Gapless Spin-Liquid Ground State in the Kagome Antiferromagnets

Tao Xiang

Institute of Physics

Chinese Academy of Sciences

txiang@iphy.ac.cn

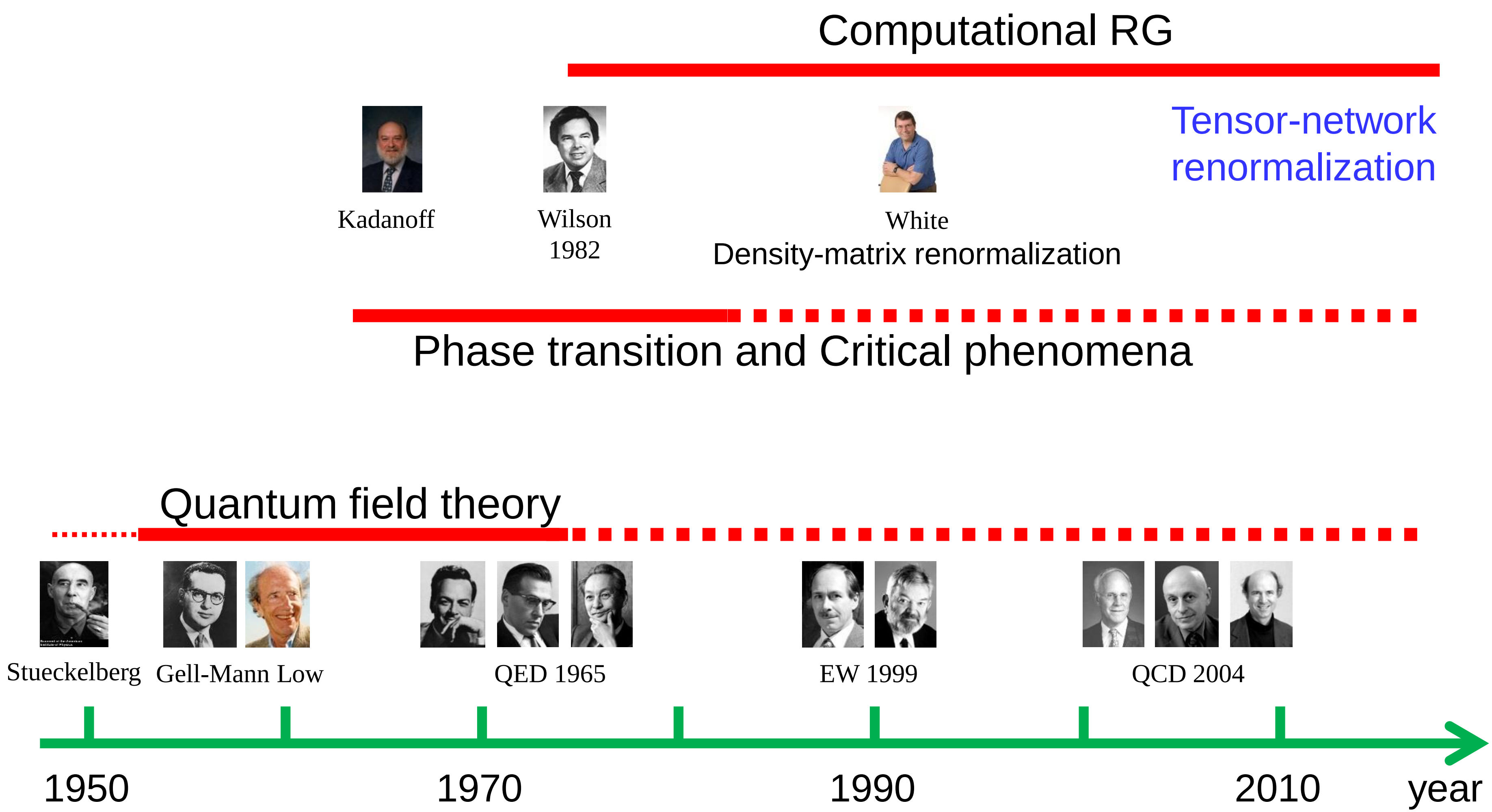
Outline

I. Brief introduction to the tensor-network states and their renormalization

II. Tensor-network renormalization group study of the Kagome Heisenberg model

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad J > 0$$

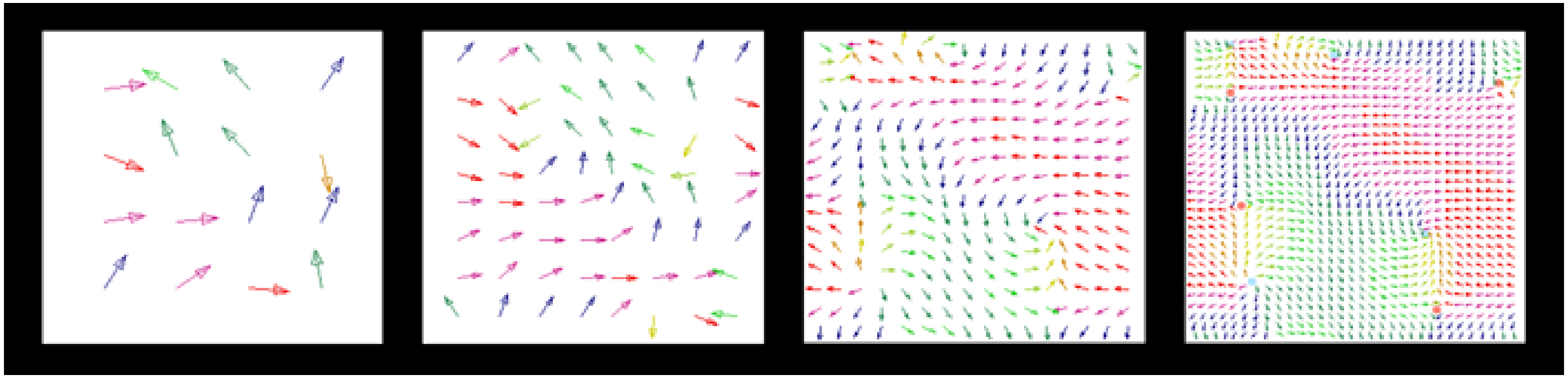
Road Map of Renormalization Group



I. Basic Idea of Renormalization Group

$$|\psi\rangle = \sum_{k=1} a_k |k\rangle \approx \sum_{k=1}^{N \ll N_{total}} a_k |k\rangle$$

To find a small but optimized set of basis states $\{|k\rangle\}$
to represent accurately a wave function



Scale transformation: refine the wavefunction by local RG transformations

Optimization of Basis States

$$|\psi\rangle = \sum_{k=1} a_k |k\rangle \approx \sum_{k=1}^{N \ll N_{total}} a_k |k\rangle$$

To find a small but optimized set of basis states $\{|k\rangle\}$
to represent accurately a wave function

Physics : compression of basis space (phase space)
i.e. compression of information

Mathematics: low rank approximation of matrix or tensor

RG versus Tensor-Network RG

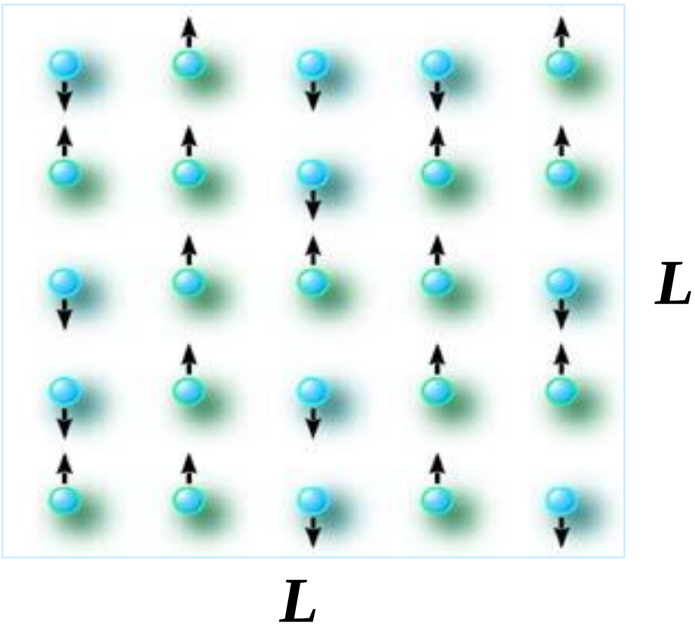
Renormalization Group (analytical)

RG equation for charge, critical exponents and other coupling constants at critical regime

Tensor-Network Renormalization Group

Direct evaluation of quantum wave function or partition function at or away from critical points

Is Quantum Wave Function Compressible?

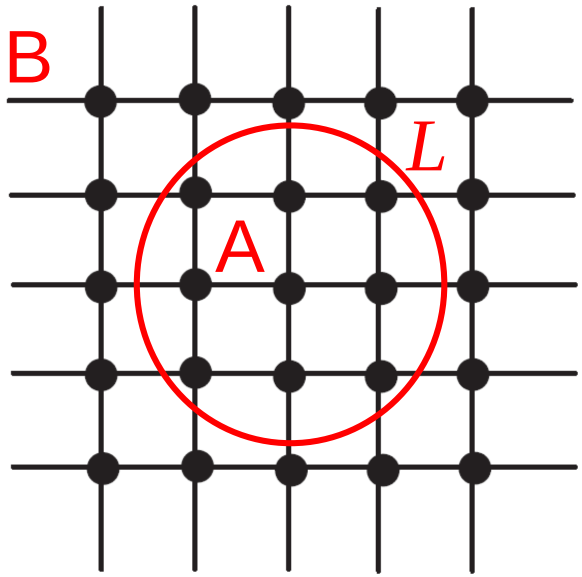


$$N_{\text{total}} = 2^{L^2}$$

$$|\psi\rangle = \sum_{k=1}^{N_{\text{total}}} a_k \, |k\rangle$$

basis states

Yes: Entanglement Entropy Area Law



$$S \propto L \propto \log N$$

$$N \sim 2^{L} \ll 2^{L^2} = N_{\text{total}}$$

Minimum number of basis states needed for accurately representing ground states

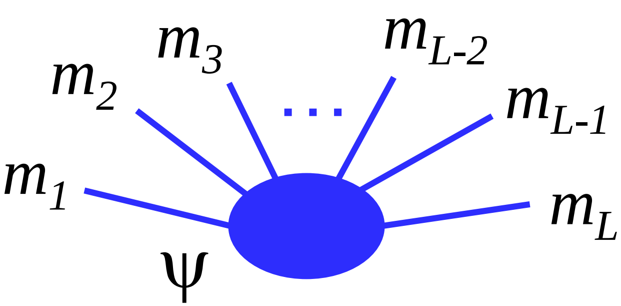
$$|\psi\rangle \approx \sum_{k=1}^{N \ll N_{\text{total}}} a_k |k\rangle$$

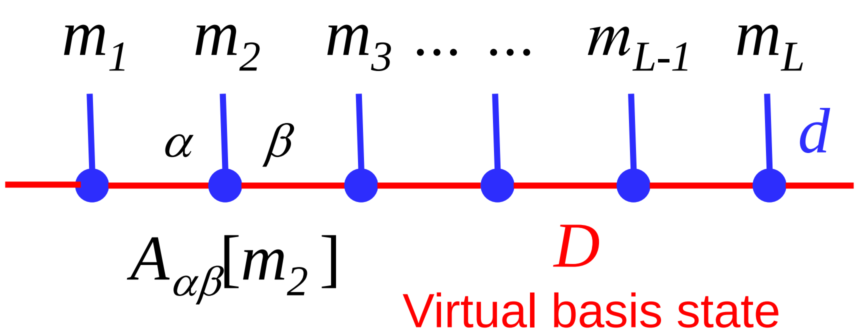
basis states

What Kind of Wavefunction Satisfies the Area Law?

The Answer: Tensor Network States

Example: Matrix Product States (MPS) in 1D





$\psi(m_1, \dots m_L)$

$\psi(m_1, \dots m_L) = TrA[m_1] \cdots A[m_L]$

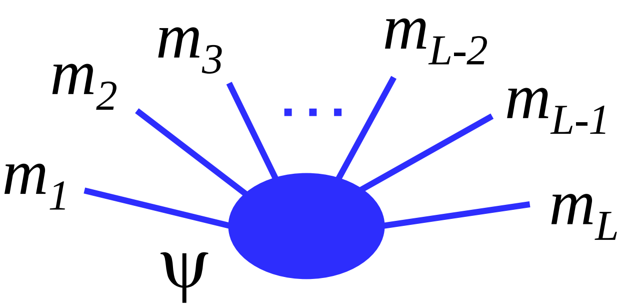
d^L **parameters**

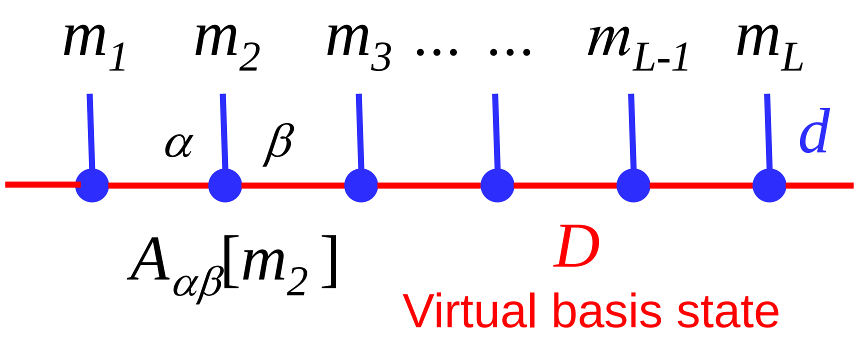
dD^2L **parameters**

Entanglement Entropy of MPS

$$S \sim \log D$$

Example: Matrix Product States (MPS)





$\psi(m_1, \ldots m_L)$

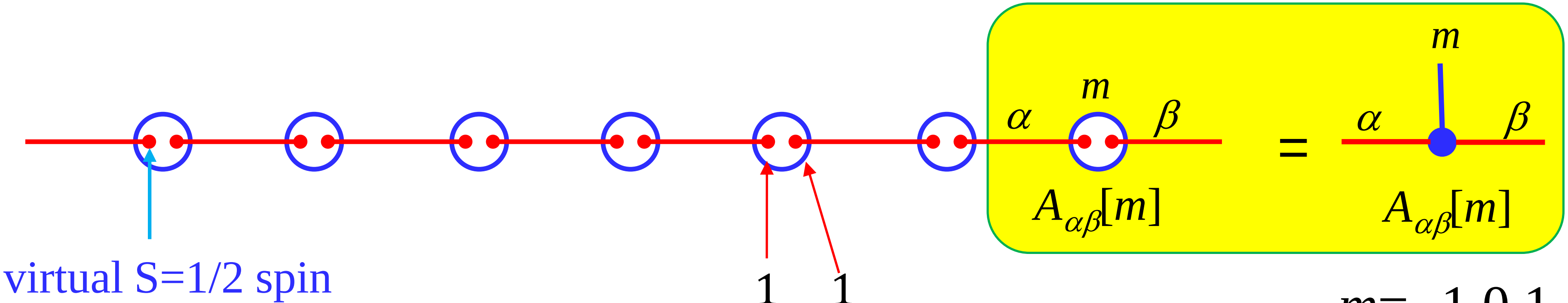
$\psi(m_1, \ldots m_L) = TrA[m_1] \cdots A[m_L]$

d^L parameters

dD^2L parameters

Example：S=1 AKLT valence bond solid state

$$H=\sum_i \frac{1}{2}\left[S_i\cdot S_{i+1}+\frac{1}{3}\left(S_i\cdot S_{i+1}\right)^2+\frac{2}{3}\right]$$



$$1=\frac{1}{2}\oplus\frac{1}{2}$$

m= -1,0,1

$$|\Psi\rangle=\sum_{m_1\ldots m_L} Tr\left(A[m_1]\ldots A[m_L]\right)|m_1\ldots m_L\rangle$$

$$A[-1]=\begin{pmatrix}0 & 0\\ \sqrt{2} & 0\end{pmatrix}\qquad A[0]=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}\qquad A[1]=\begin{pmatrix}0 & \sqrt{2}\\ 0 & 0\end{pmatrix}$$

$A_{\alpha\beta}[m]$:

To project two virtual S=1/2 states, α and β, onto a S=1 state m

Affleck, Kennedy, Lieb, Tasaki, PRL **59**, 799 (1987)

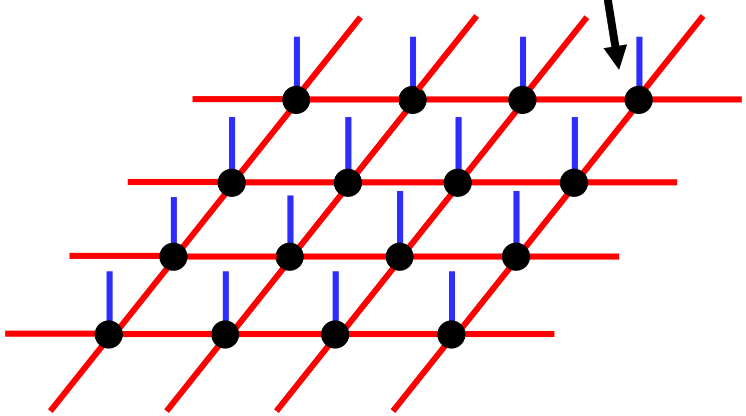
2D: Projected Entangled Pair State

$$|\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'}[m_i] |m_i\rangle$$

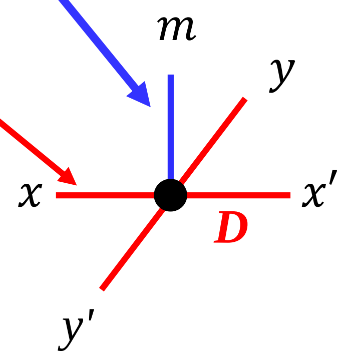
Local tensor

Virtual basis

Physical basis



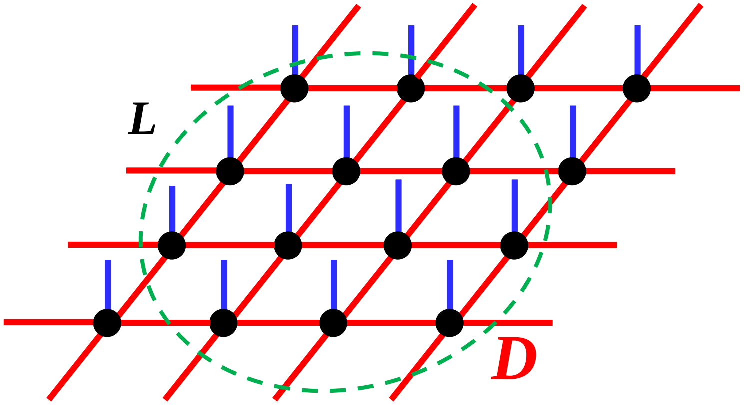
$$T_{xx'yy'}[m] =$$



F. Verstraete and J. Cirac, cond-mat/0407066

Entanglement Entropy of PEPS

$$S = \alpha L \sim L \log D$$



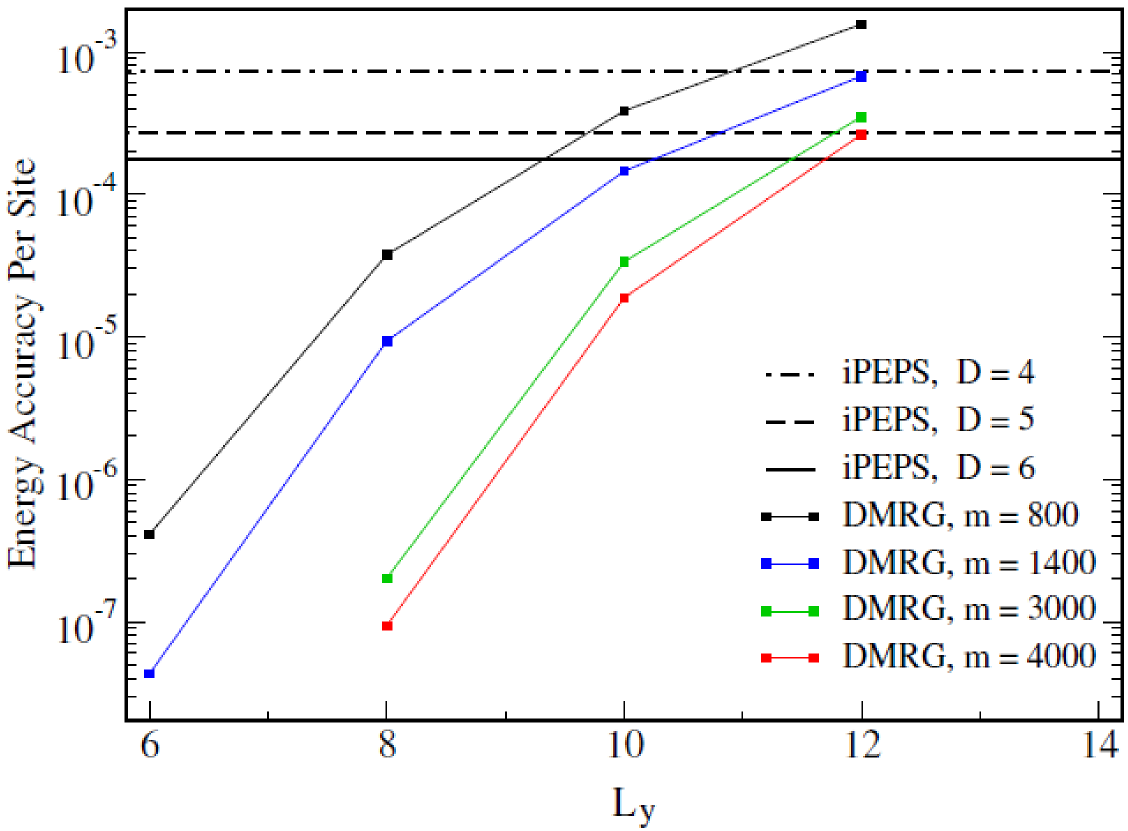
$$|\Psi\rangle = Tr \prod T_{x_i x'_i y_i y'_i}[m_i] |m_i\rangle$$

Local tensor **Virtual basis** **Physical basis**

PEPS becomes exact in the limit $D \to \infty$

PEPS versus MPS (DMRG)

PEPS is more suitable for studying large 2D lattice systems



S=1/2

Heisenberg model on

$L_x \times L_y$ square lattice

Reference energy: VMC

Sandvik PRB **56**, 11678 (1997)

Stoudenmire and White, Annu. Rev. CMP **3**, 111(2012)

Tensor Network States

- **Partition functions of all classical and quantum lattice models can be represented as tensor network models**

$$Z = Tr \prod_i T_{x_i x'_i y_i y'_i}$$

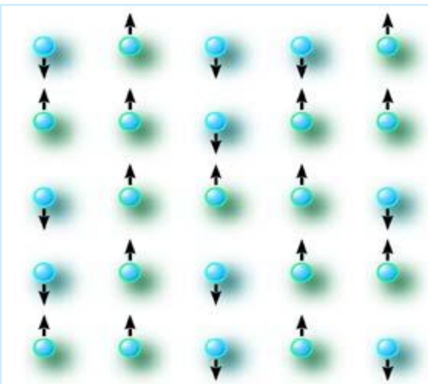
- **Ground state wave function can be represented as tensor-network state**

$$|\Psi\rangle = Tr \prod T_{x_i x'_i y_i y'_i}[m_i]|m_i\rangle$$

***d*-dimensional quantum system = (*d+1*)-dimensional classical model**

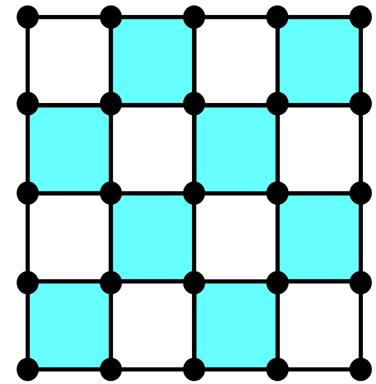
Partition Function: Tensor Representation of Ising model

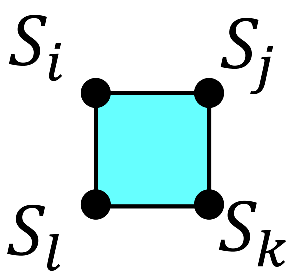
$$H = -J\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z$$



$\sigma_i^z = -1, 1$

$$Z = \mathrm{Tr}\exp(-\beta H)$$
$$= \mathrm{Tr}\prod_{\blacksquare}\exp(-\beta H_{\blacksquare})$$
$$= \mathrm{Tr}\prod_{\{S\}} T_{S_iS_jS_kS_l}$$

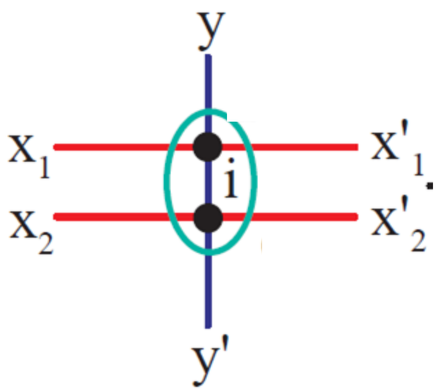




$$= T_{S_iS_jS_kS_l} = \exp(-\beta H_{\blacksquare})$$

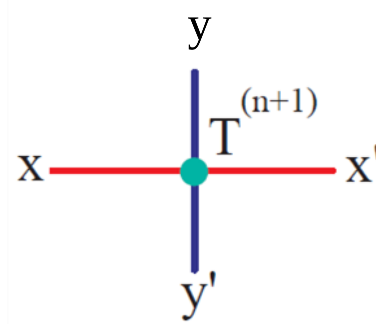
How to renormalize a tensor-network model

Z. Y. Xie et al, PRB **86**, 045139 (2012)

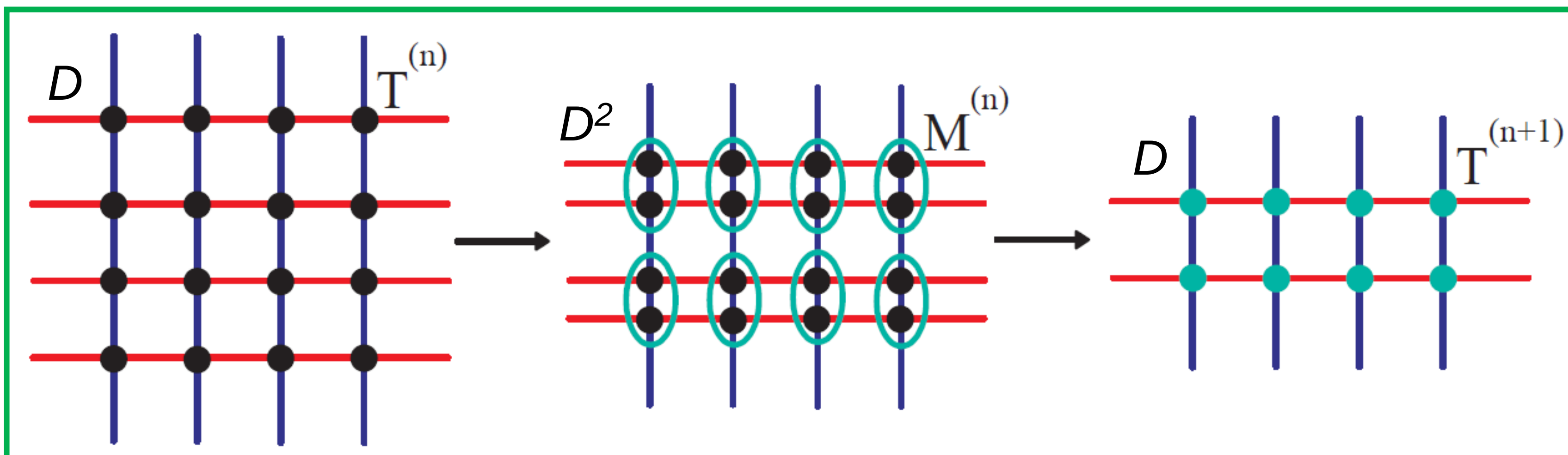


Higher-order singular value decomposition (HOSVD)

Truncation:
Lower-rank approximation

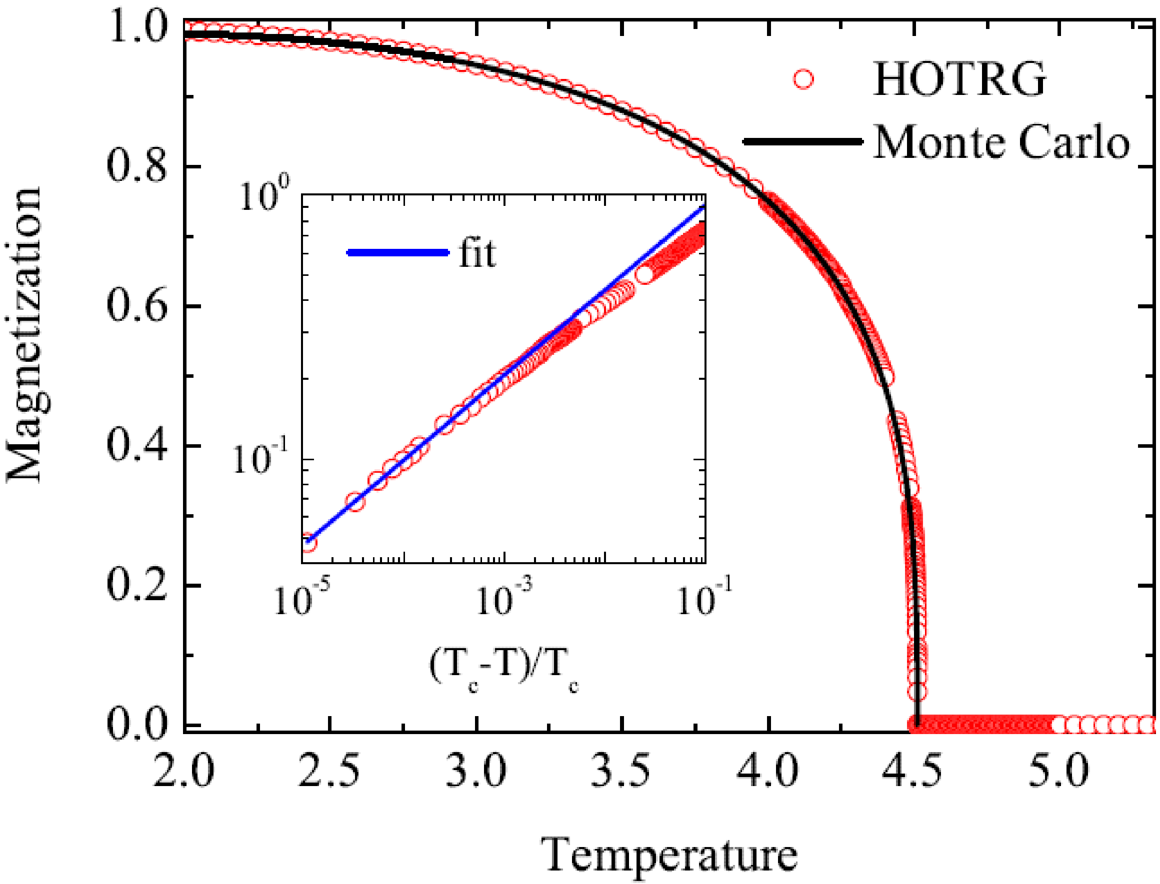


$$M^{(n)}_{(x_1 x_2),(x_1' x_2'),y,y'} \qquad T^{(n+1)}_{x,x',y,y'}$$



Magnetization of 3D Ising model

Xie et al, PRB 86,045139 (2012)



$$M \sim t^{\beta}$$

HOTRG (D=14): 0.3295

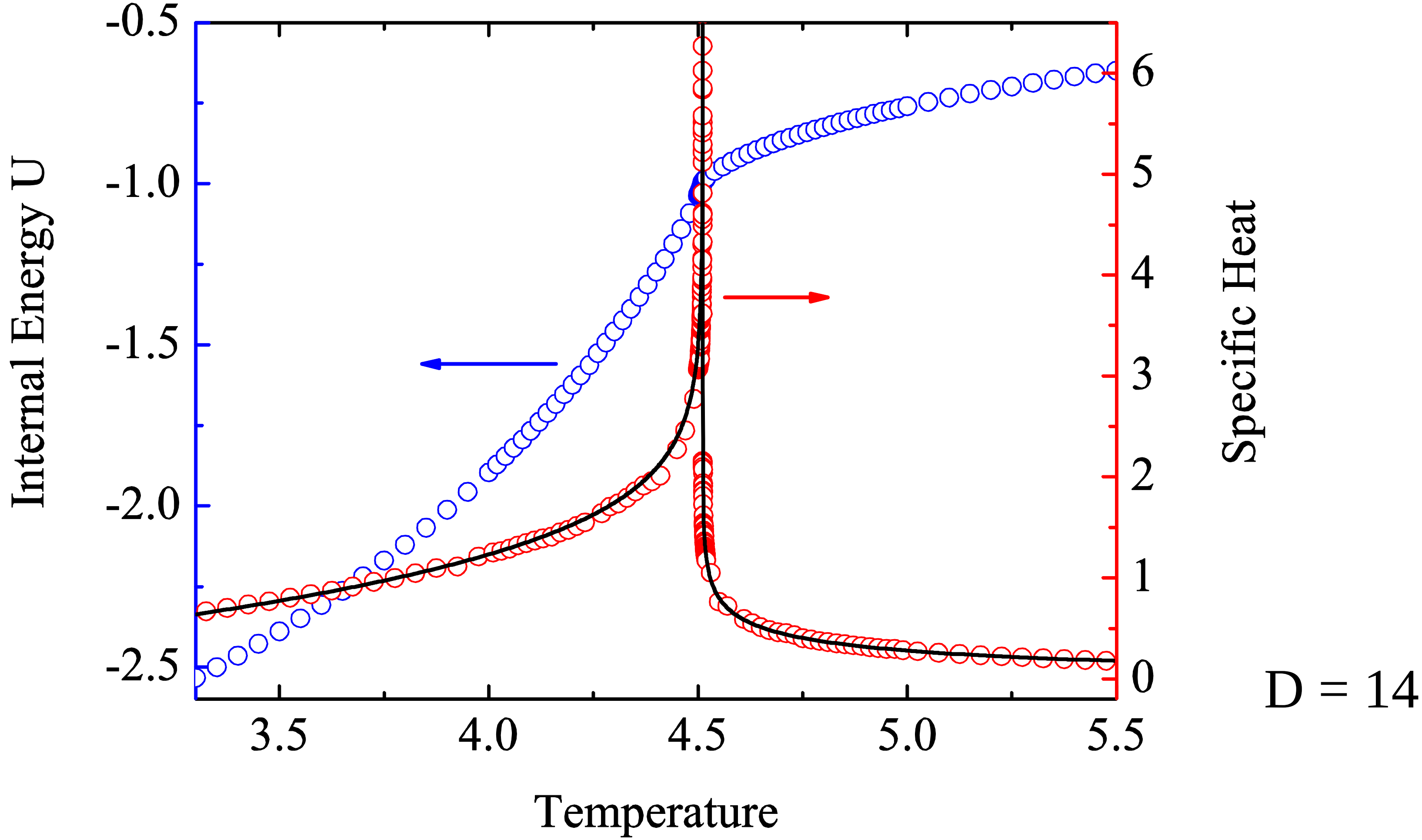
Monte Carlo: 0.3262

Series Expansion: 0.3265

Relative difference is less than 10^{-5}

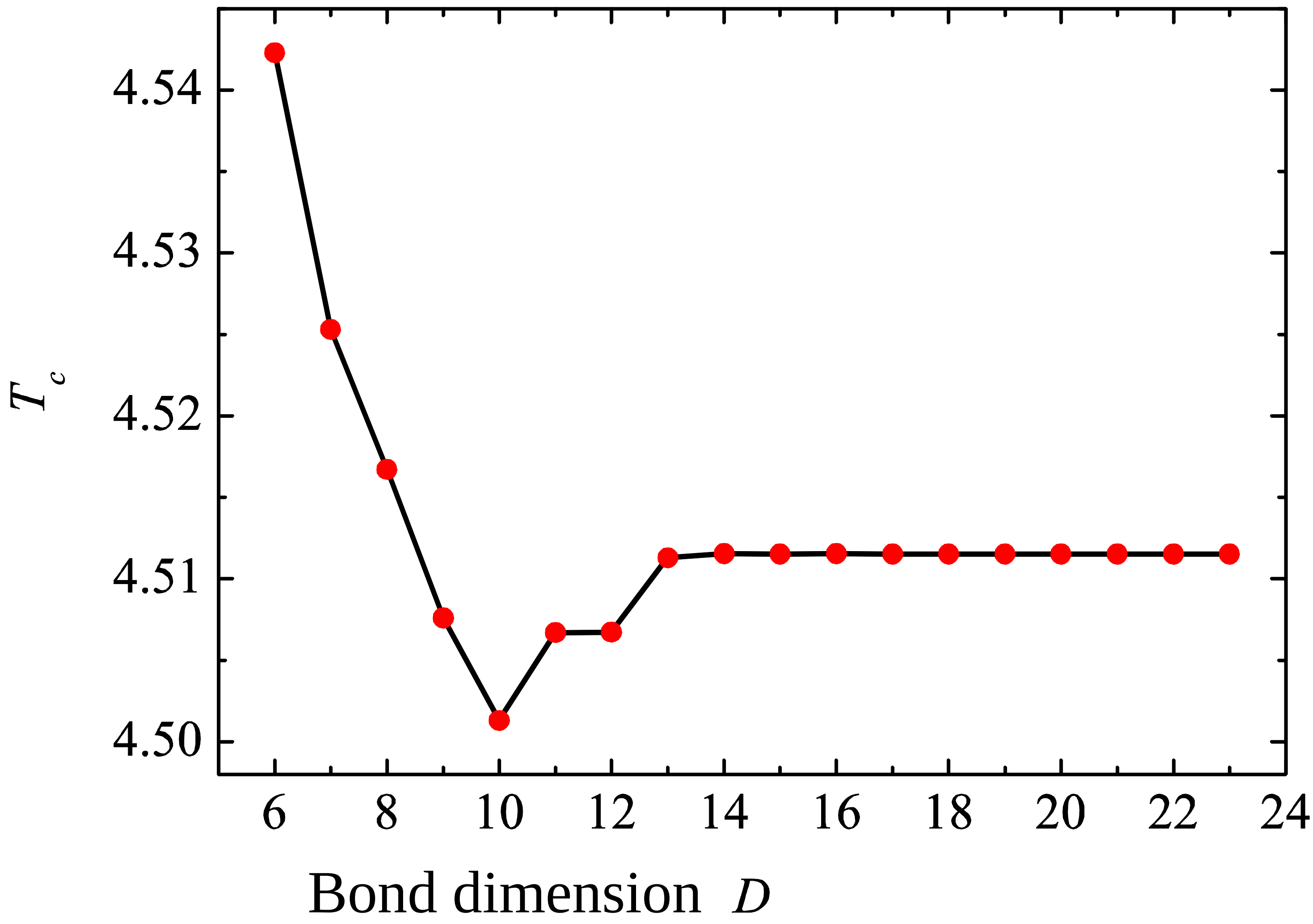
MC data: A. L. Talapov, H. W. J. Blote, J. Phys. A: Math. Gen. 29, 5727 (1996).

Specific Heat of 3D Ising model



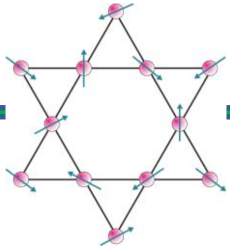
Solid line: Monte Carlo data from X. M. Feng, and H. W. J. Blote, Phys. Rev. E 81, 031103 (2010)

Critical Temperature of 3D Ising model



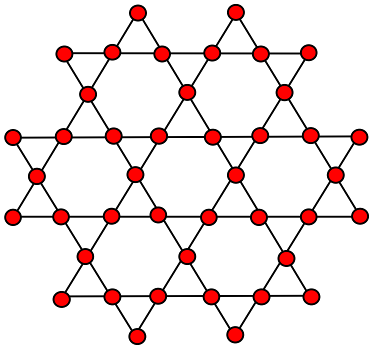
Critical Temperature of 3D Ising model

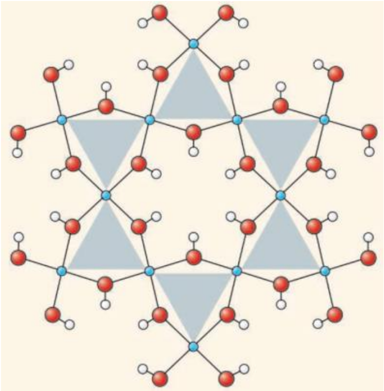
method	year	T_c
HOTRG D = 16	2012	4.511544
D = 23	2014	4.51152469(1)
NRG of Nishino et al	2005	4.55(4)
Monte Carlo Simulation	2010	4.5115232(17)
	2003	4.5115248(6)
	1996	4.511516
High-temperature expansion	2000	4.511536



II. Ground State of Kagome Antiferromagnets

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





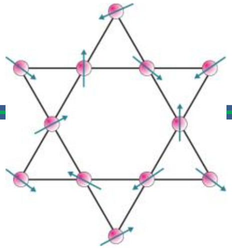
Herbertsmithite: *$ZnCu_3(OH)_6Cl_2$*

S=1/2 Kagome Heisenberg

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad J > 0$$

Is the ground state

1. **gapped or gapless?**
2. **quantum spin liquid?**

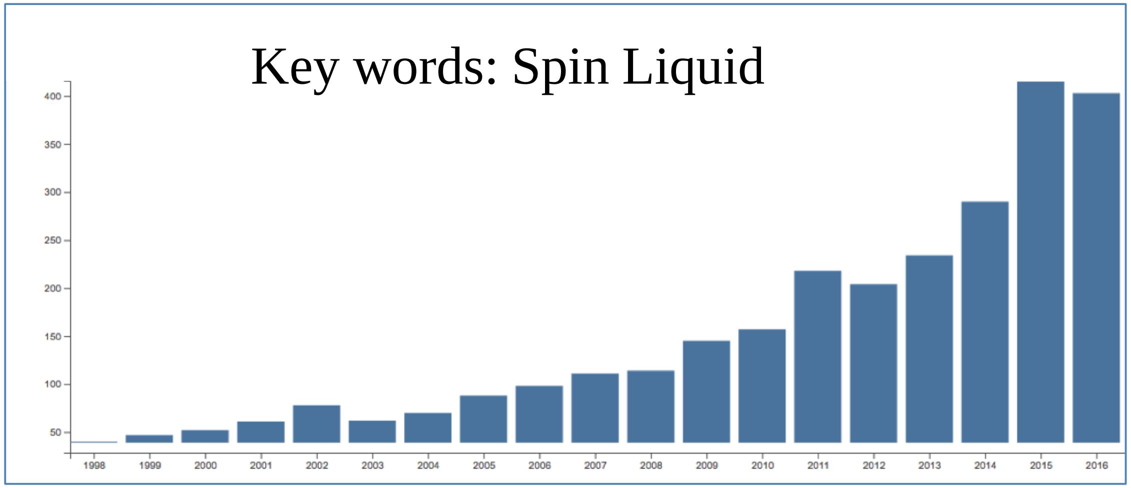


Quantum Spin Liquid

- ✓ Novel quantum state possibly with topological order
- ✓ Mott insulator without antiferromagnetic order
- ✓ Geometric or quantum frustrations are important

Quantum spin liquid has attracted great interests in recent years

Publication Number



Web of Science

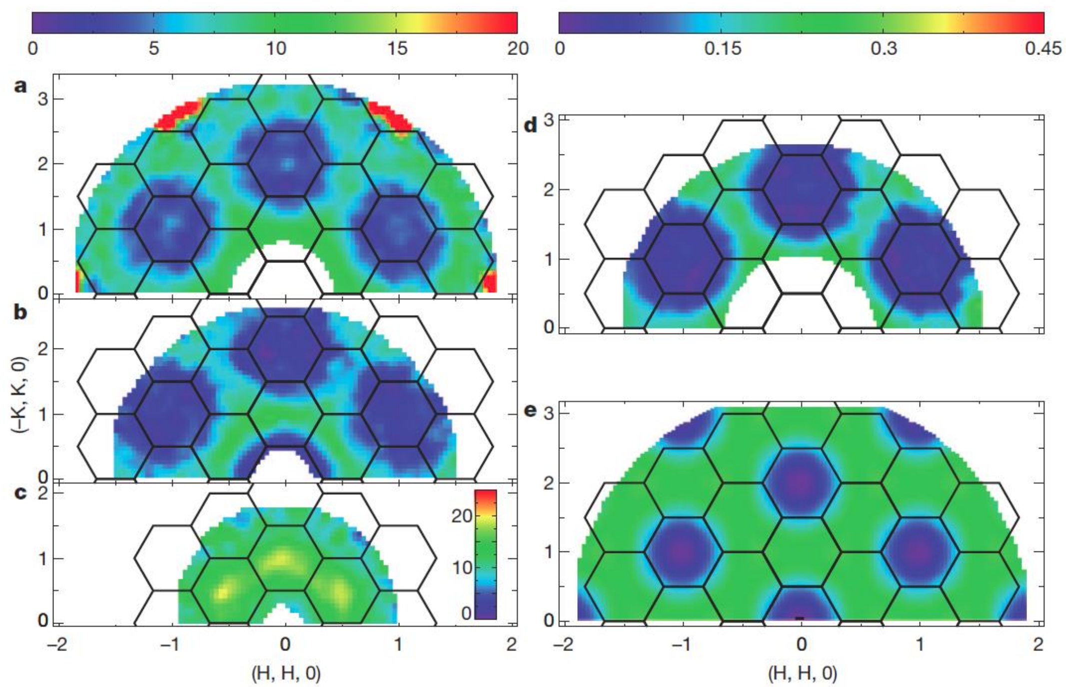
Hints from Experiments

Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet

Tian-Heng Han[1], Joel S. Helton[2], Shaoyan Chu[3], Daniel G. Nocera[4], Jose A. Rodriguez-Rivera[2,5], Collin Broholm[2,6] & Young S. Lee[1]

Nature 492 (2012) 406

Gapless spin liquid



Along the (H, H, 0) direction, a broad excitation continuum is observed over the entire range measured

Herbertsmithite $ZnCu_3(OH)_6Cl_2$: Neutron scattering

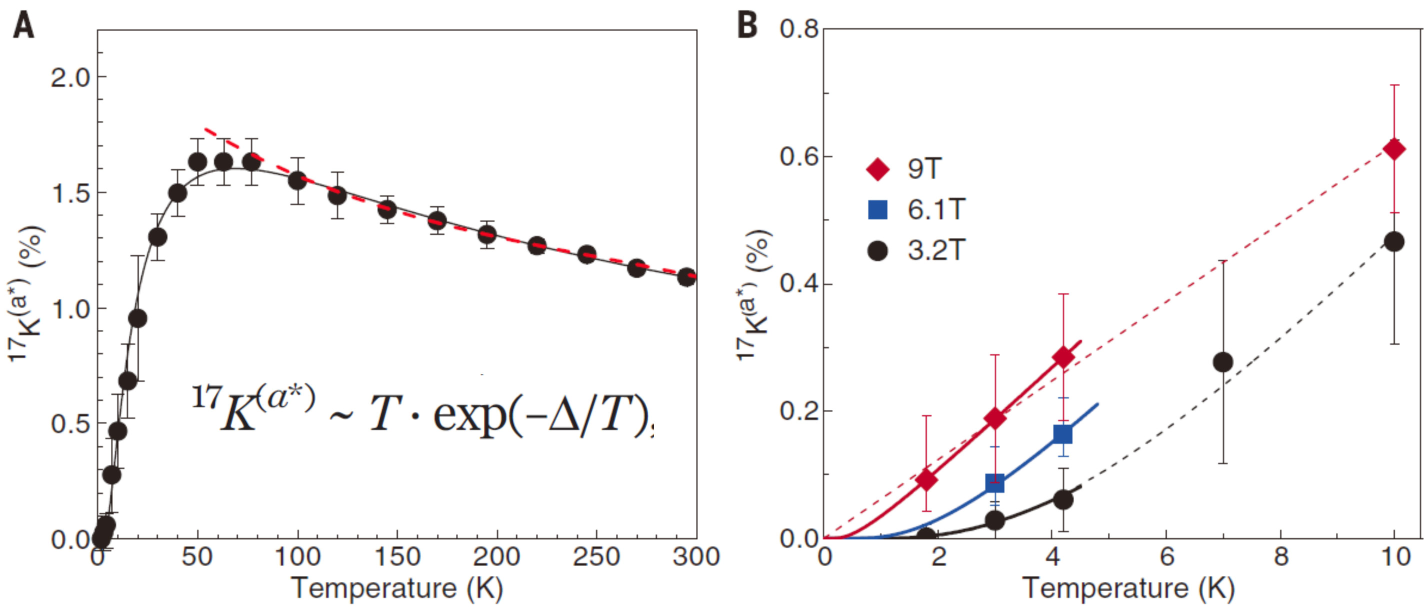
Hints from Experiments

Evidence for a gapped spin-liquid ground state in a kagome Heisenberg antiferromagnet

Mingxuan Fu,[1] Takashi Imai,[1,2*] Tian-Heng Han,[3,4] Young S. Lee[5,6]

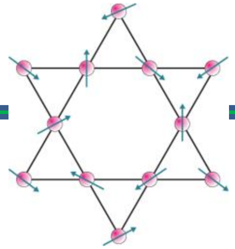
Science **360** (2016) 655

Gapped spin liquid



NMR Knight shift

$$\Delta(0)/J = 0.03 \text{ to } 0.07$$



Kagome AFM: Theoretical Study

A question under debate for many years

Not Spin Liquid

Valence-bond Crystal

Marston *et al.*, J. Appl. Phys. 1991

Zeng *et al.*, PRB 1995

Nikolic *et al.*, PRB 2003

Singh *et al.*, PRB 2008

Poilblanc *et al.*, PRB 2010

Evenbly *et al.*, PRL 2010

Schwandt *et al.*, PRB 2011

Iqbal *et al.*, PRB 2011

Poilblanc *et al.*, PRB 2011

Iqbal et al., New J. Phys. 2012

……

Spin Liquid

Gapped

Jiang, *et al.*, PRL 2008

Yan, *et al.*, Science 2011

Depenbrock, *et al.*, PRL 2012

Jiang, *et al.*, Nature Phys. 2012

Nishimoto, Nat. Commu. (2013)

Gong, *et al.*, Sci. Rep. 2014

Li, arXiv 2016

Mei, *et al.*, PRB 2017

……

Gapless

Hastings, PRB 2000

Hermele, *et al.*, PRB 2005

Ran, *et al.*, PRL 2007

Hermele, *et al.*, PRB 2008

Tay, *et al.*, PRB 2011

Iqbal, *et al.*, PRB 2013

Hu, *et al.*, PRB 2015

Jiang, *et al.*, arXiv 2016

Liao, *et al.***, PRL 2017**

He, *et al.*, PRX 2017

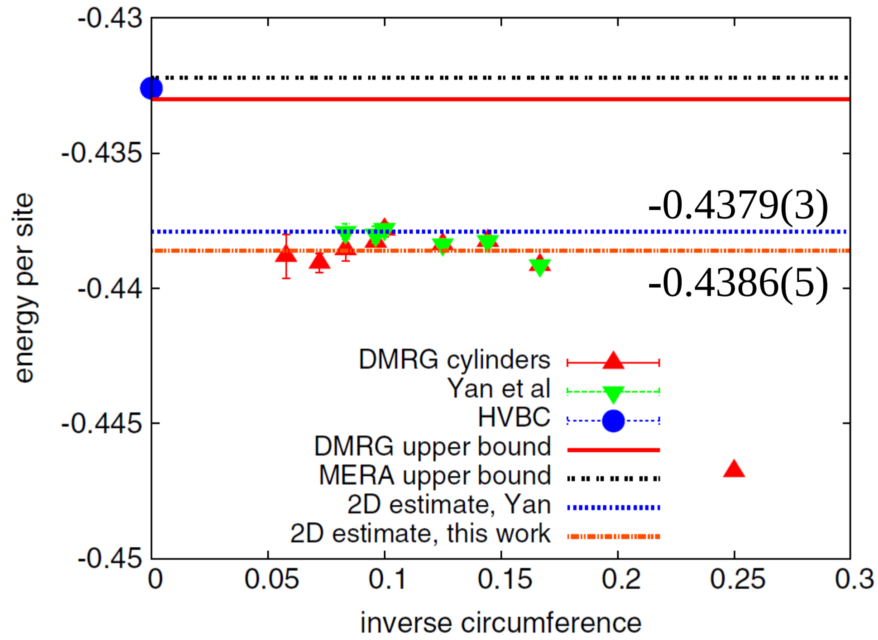
……

Problems in the theoretical studies

✓ Density Matrix Renormalization Group (DMRG):

strong finite size effect

error grows exponentially with the system size



Depenbrock et al, PRL **109**, 067201 (2012)

Problems in the theoretical studies

✓ Density Matrix Renormalization Group (DMRG):

strong finite size effect

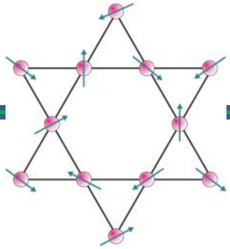
error grows exponentially with the system size

✓ Variational Monte Carlo (VMC)

need accurate guess of the wave function

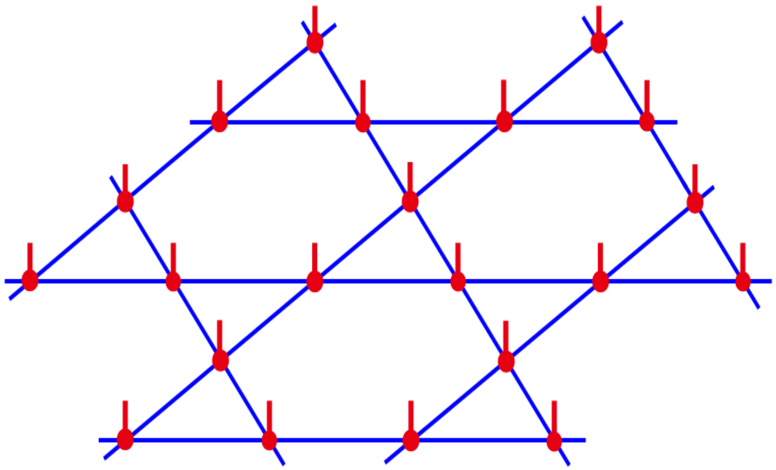
✓ Quantum Monte Carlo

Minus sign problem



Can we solve this problem using PEPS?

$$|\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'}[m_i] |m_i\rangle$$

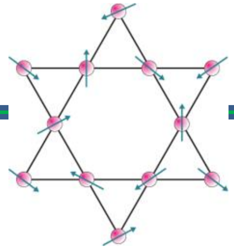


Local tensors

Rank-5 tensors

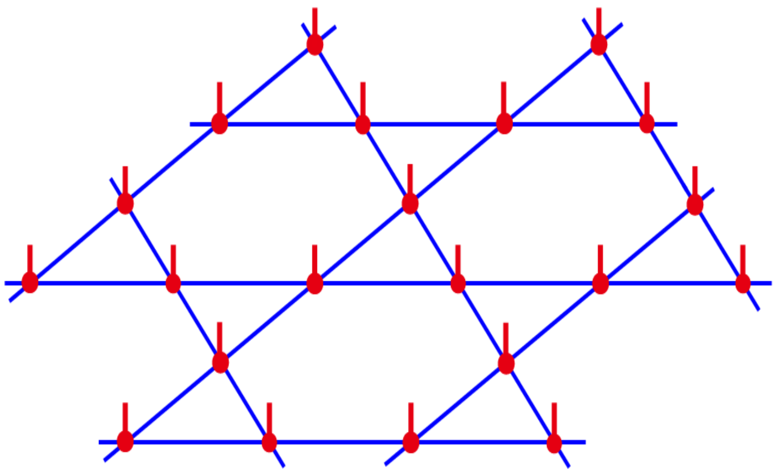
Projected Entangled Pair State (PEPS):

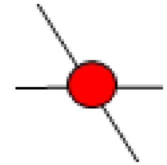
Virtual spins at two neighboring sites form a maximally entangled state

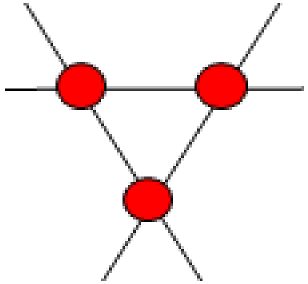


Can we solve this problem using PEPS?

$$|\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'}[m_i]|m_i\rangle$$

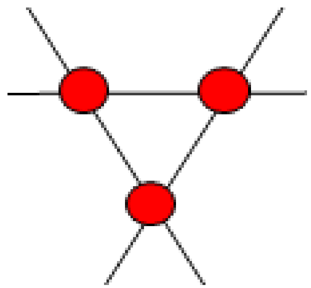


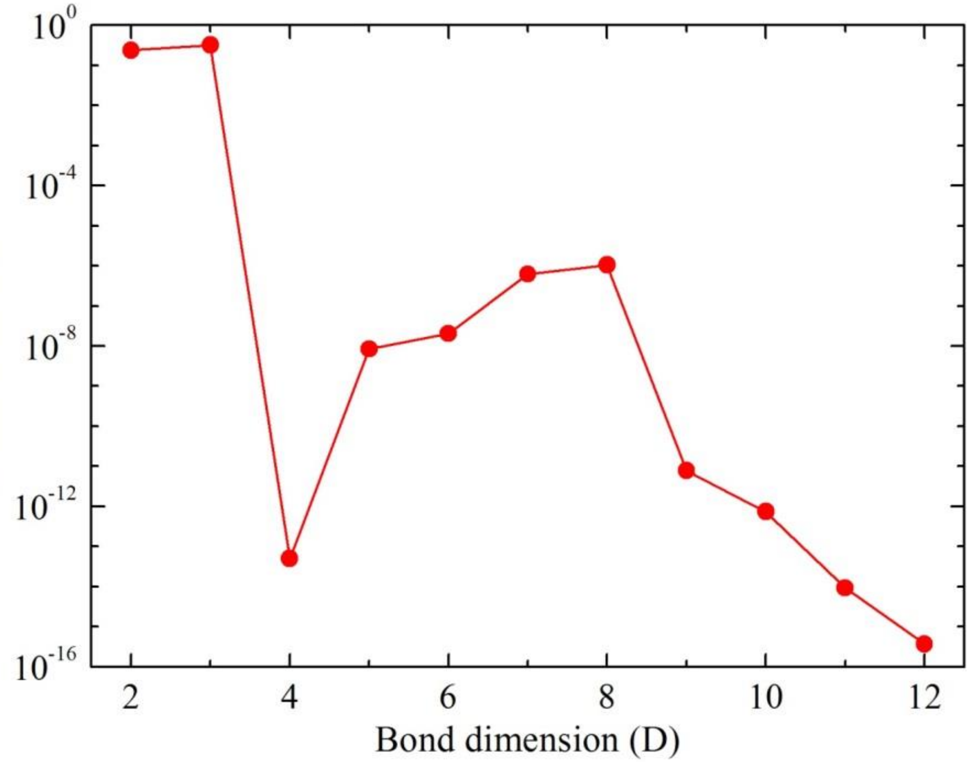
Max **(**  ***) ~ 1***

Max **(**  ***) < 10^-6***

- ✓ **There is a serious cancellation in the tensor elements if three tensors on a simplex (triangle here) are contracted**
- ✓ **3-body (or more-body) entanglement is important**

Cancellation in the PEPS

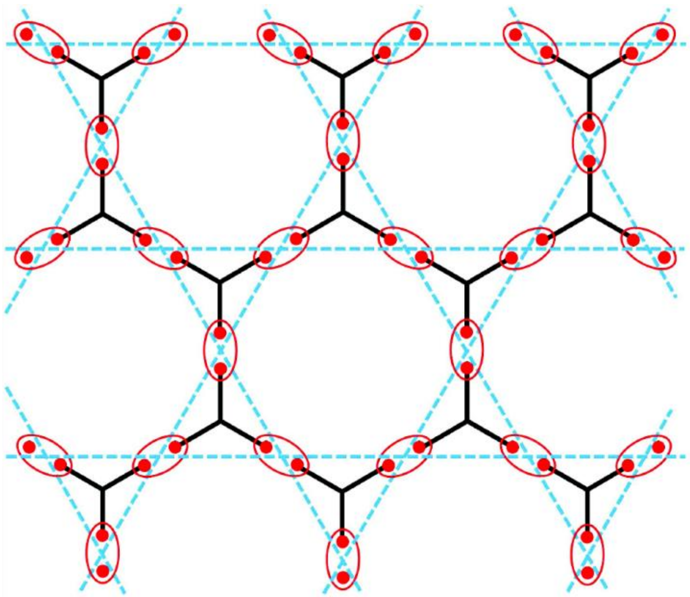
Max **(**  **)**

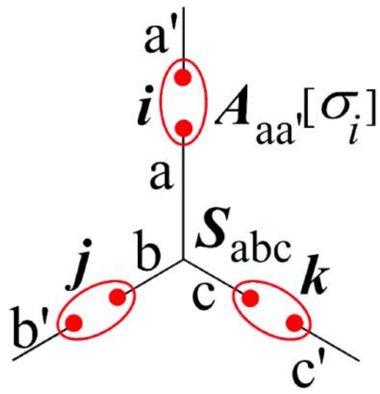


$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad J > 0$$

Solution: Projected Entangled Simplex States (PESS)

Z. Y. Xie et al, PRX 4, 011025 (2014)

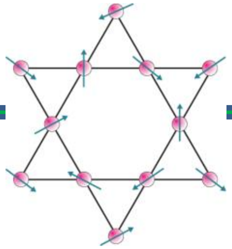




Projection tensor

Simplex tensor

- ✓ **Virtual spins at each simplex form a maximally entangled state**
- ✓ **Remove the geometry frustration: The PESS is defined on the decorated honeycomb lattice**
- ✓ **Only 3 virtual bonds, low cost**



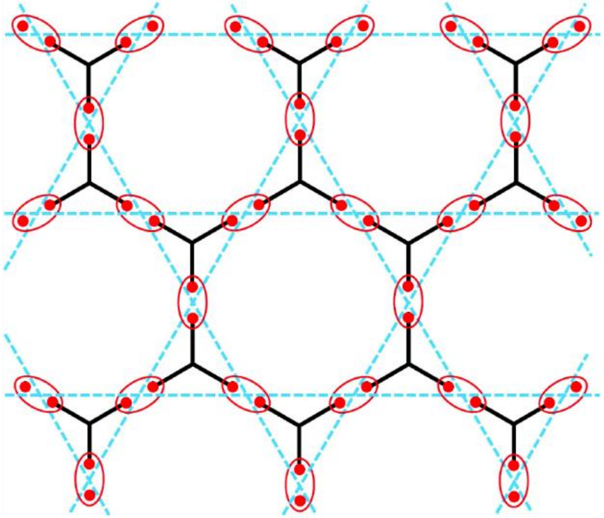
PESS: exact wave function of Simplex Solid States

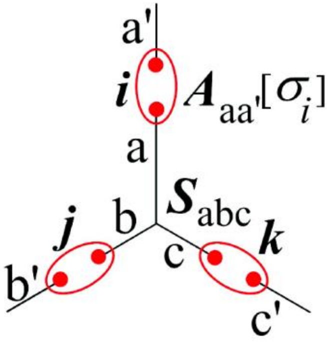
D. P. Arovas, Phys. Rev. B **77**, 104404 (2008)

Example: **S = 2** spin model on the Kagome lattice

A **S = 2** spin is a symmetric superposition of two virtual **S = 1** spins

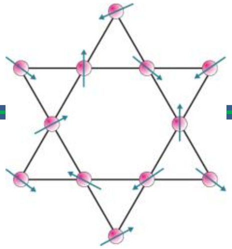
Three virtual spins at each triangle form a spin singlet





Projection tensor

Simplex tensor



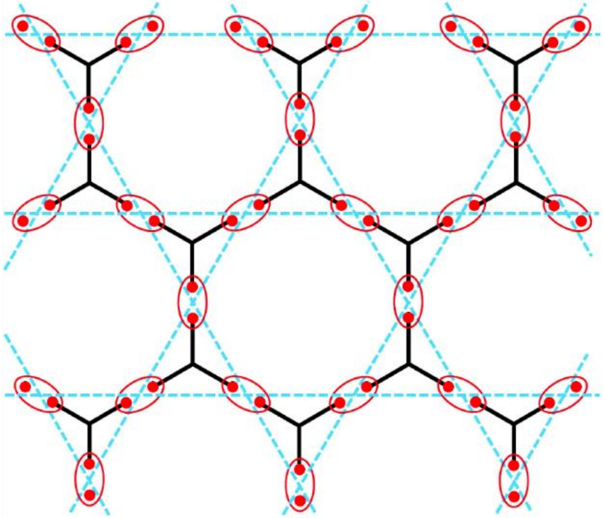
S=2 Simplex Solid State

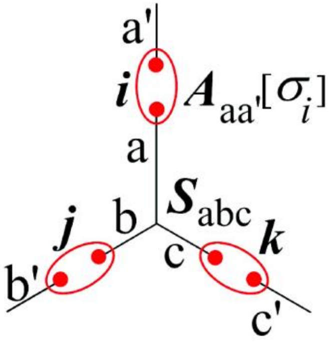
Local tensors

$$|0,0\rangle = \frac{1}{\sqrt{6}} \sum_{s_i s_j s_k} \varepsilon_{s_i s_j s_k} |s_i\rangle |s_j\rangle |s_k\rangle$$

$S_{ijk} = \varepsilon_{ijk}$ antisymmetric tensor

$A_{ab}[\sigma] = \begin{pmatrix} 1 & 1 & 2 \\ a & b & \sigma \end{pmatrix}$ C-G coefficients





Projection tensor

Simplex tensor

Advantage for using PESS

1. No finite size effect: PESS can be defined on an infinite lattice

2. More accurate for studying large lattice size systems

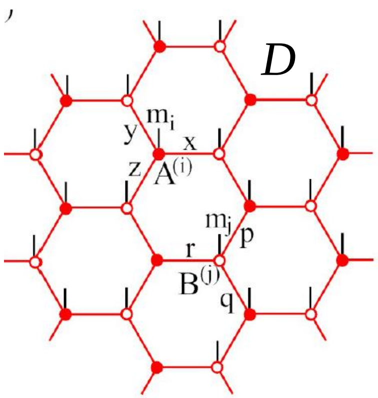
3. The ground state energy converges fast with the increase of the bond dimension ***D***

   - **Converge exponentially with *D* if the ground state is gapped**
   - **Converge algebraically with *D* if the ground state is gapless**

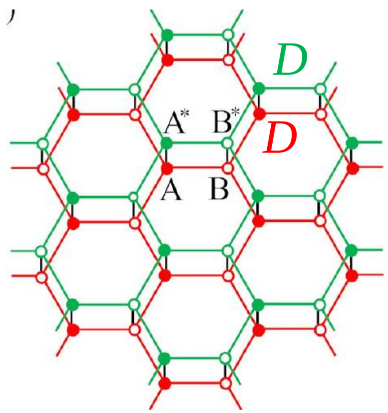
   This property is used to determine whether the ground state is gapped or gapless

Main Difficulty in the Calculation of TNS

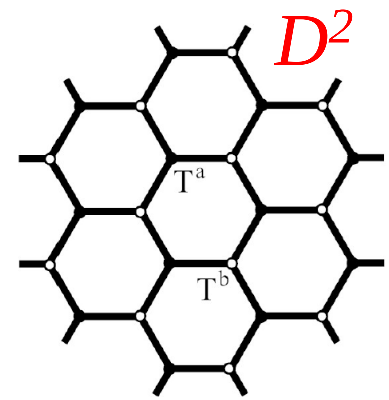
Conventional Double-Layer Contraction Approach



$|\Psi\rangle$



$\langle\Psi| * |\Psi\rangle$



$\langle\Psi|\Psi\rangle$

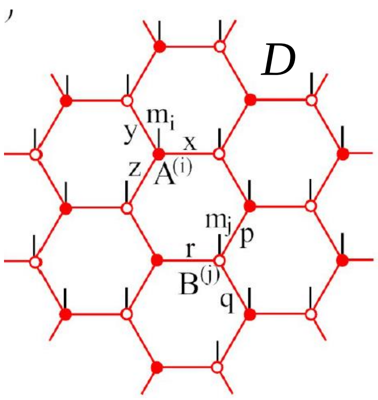
Computational time scales as $\boldsymbol{D^{12}}$

maximal $\boldsymbol{D}$ that can be handle is ***13***

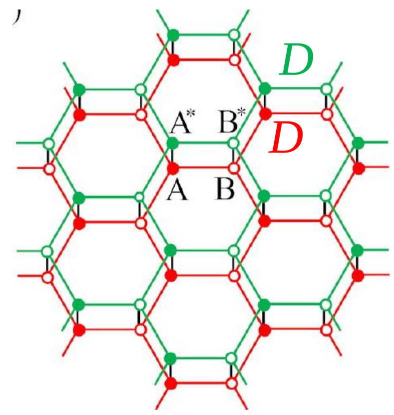
Solution

Reduce the Cost by Dimension Reduction

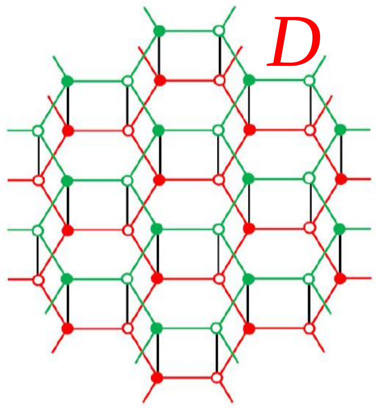
Shifted Single-Layer Approach: Nested Honeycomb Lattice



$|\Psi\rangle$



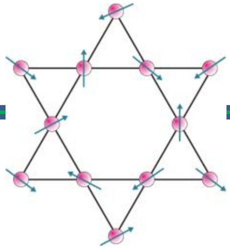
$\langle\Psi| * |\Psi\rangle$



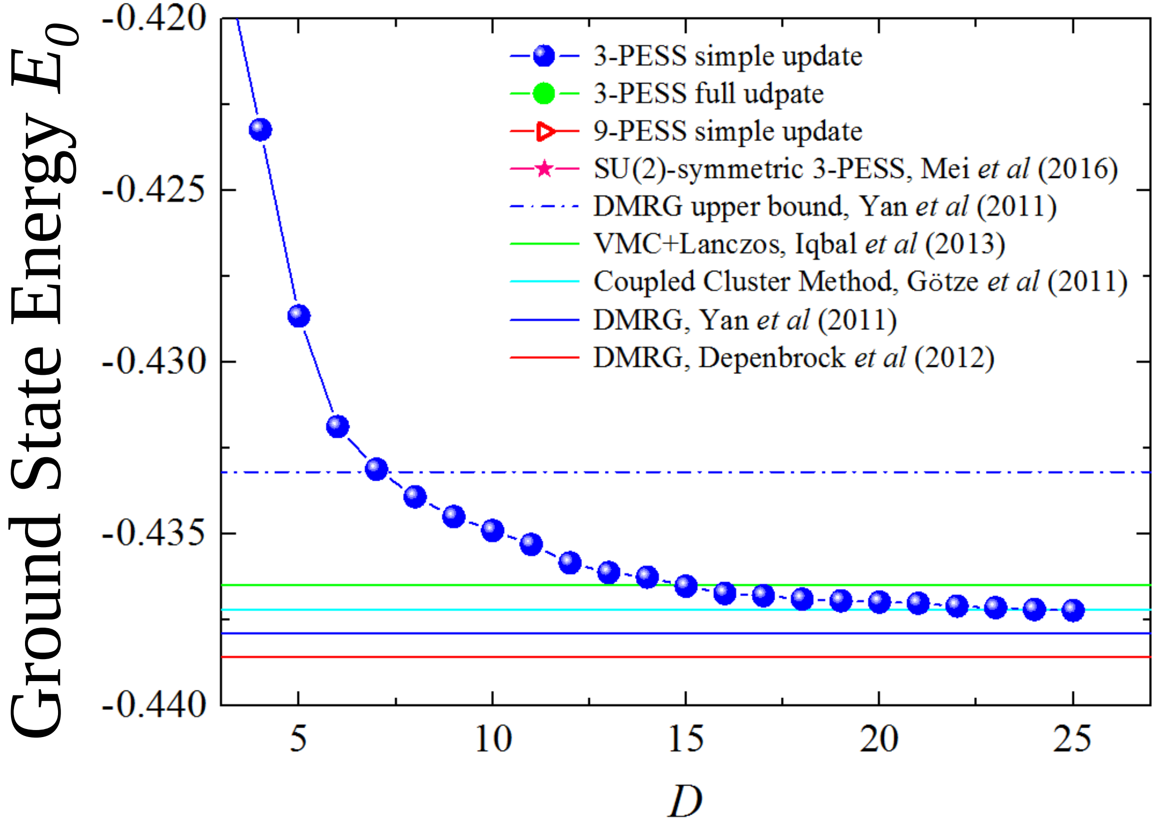
$\langle\Psi|\Psi\rangle$

Computational time scales as $\boldsymbol{D^8}$

maximal $\boldsymbol{D}$ reaches *25*



Kagome Heisenberg: Ground State Energy

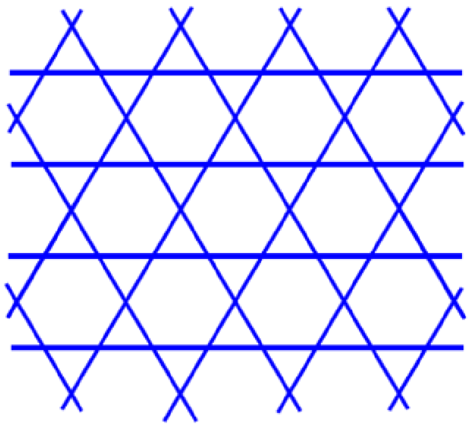


Ground state energy shows a power law behavior

Question: Is ***D*=25** large enough?

Take A Reference: Husimi lattice

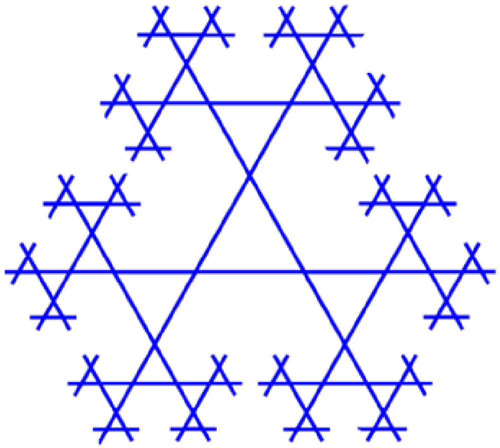
Make comparison between Kagome and Husimi results



Kagome Lattice

Same local structure

Gain insight for the kagome system



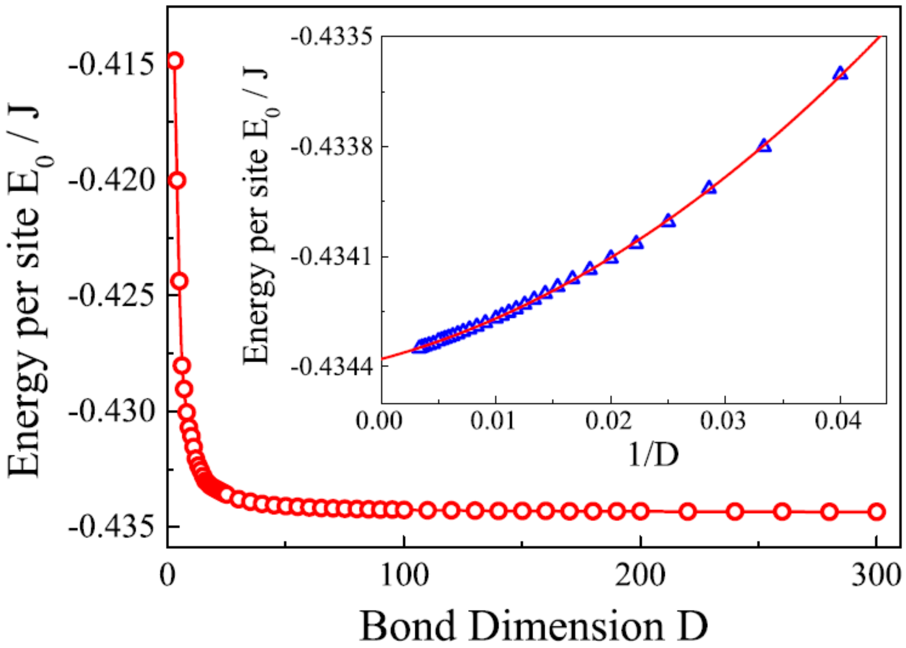
(b) Husimi Lattice

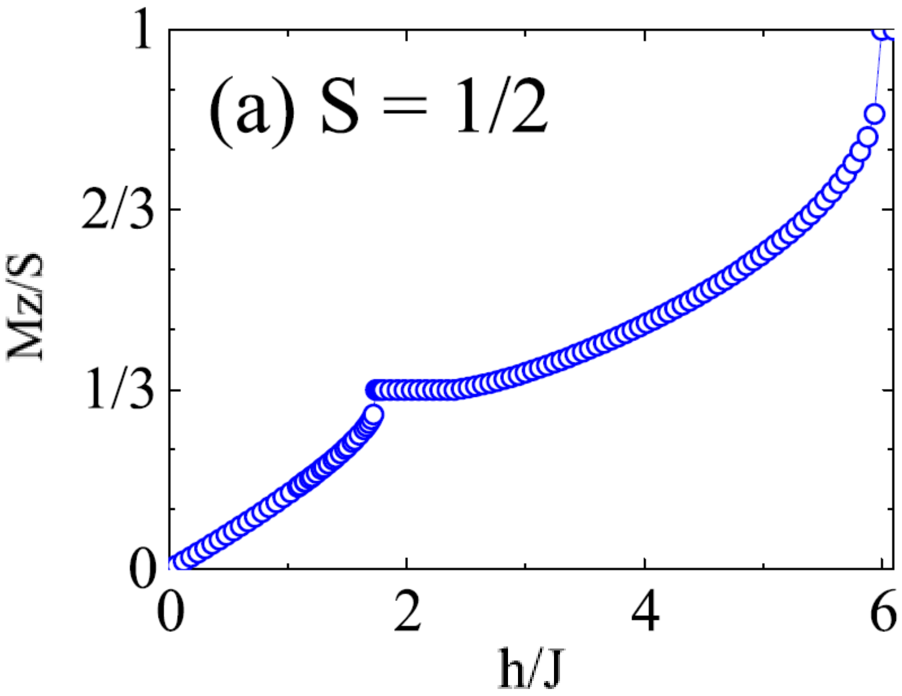
- ✓ Highly frustrated
- ✓ ***D*** is generally small

- ✓ Tree Structure
- ✓ Tensor renormalization is rigorous, ***D*** can reach 1000

S=1/2 Husimi Lattice: Gapless Ground State

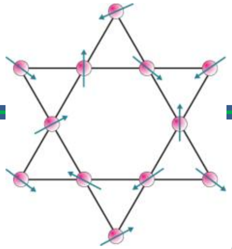
S = 1/2 Husimi Heisenberg model

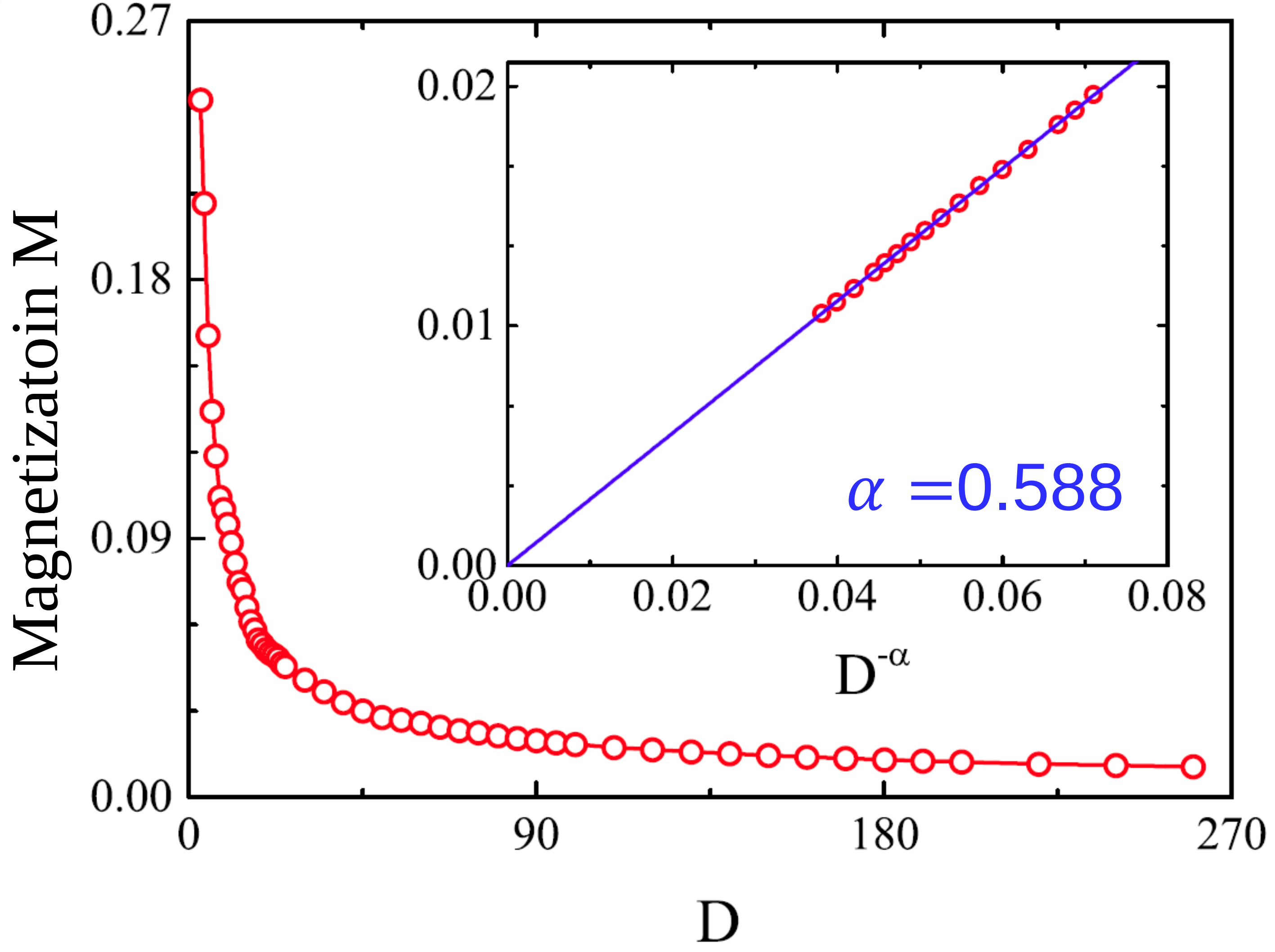




Energy algebraically converge with the bond dimension

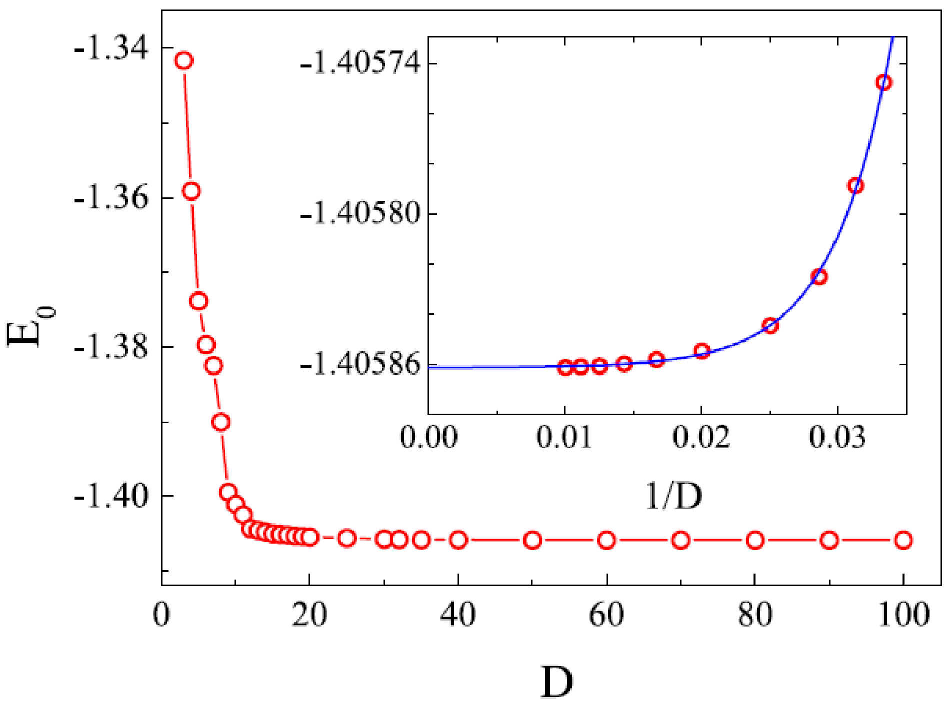
S=1/2 Husimi Lattice: Magnetization Free

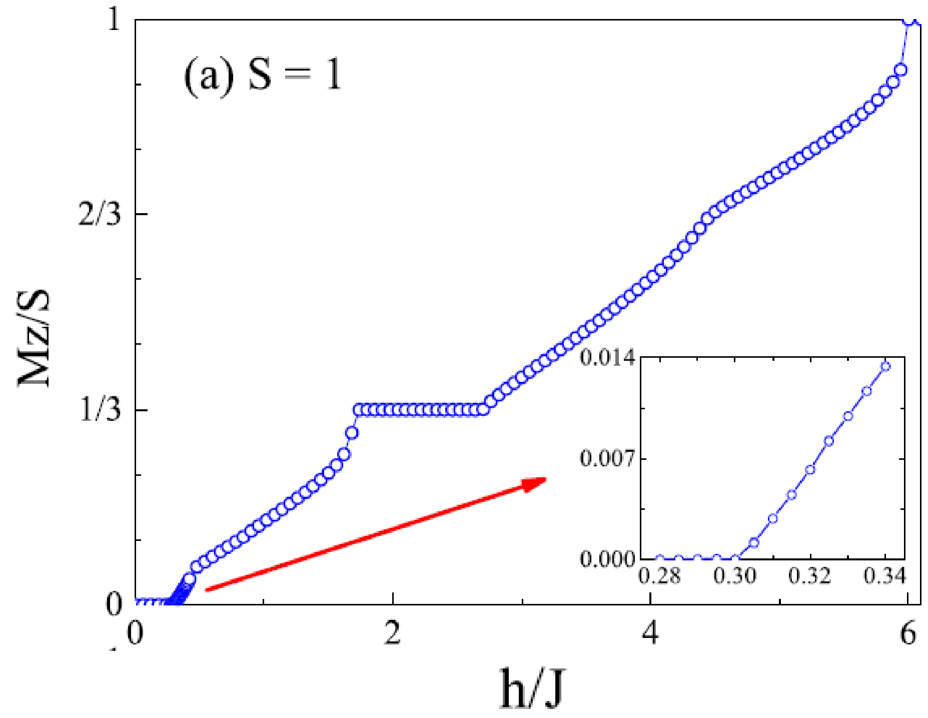




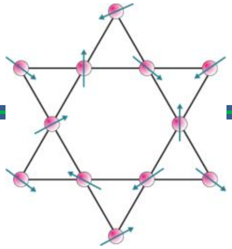
S=1 Husimi: Gapped Ground State

Ground state: trimerized

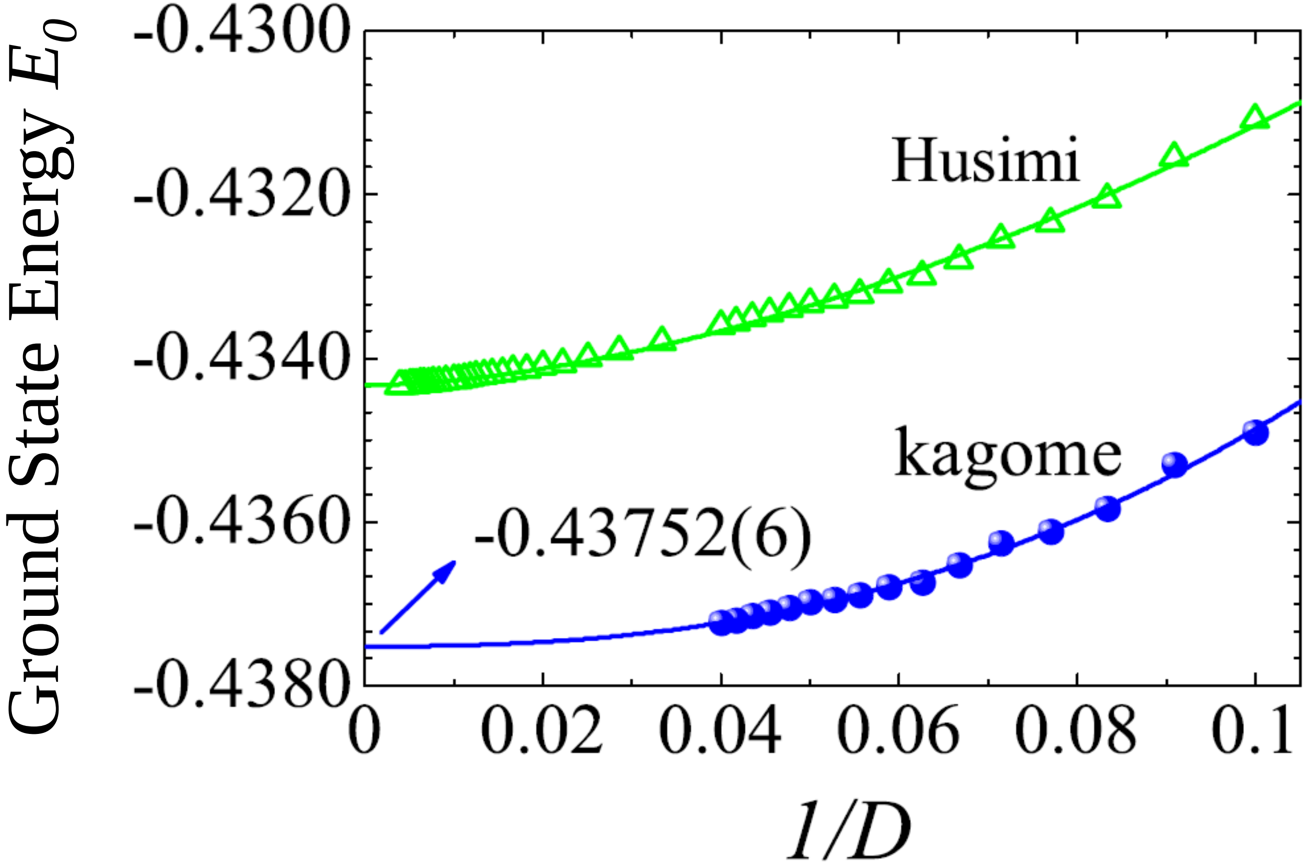




Energy converges exponentially with the bond dimension



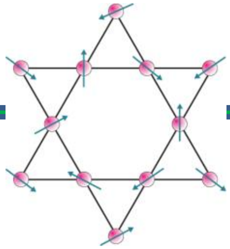
Kagome Heisenberg: Gapless



Upper bound of the energy Gap:

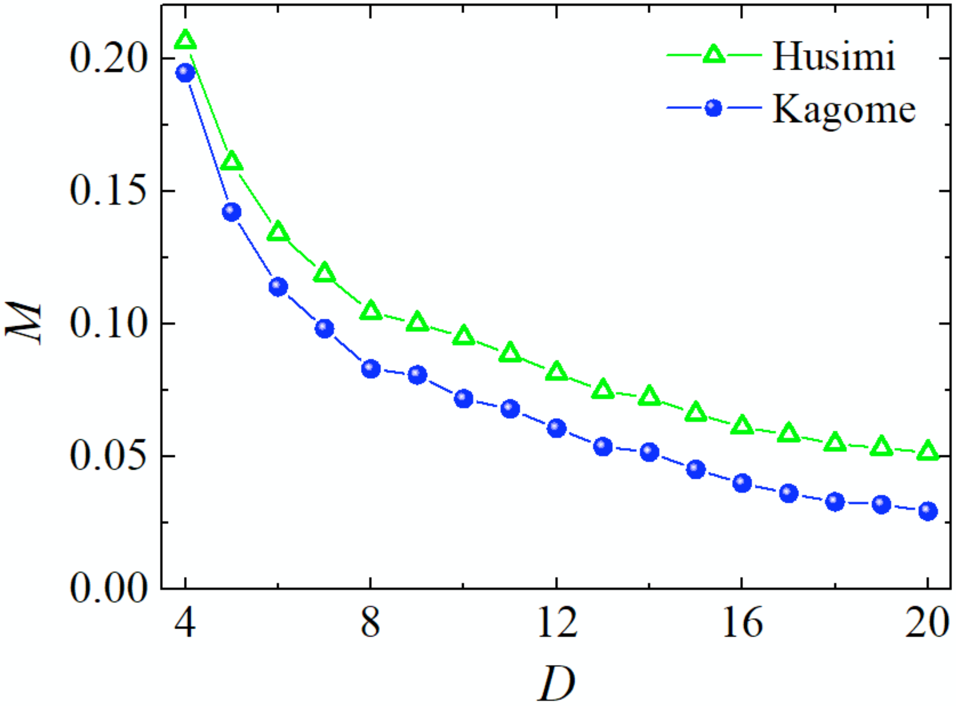
less than 10^{-4}

Energy converges algebraically with the bond dimension

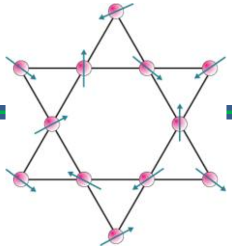


Kagome Antiferromagnetic: Magnetic free?

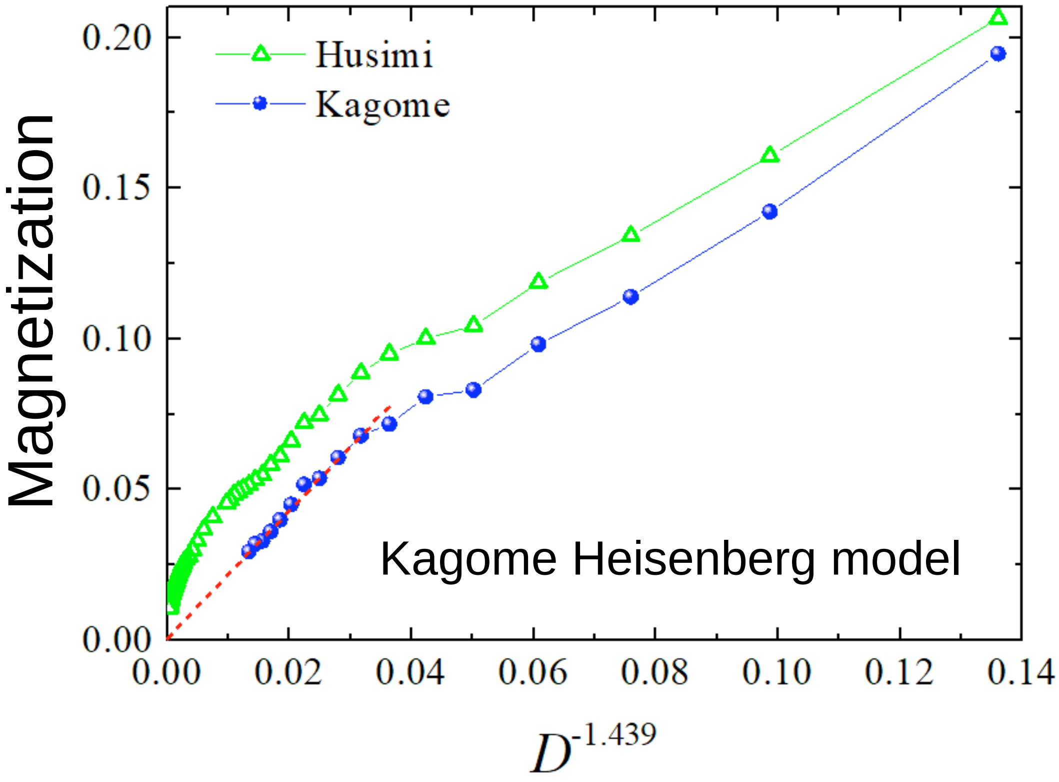
$$M_{Kagome} < M_{Husimi}$$



Magnetization: decays algebraically with *D*



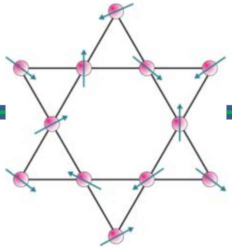
Kagome Antiferromagnetic: Magnetic free?



The magnetic long-range order vanishes in the infinite ***D*** limit

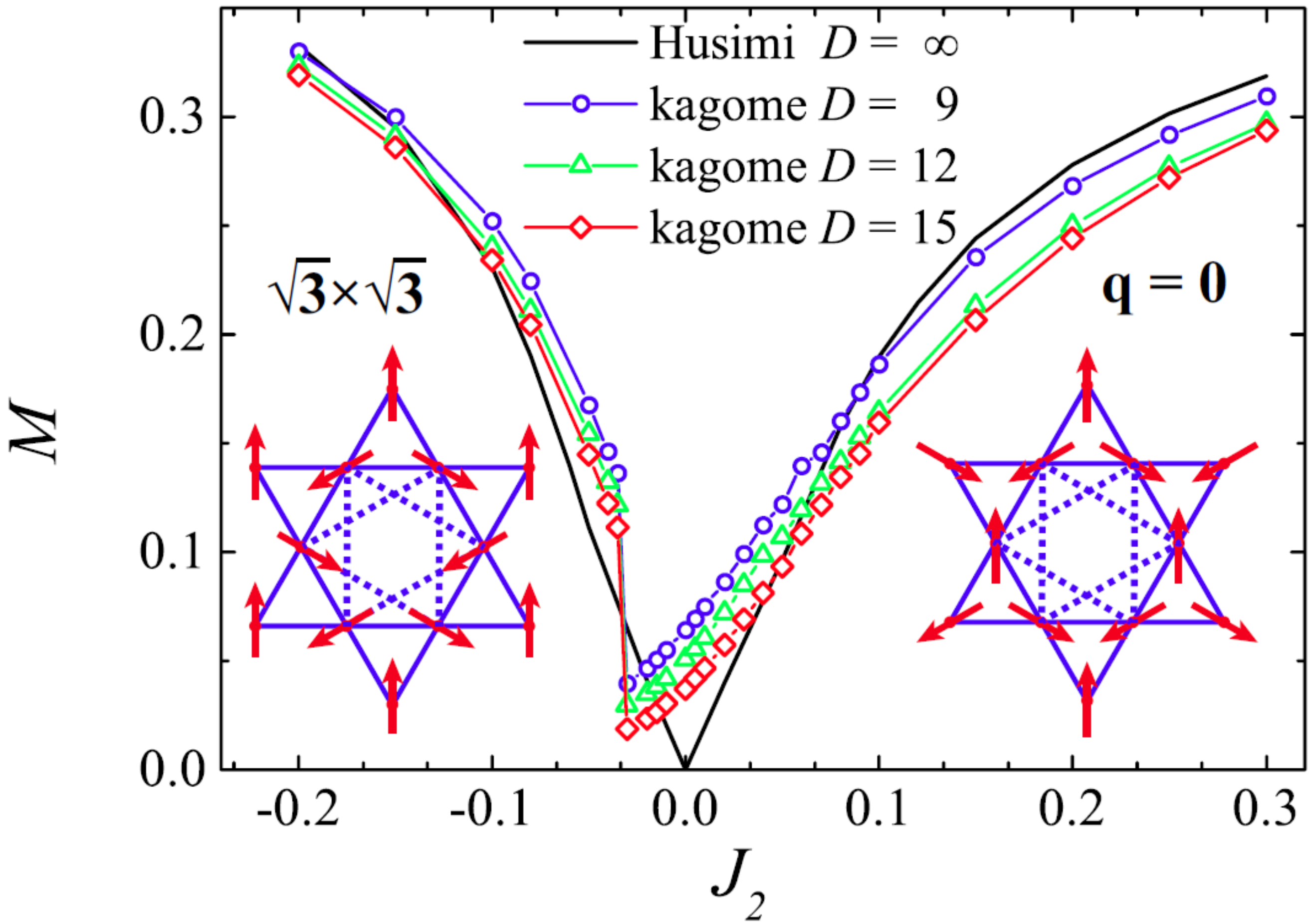
↓

The ground state of the Kagome Heisenberg model is a spin liquid.

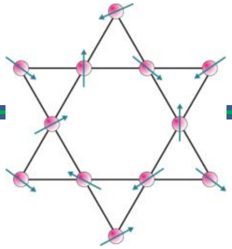


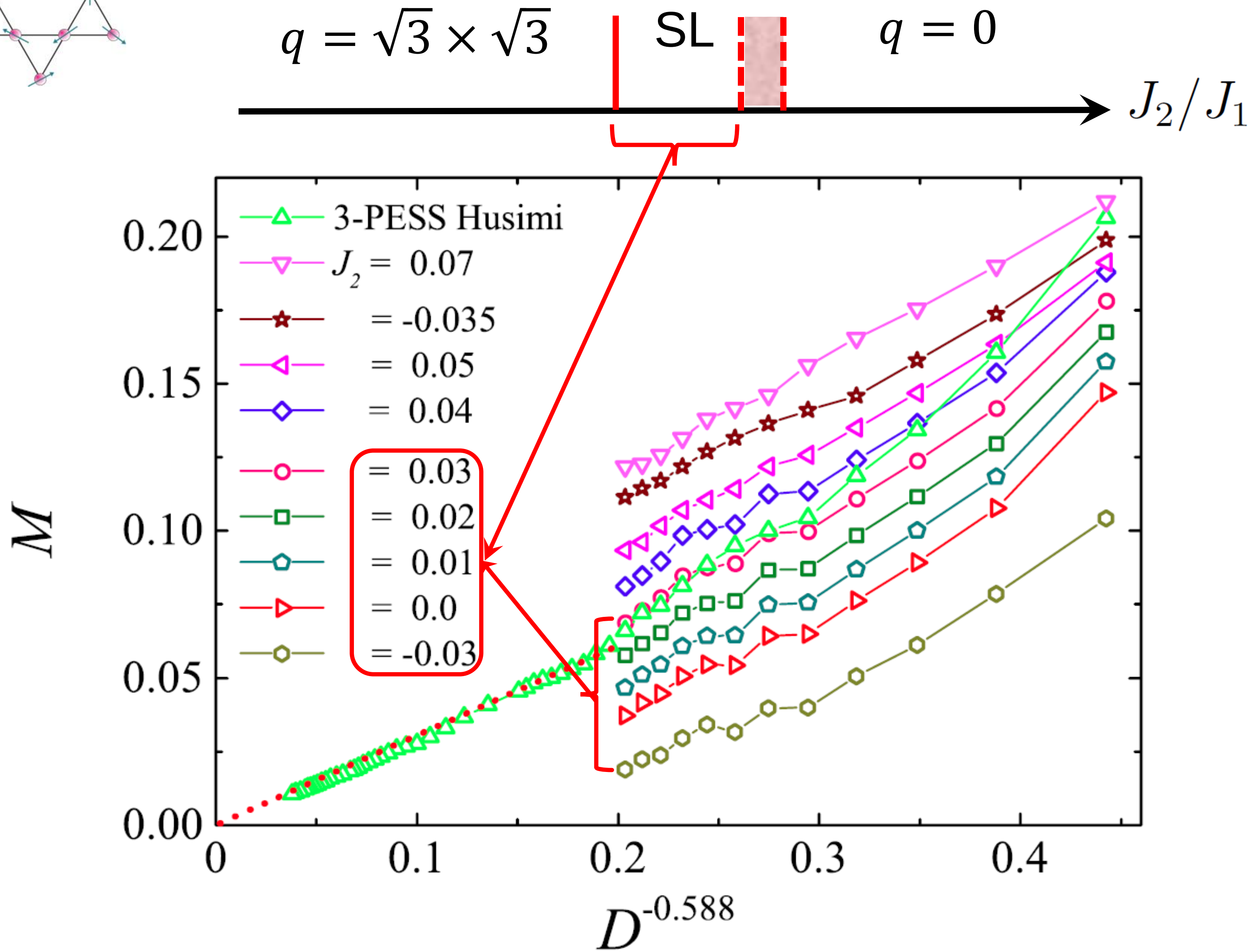
Stability against other interactions

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

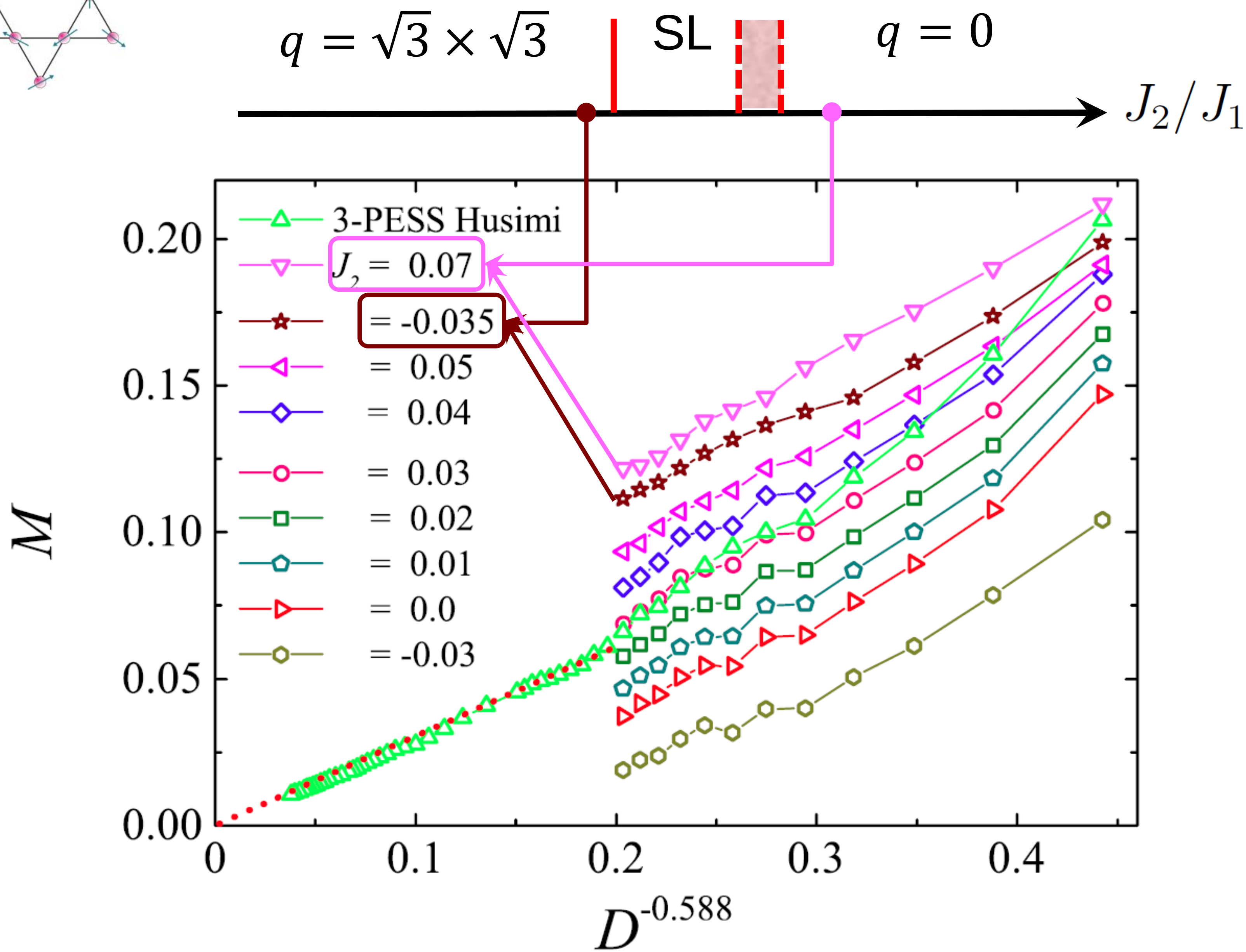


Bond dimension dependence of the magnetic order

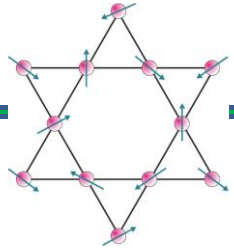


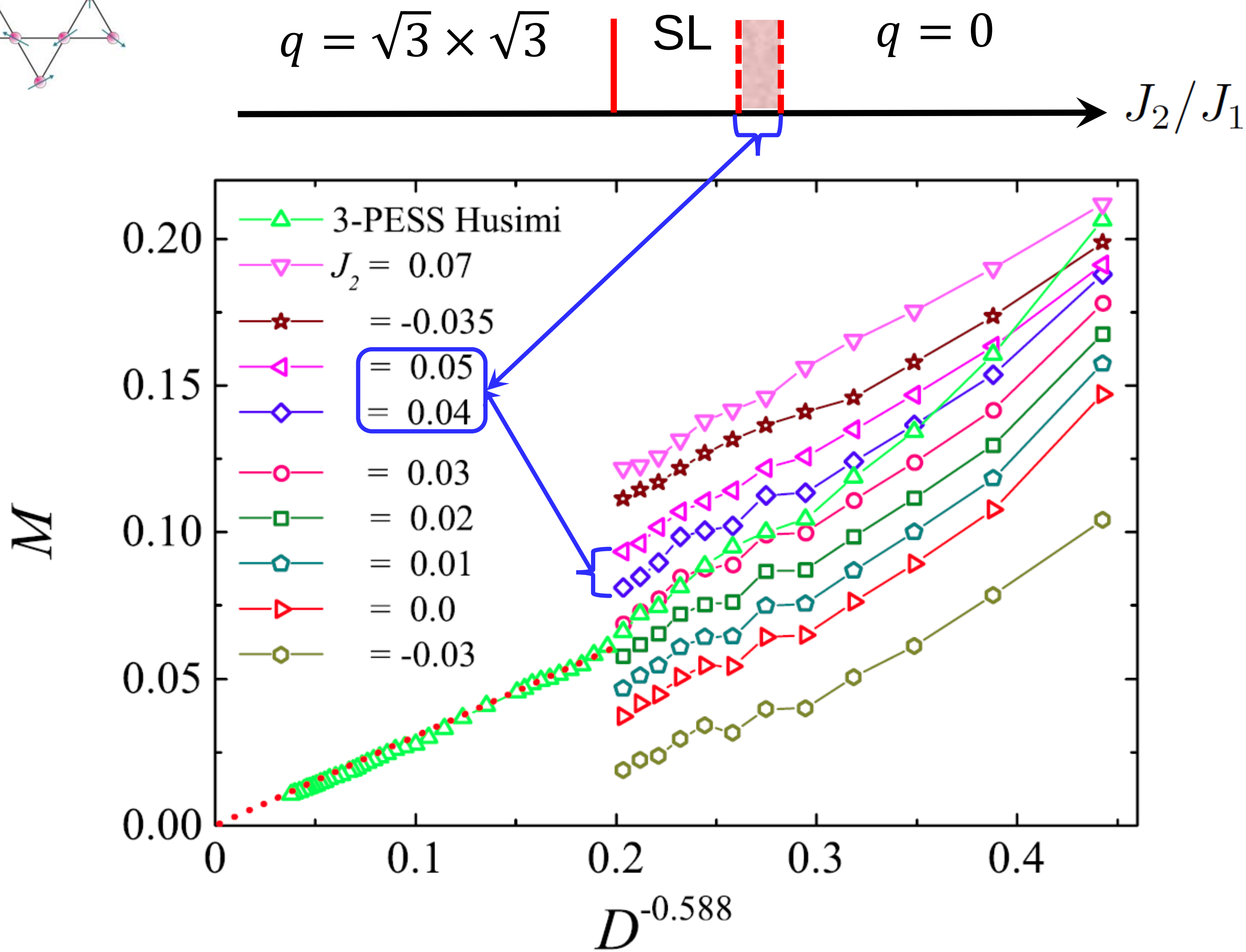


Bond dimension dependence of the magnetic order

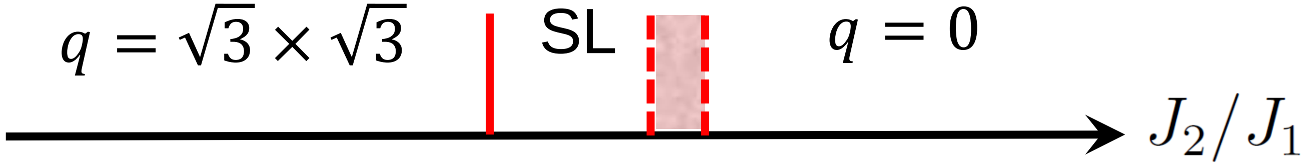


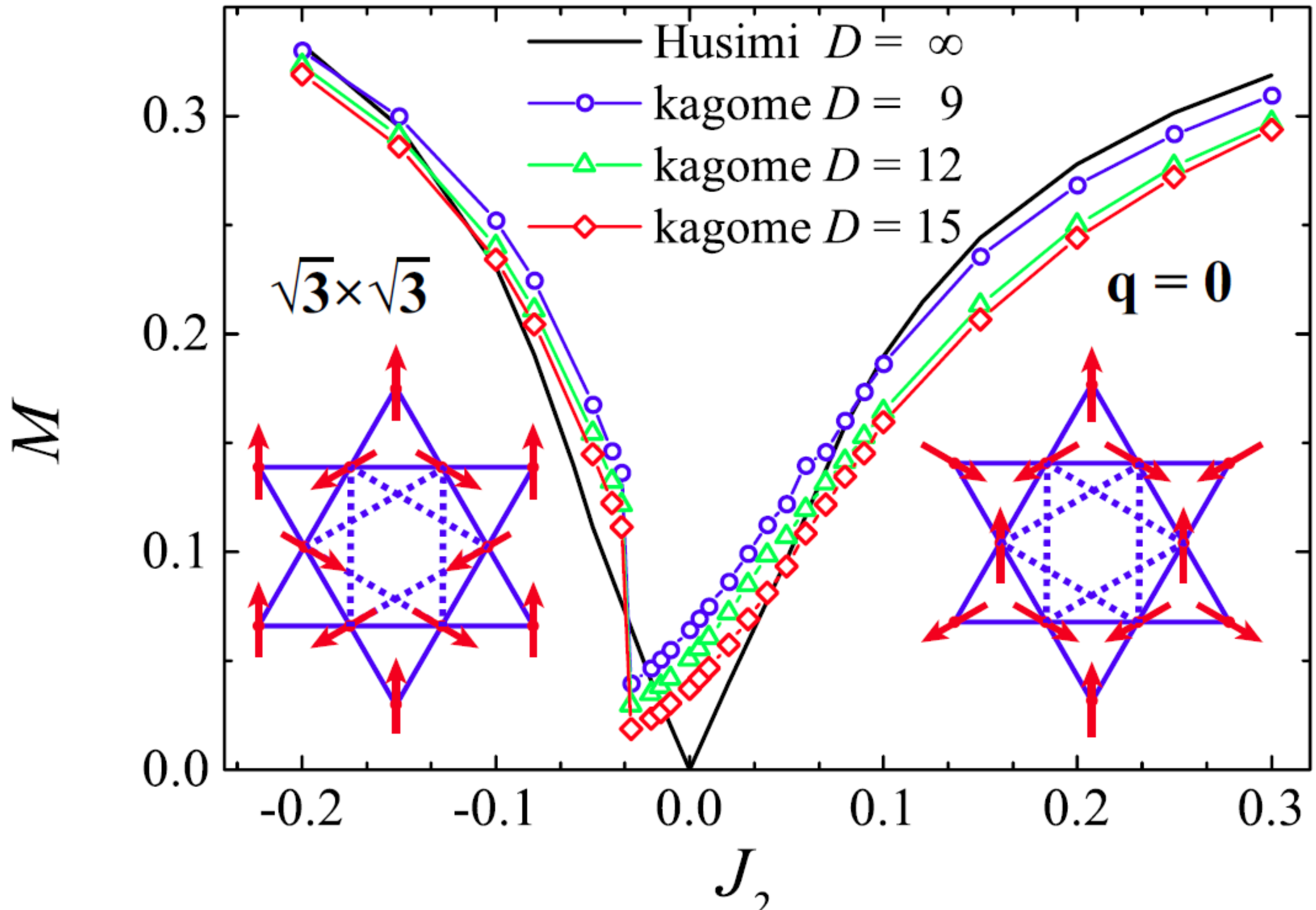
Bond dimension dependence of the magnetic order

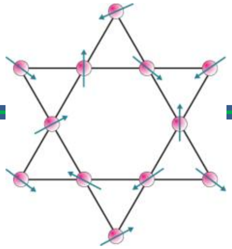




Phase Diagram







Summary

- **Tensor-network renormalization provides a powerful tool for studying correlated many body problems**

- **The ground state of the Kagome Heisenberg model is likely a gapless spin liquid**

Bruce Normand

PSI

Haijun Liao

Haidong Xie

Ruizhen Huang

Institute of Physics, CAS

Zhiyuan Xie

Renmin Univ China