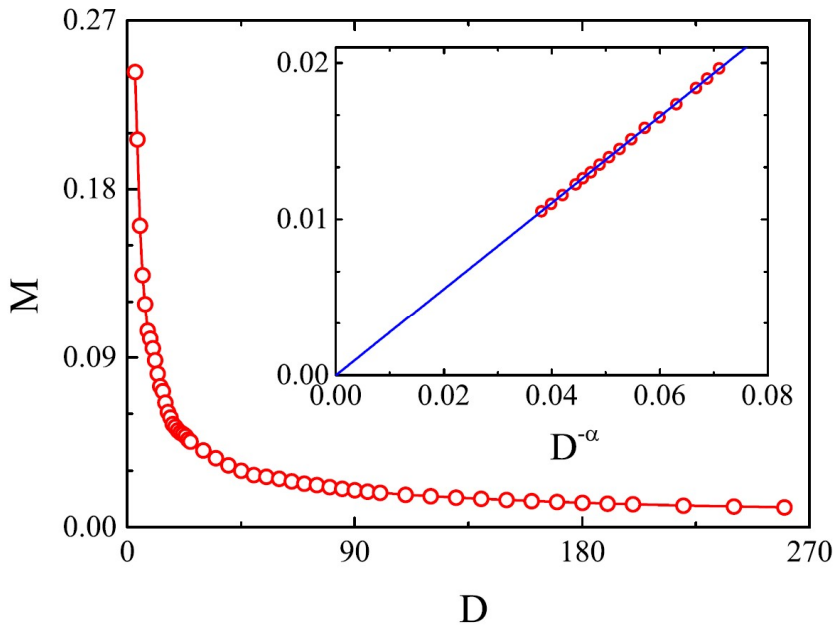
Gapless/critical system: polynomial  
Gapped system: exponential



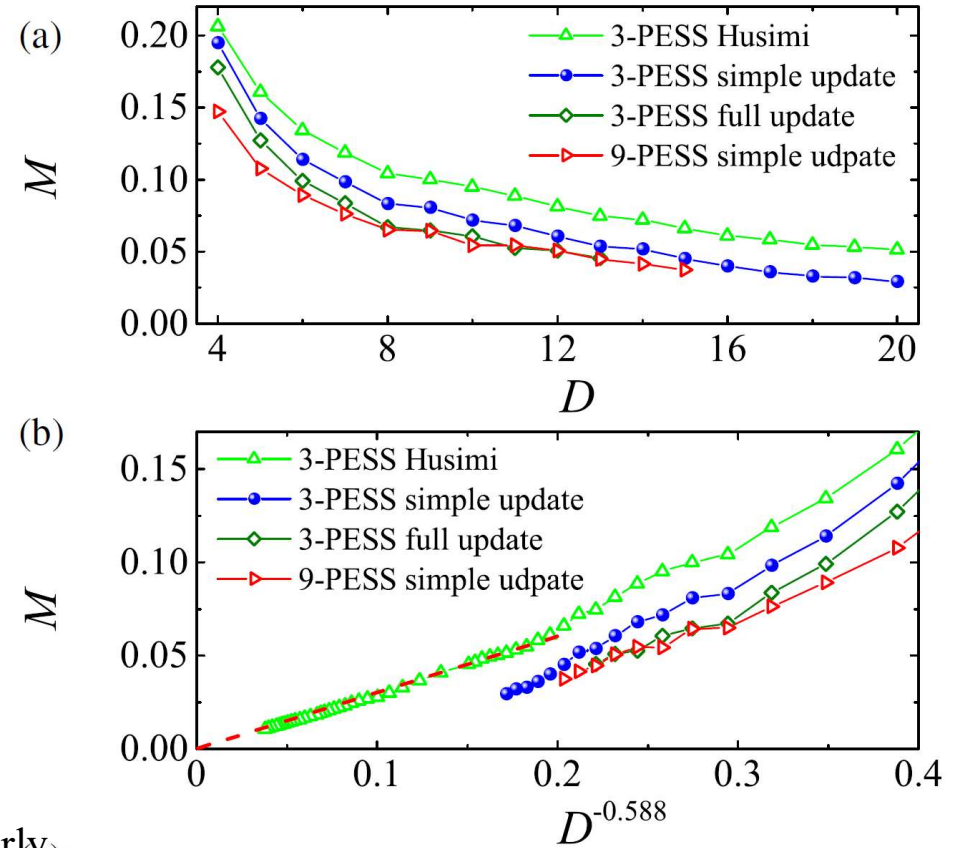
➤ Full update ( $D \sim 13$ ), large cluster ( $D \sim 15$ ) does not change too much



Husimi lattice



Comparison between Husimi and Kagome



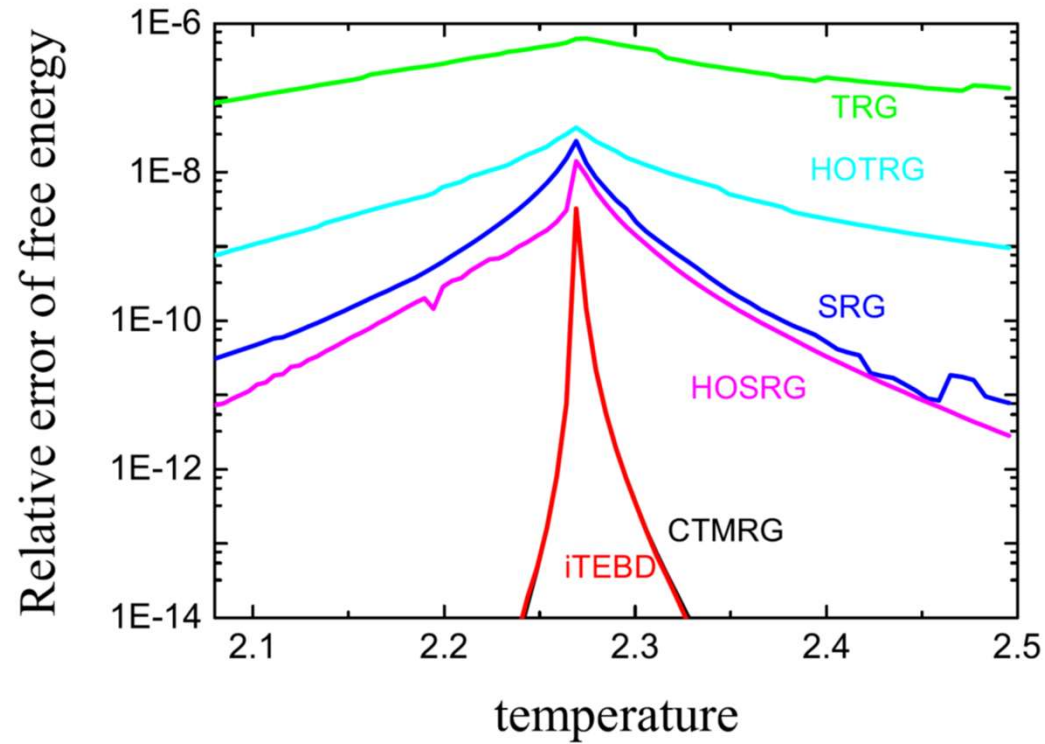
✓ At finite  $D$ , both of them are ordered, and behaves very similarly.

✓ At infinite  $D$  limit, Husimi is of no order, i.e.,  $M = 0$

❑ If Husimi Mag is still upper bound when  $D$  approaches infinity, then Kagome Mag should also vanish!

❑ If there is no finite- $D$  transition, then probably gapless.

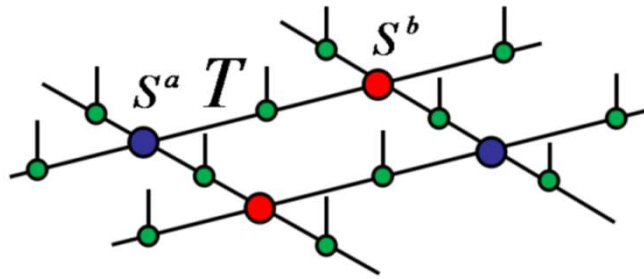
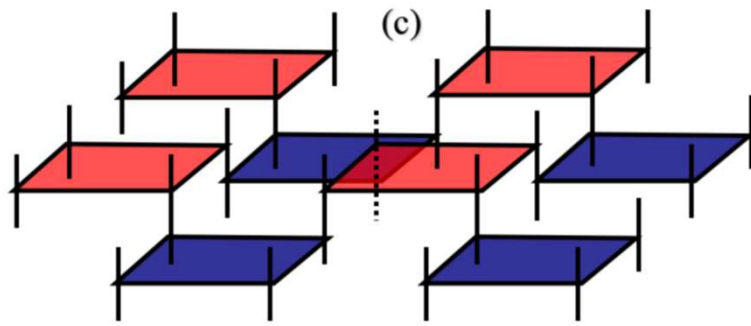
## Application 2: Ising model on cubic lattice



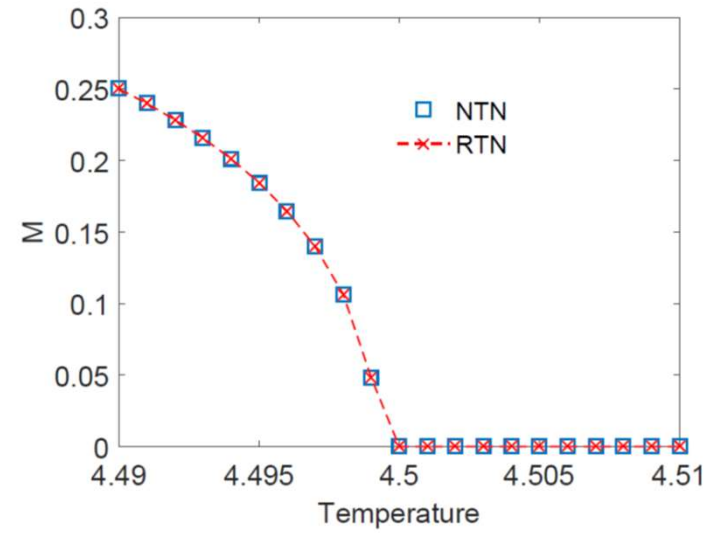
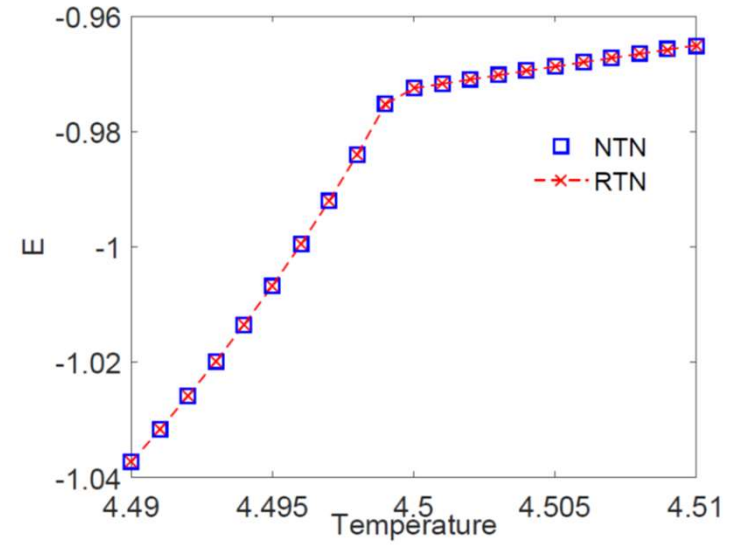
Motivation:

1. HOTRG works well in 3D  
iTEBD should work better
2. Gain insight for quantum lattice model  
(more efficient wavefunction update scheme)

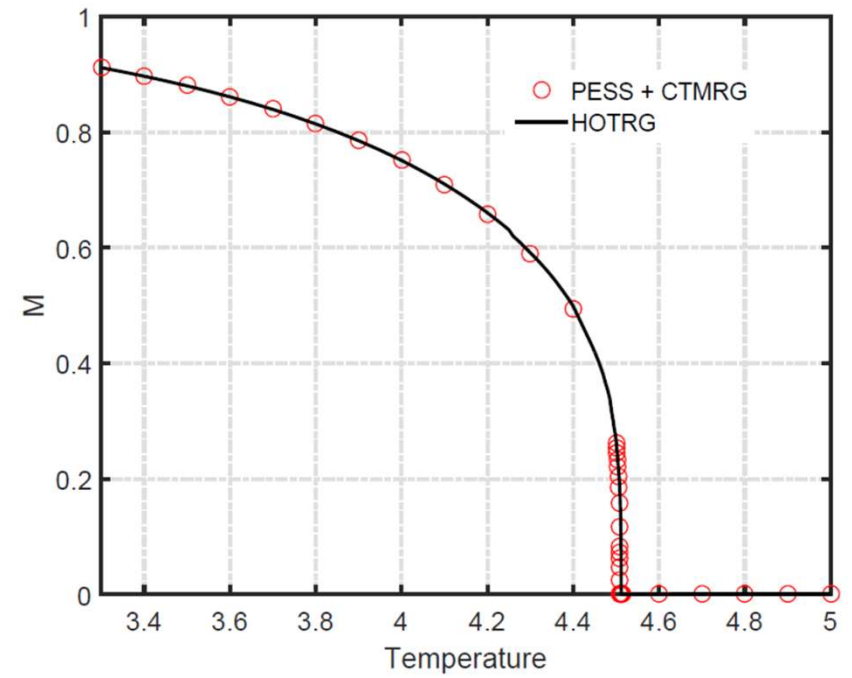
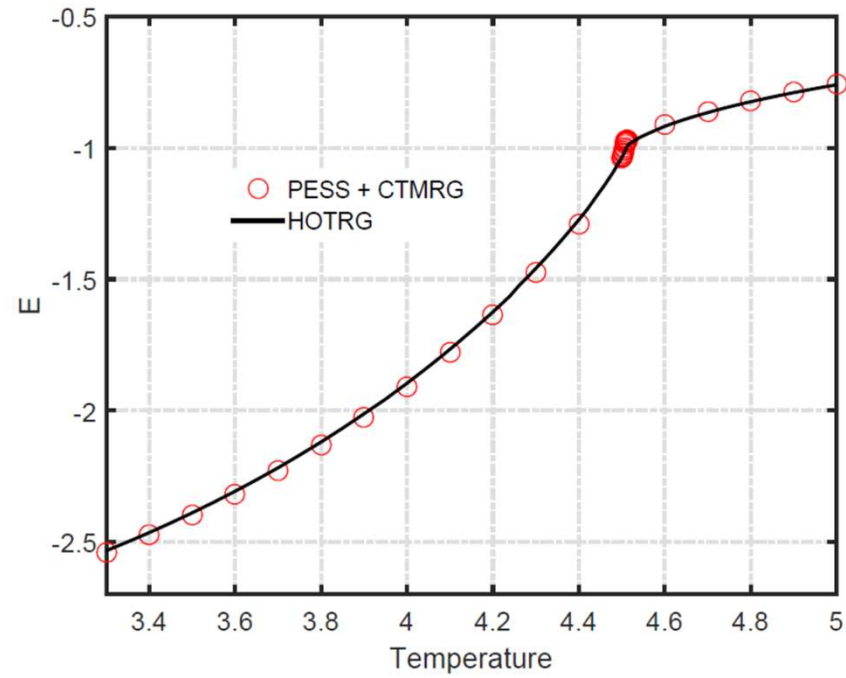
Ising model on square lattice:  $D = 30$



$D = 4, x = 20$



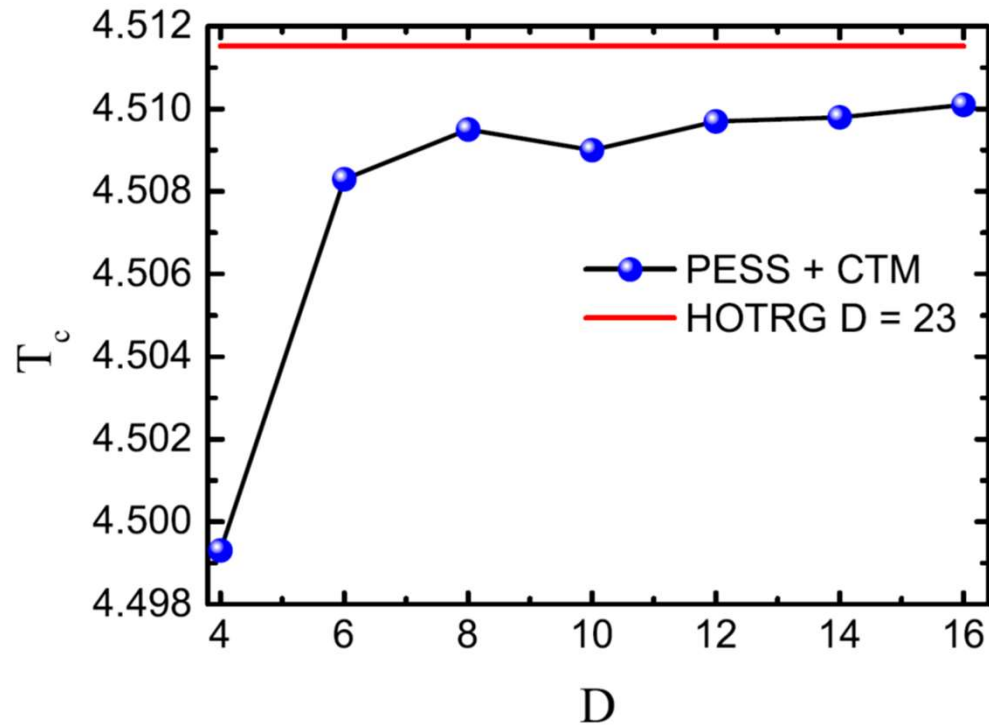
Produce reliable tensor-network state result, [probably the 1<sup>st</sup> time](#)



$D = 10$ ,  $x = 160$  (guaranteed to be very accurate)

Wavefunction-based method **can** also work well in 3D, **if the wf ansatz is properly chosen**

Z. Y. Liu, *et al*, in preparation



| Method                                   | $T_c$         |
|--|---------------|
| TPVA (2001) <sup>[38]</sup>              | 4.5393        |
| Series Expansion (2000) <sup>[165]</sup> | 4.511536(21)  |
| Monte Carlo (2010) <sup>[164]</sup>      | 4.5115232(17) |
| HOTRG (2014) <sup>[104]</sup>            | 4.51152469(1) |
| PESS + CTMRG(D = 16, this work)          | 4.5101(1)     |

PESS wavefunction ansatz is important  
Can be improved by better update method

## Summary

- Calculation of the wavefunction overlap (or inner product) is a central part of TRG for quantum lattice models, and also a **main bottleneck of almost all TRG methods**.
- **Nested Tensor Network** method aims to solve the problem
  - Idea: change the order of summation over the local tensors
  - **Memory:  $D^2$ , computation:  $D^3$ , accuracy: improved by much larger  $\chi$  (10 times)**
- **Critical 1**: Anti-ferromagnetic Kagome Heisenberg Model: **PESS wf**
  - More reliable grdst Energy:  $-0.43752(6)$ ,  **$D=25$** ,  $x=1500$
  - Finite  $D$ :  $q=0$  ordered state, extrapolation: **gapless** SL **E/M converge polynomially** (U(1)-Dirac-fermion)
- **Critical 2**: Ising model on cubic lattice: **PESS wf**
  - **Produce reliable result** for thermodynamic quantities (E, M): **This is first!**
  - Obtain comparable  $T_c$  with other techniques, promising for better update,  **$D=16$**

Main Collaborators in this talk:



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IOPCAS, China



Prof. Bruce Normand  
PSI, Switzerland



Dr. Haijun Liao  
IOPCAS, China



Dr. Jing Chen  
IOPCAS, China



Dr. Zhiyuan Liu  
ITPCAS, China

Main Refs: ZYXie, H. J. Liao, R. Z. Huang, H. D. Xie, J. Chen, Z. Y. Liu, T. Xiang, **Phys. Rev. B** 96, 045128 (2017)

H. J. Liao, ZYXie, J. Chen, Z. Y. Liu, H. D. Xie, R. Z. Huang, B. Normand, T. Xiang, **Phys. Rev. Lett.** 118, 137202 (2017)

ZYXie, J. Chen, J. F. Yu, X. Kong, B. Normand, T. Xiang, **Phys. Rev. X** 4, 011025 (2014)

Z. Y. Liu, ZYXie, T. Xiang, **to appear**

*Thanks!*

Next, we calculate the Kitaev model on the honeycomb lattice [52] with an equal amplitude of bond couplings defined by

$$H = \frac{1}{2} \sum_{\langle i,j \rangle_\gamma} \sigma_i^\gamma \sigma_j^\gamma, \quad \gamma = z, x, y \quad (47)$$

where the Ising anisotropy depends on the three different directions of bonds of the honeycomb lattice. Here,  $\sigma_i^\gamma$  represents the Ising spin at  $i$  site with the Ising anisotropy axis in the  $\gamma$  direction. This model is exactly solvable at any lattice size with any kind of the PBC [52]. The exact ground state is a highly frustrated spin liquid and it is gapless in the thermodynamic limit. The infinite PEPS calculation [53] shows good agreement with the exact ground-state energy in the infinite lattice, although the lattice rotational symmetry is artificially broken due to the mapping from honeycomb lattice to brick-wall lattice.

The Lieb-Schultz-Mattis (LSM) theorem [1], and its higher-dimensional generalizations [2,3], state that if a quantum spin system defined on a lattice has odd number of spin- $\frac{1}{2}$  per unit cell, then any local spin Hamiltonian which preserves the spin and translation symmetry cannot have a featureless (gapped and nondegenerate) ground state. This implies that any symmetry-allowed Hamiltonian on the spin Hilbert space defined above can only have the following possible scenarios: (i) its ground state spontaneously breaks either the spin symmetry or the lattice symmetry, hence leads to degenerate ground states and possible gapless Goldstone modes; (ii) it has gapped and degenerate ground states without breaking any symmetry, i.e., its ground state develops a topological order (the second possibility can only happen in two- and higher-dimensional systems); (iii) its ground state has algebraic (power-law) correlation function of physical quantities, and the spectrum is again gapless [this scenario happens most often in one-dimensional (1D) spin systems, while still possible in higher dimensions].

E.H. Lieb, T.D. Schultz, and D.C. Mattis, *Ann. Phys.* **16**, 407 (1961)

M. B. Hastings, *Phys. Rev. B* **69**, 104431 (2004).



# Lieb-Schultz-Mattis-Hasting Theorem

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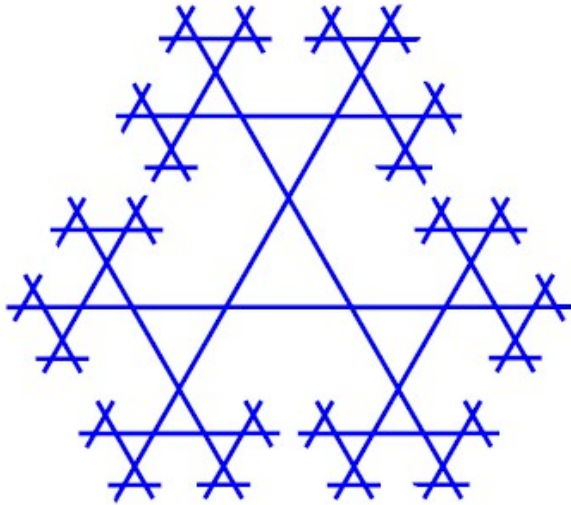
**LSMH theorem:** SU(2) invariant Hamiltonian with odd-half-integer spin per unit cell, which implies following three cases:

- symmetry-breaking: goldstone mode
- Gaped spin liquid with degenerate ground states
- Gapless spin liquid

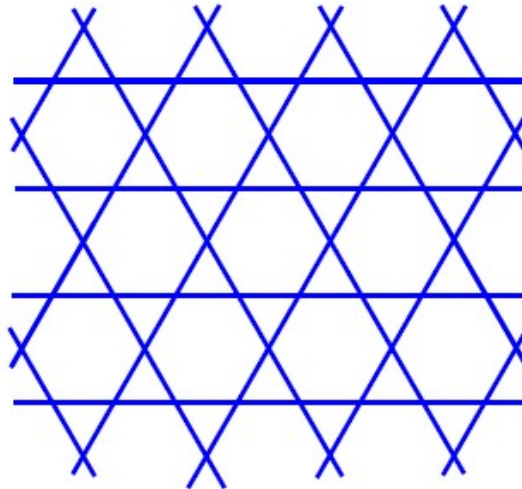
E.H. Lieb, T.D. Schultz, and D.C. Mattis, *Ann. Phys.* **16**, 407 (1961)

M. B. Hastings, *Phys. Rev. B* **69**, 104431 (2004) .

## Some evidence of the scaling-gap relation



(p=3,q=2) Husimi



Kagome

Husimi:

each bond belongs to a single polygon/loop

*much less frustrated*, and *much easier to study!*

1D: much evidence

2D: less evidence (due to small D), well believed

Simple argue band not rigourouse at all:  
for gapped system

$$S = \alpha L^{d-1}$$

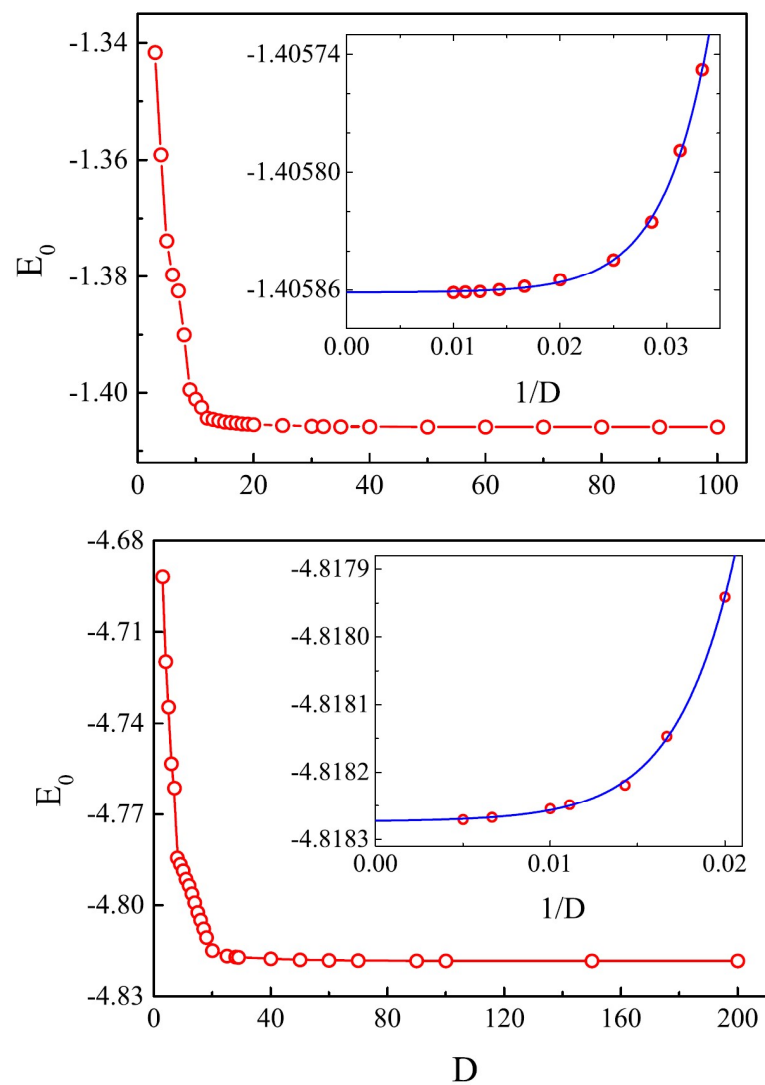
$$S_D = L^{d-1} \log D$$

$$\varepsilon = 1 - S_D/S = 1 - \frac{\log D}{\alpha} \sim \log \frac{1}{D}$$

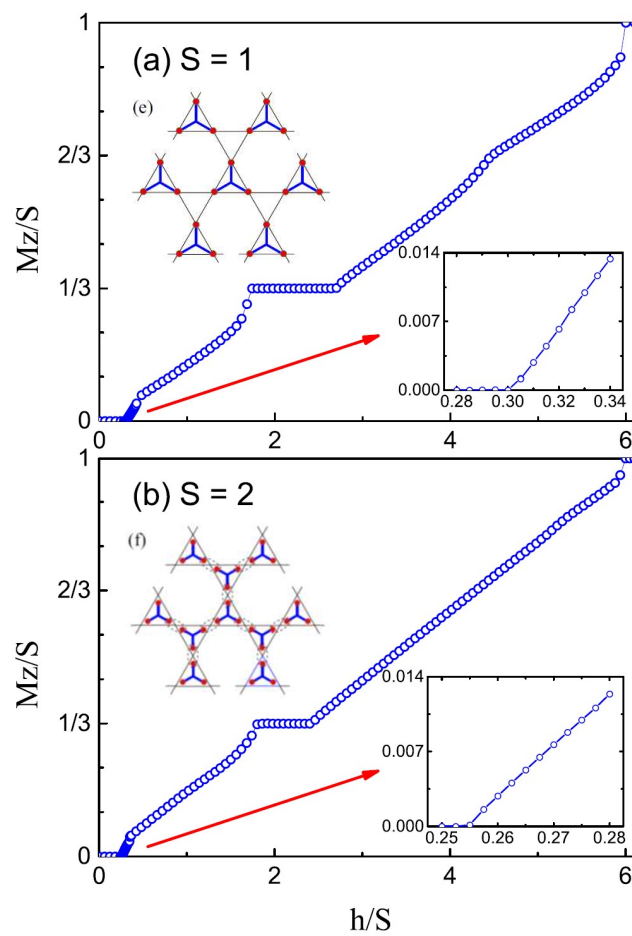
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i \mathbf{S}_i^z,$$

HJLiao, *et al*, PRB 93, 075154 (2016)

# About the scaling-gap relation



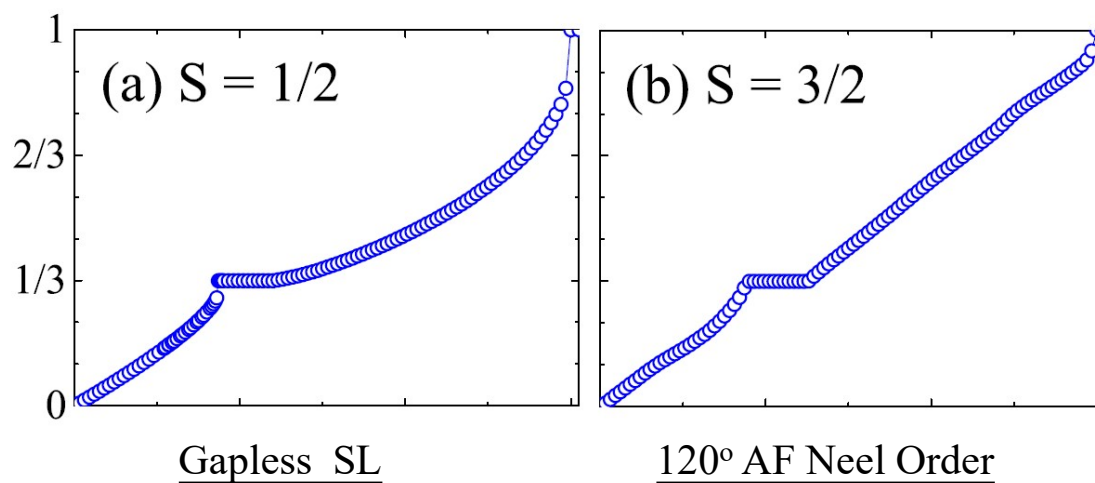
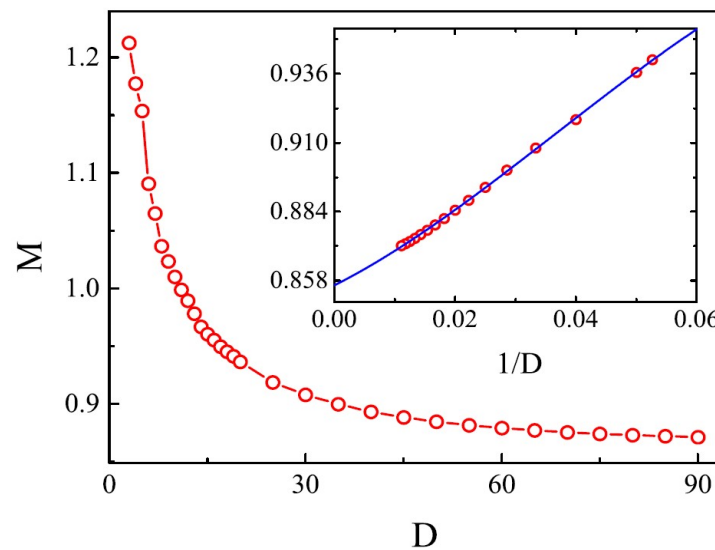
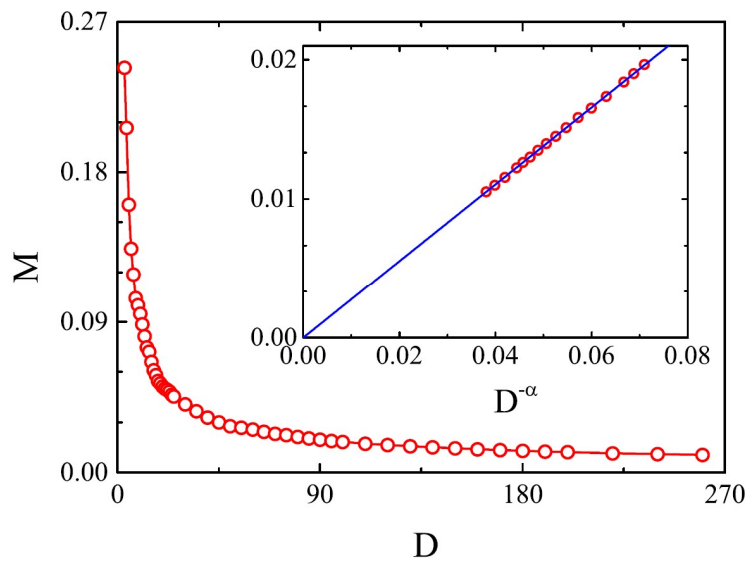
## Gapped SSS (trimerized, non-uniform)



## Gapped SSS (uniform)

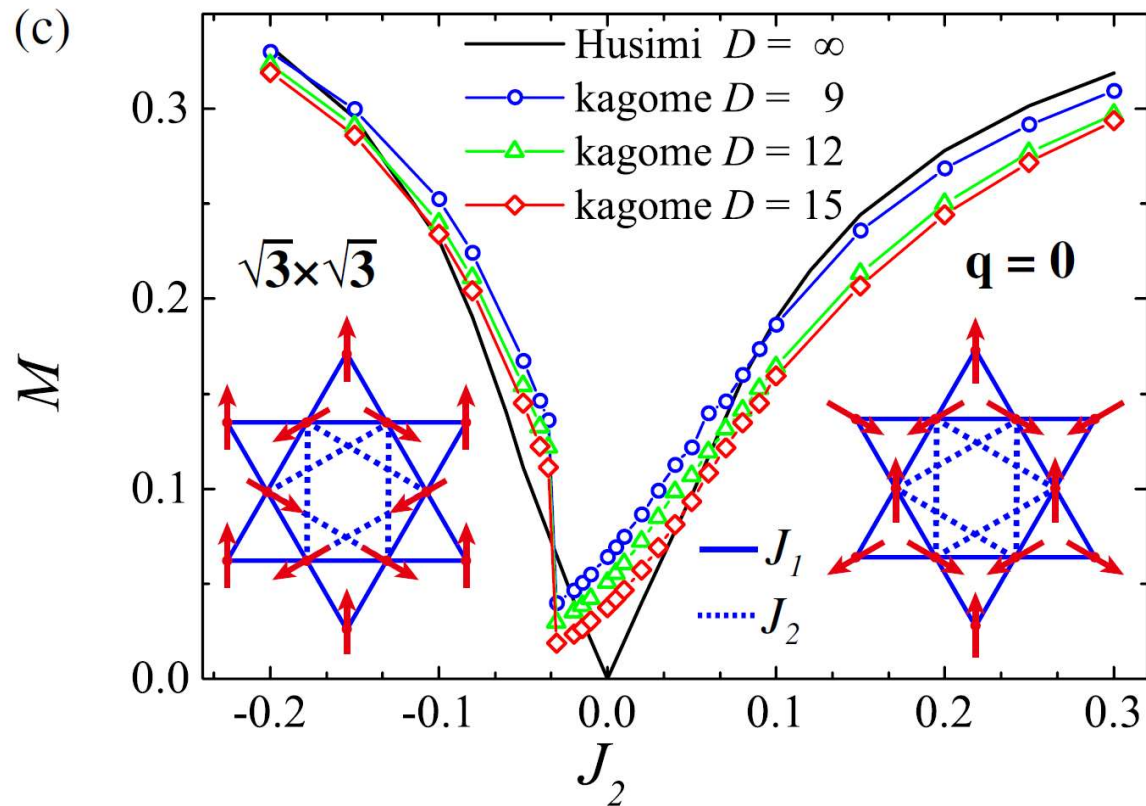
HJLiao, *et al*, PRB 93, 075154 (2016)

## Quasi-2D Example: About the scaling-gap relation



Just to mention:  
 $S > 2$ , always ordered  
 Just like  $S = 3/2$  (gapless)

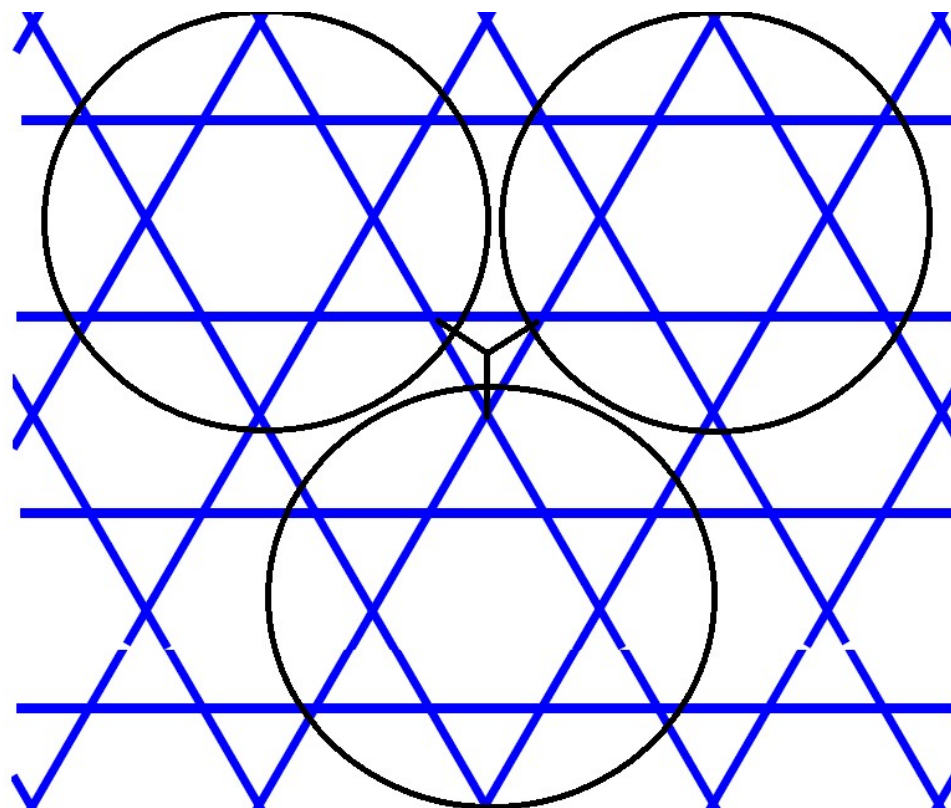
Supplementary Information:  
simple update with second neighbor coupling  $J_2$



Seems like a stable phase:  $(-0.03, 0.04)$

Unsuitable channel: always ( $q=0$ ) ordered at finite D!

**36-PES**



## Fermions with 2D tensor networks

**Simulate fermions in 2D?**

Before April 2009: **NO!**

Since April 2009: **YES!**

### **Different formulations:**

P. Corboz and G. Vidal, Phys. Rev. B 80, 165129 (2009)

T. Barthel, C. Pineda, and J. Eisert, Phys. Rev. A 80, 042333 (2009)

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, Phys. Rev. A 81, 052338 (2010)

Q.-Q. Shi, S.-H. Li, J.-H. Zhao, and H.-Q. Zhou, arXiv:0907.5520

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, Phys. Rev. A 81, 010303(R) (2010)

C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A 81, 050303(R) (2010)

P. Corboz, R. Orus, B. Bauer, G. Vidal, PRB 81, 165104 (2010)

I. Pizorn, F. Verstraete, Phys. Rev. B 81, 245110 (2010)

Z.-C. Gu, F. Verstraete, X.-G. Wen. arXiv:1004.2563

# Classification by entanglement

