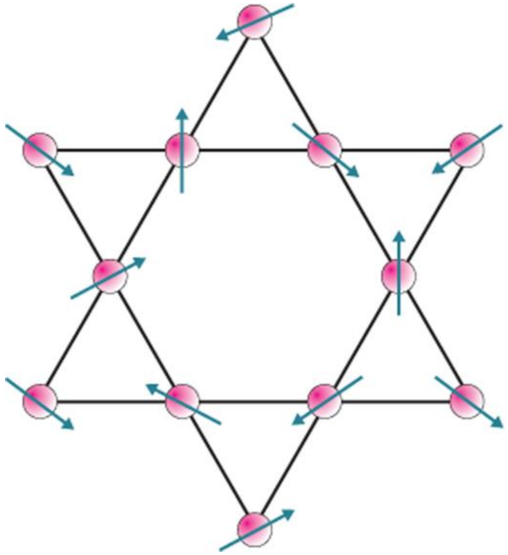
Gapless Spin Liquid Ground State in the S=1/2 Kagome Antiferromagnet



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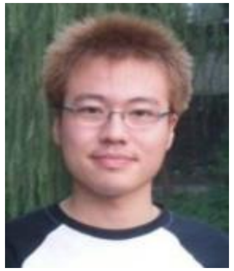
Acknowledgment



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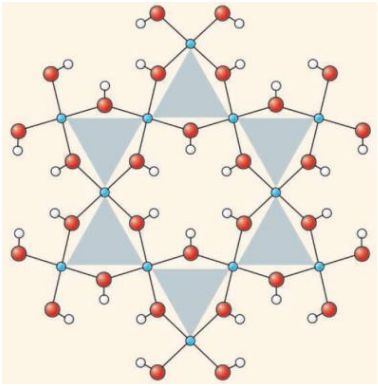
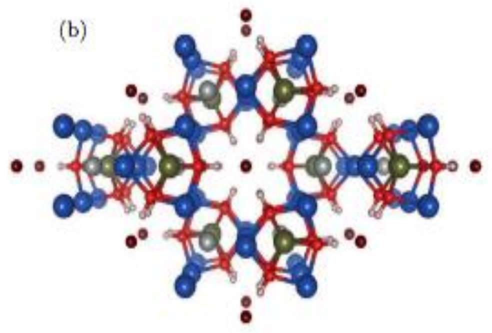
1. H. J. Liao, et al, PRL 118, 137202 (2017)
2. Z. Y. Xie, et al, PRB 96, 045128 (2017)
3. H. J. Liao, et al, PRB 93, 075154 (2016)
4. Z. Y. Xie, et al, PRX 4, 011025 (2014).

Questions to Address



Herbertsmithite: $ZnCu_3(OH)_6Cl_2$

Shores, *et al.*, J. Am. Chem. Soc. (2005)



$ZnCu_3(OH)_6FBr$

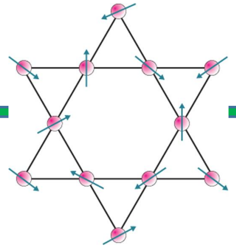
Feng Z, *et al.*, Chin. Phys. Lett. (2017)

S=1/2 Kagome Heisenberg

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

What is its ground state

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

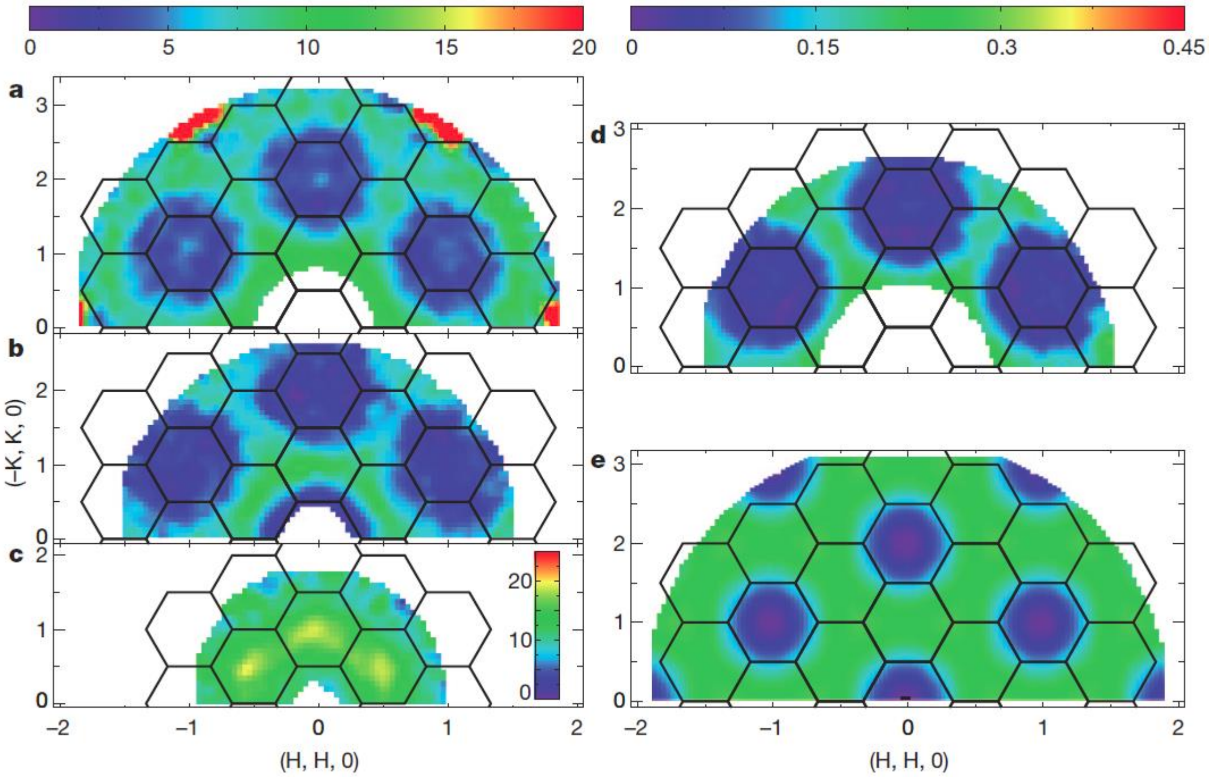


Hints from Experiments： Neutron Scattering

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]

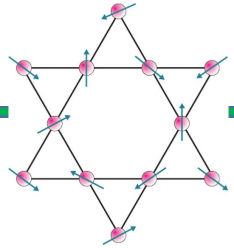
Nature 492 (2012) 406



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

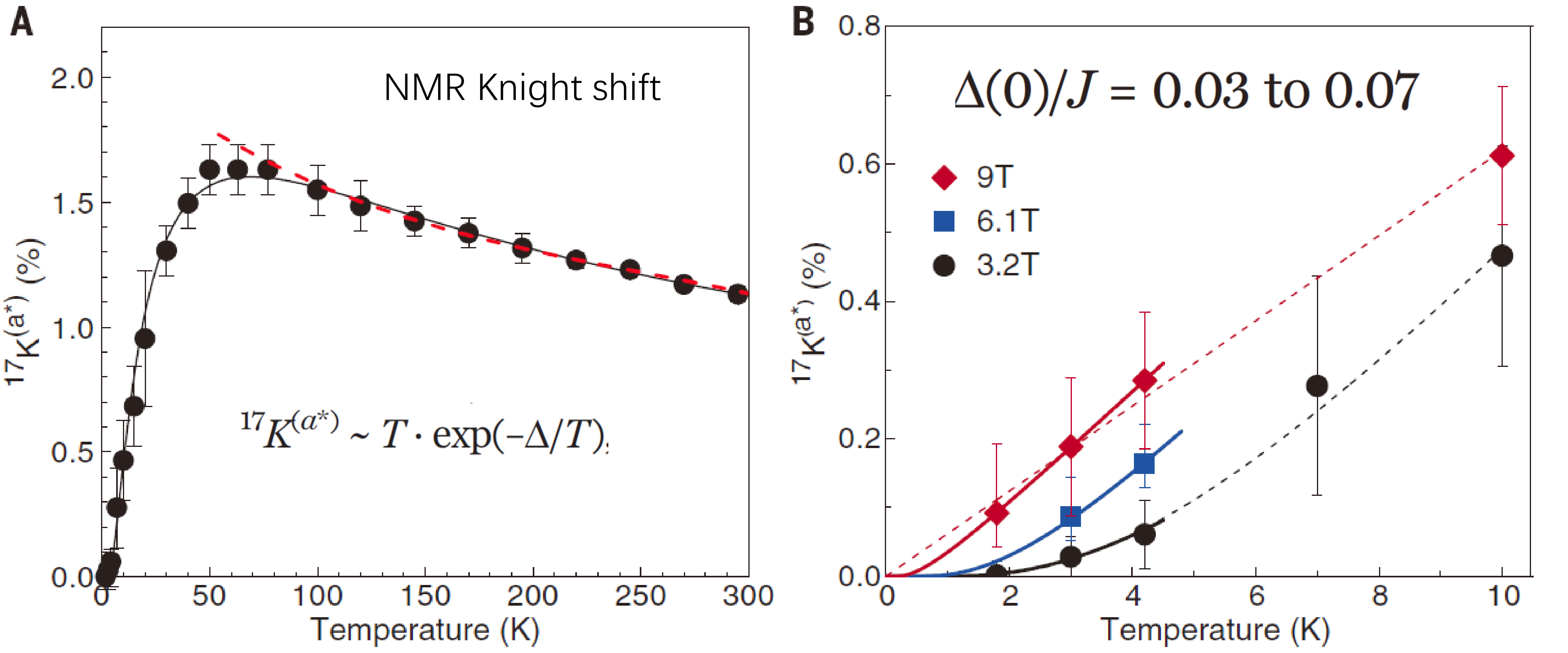


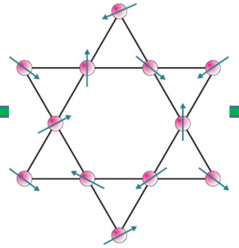
NMR：Gapped Spin Liquid

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





Kagome AFM: Theoretical Study

A question under debate for more than 30 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

……

QuantumSpin 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

……

Difficulties 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

How Do We Solve This Problem?

- **Use the Renormalization Group Method of Tensor-Network States (TRG)**

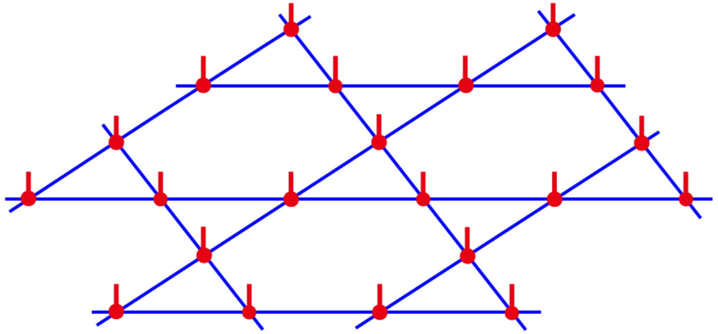
  The most accurate method for studying large-lattice size systems

- **Gain insight by making comparison with a reference system: Husimi Lattice, which can be almost exactly solved by TRG.**

  Husimi Lattice: locally similar to but less frustrated than Kagome lattice

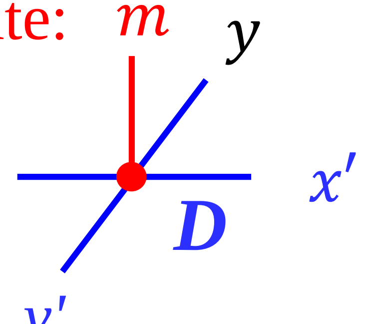
Tensor-Network States

Variational wave function that can be systematically improved by increasing the virtual basis states *D* (exact in the infinite *D* limit)



Physical state: m

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



Virtual basis state: y'

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

Each local tensor contains

$2D^4$ variational parameters

Renormalization of Tensor-Network States

✓ **No finite lattice size effect: TNS is defined on an infinite lattice**

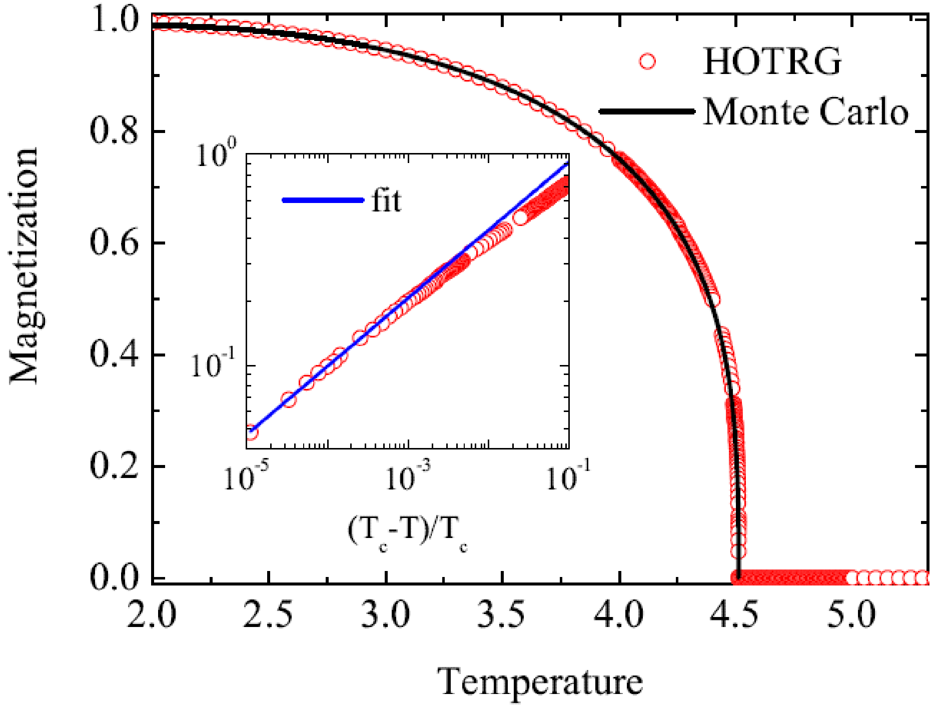
✓ **Ground state energy converges fast with the increase of the bond dimension *D***

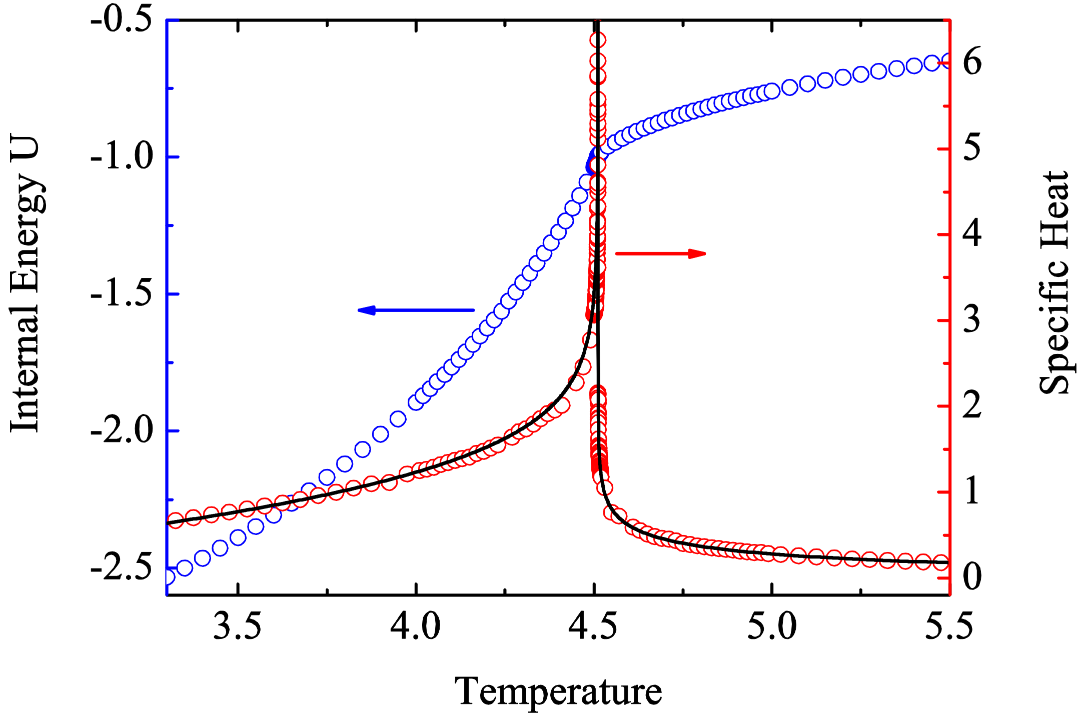
- **Converge exponentially with *D* if the ground state is gapped**
- **Converge algebraically with *D* if the ground state is gapless**

We use this to determine whether the ground state is gapped or gapless

TRG Result for the 3D Ising model

Xie et al, PRB 86,045139 (2012)





D=14

Relative difference is less than 10^{-5}

MC data:

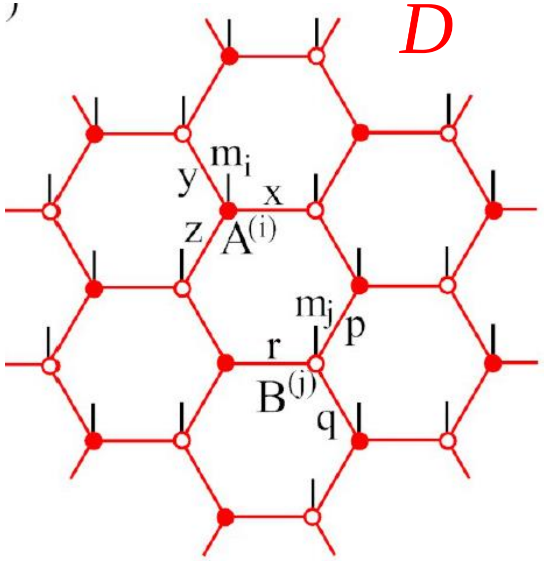
A. L. Talapov, H. W. J. Blote, J. Phys. A: Math. Gen. 29, 5727 (1996)　　**X. M. Feng, and H. W. J. Blote, Phys. Rev. E 81, 031103 (2010)**

Critical Temperature of 3D Ising model

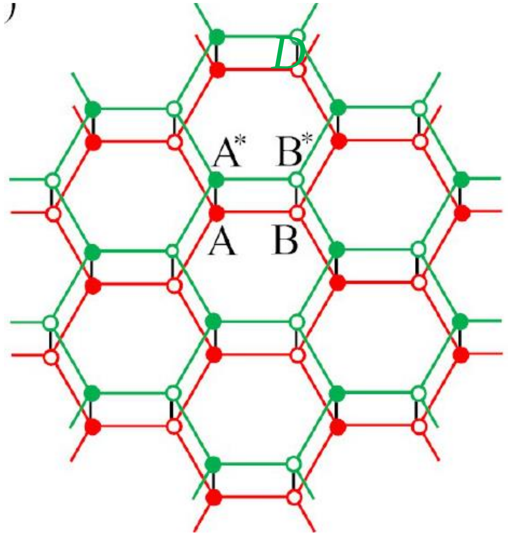
method	year	T_c
TRG (D = 23)	2014	4.51152469(1)
NRG (Nishino et al)	2005	4.55(4)
Monte Carlo Simulation	2017	4.5115232(1)
	2010	4.5115232(17)
	2003	4.5115248(6)
	1996	4.511516
High-temperature expansion	2000	4.511536

Key Problem We Solved in the Use of TNS

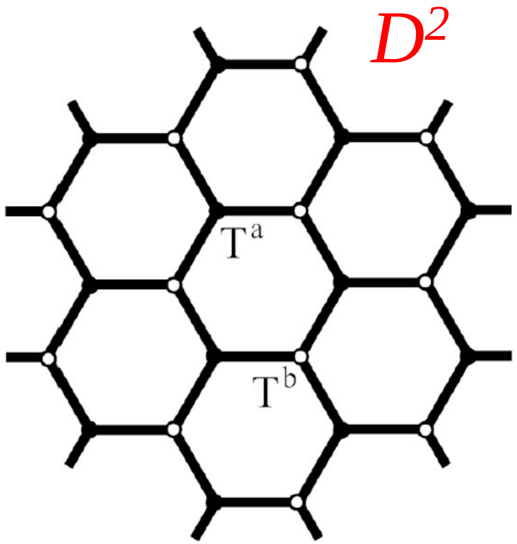
Conventional Double-Layer Approach



$|\Psi\rangle$



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



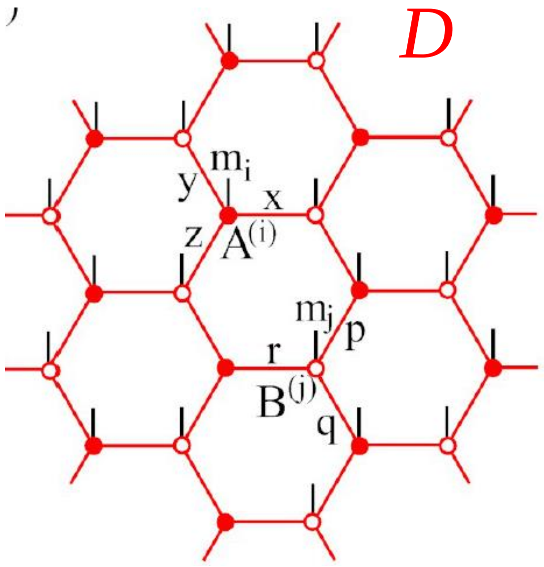
$\langle\Psi|\Psi\rangle$

Computational Cost scales as D^{12}

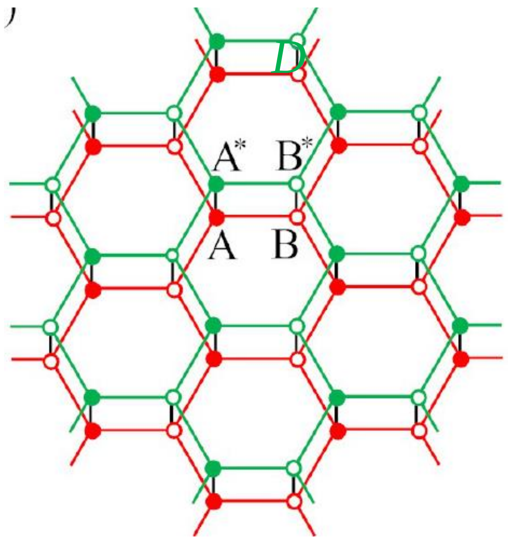
maximal D that can be reached = *13*

Solve This Problem By Dimension Reduction

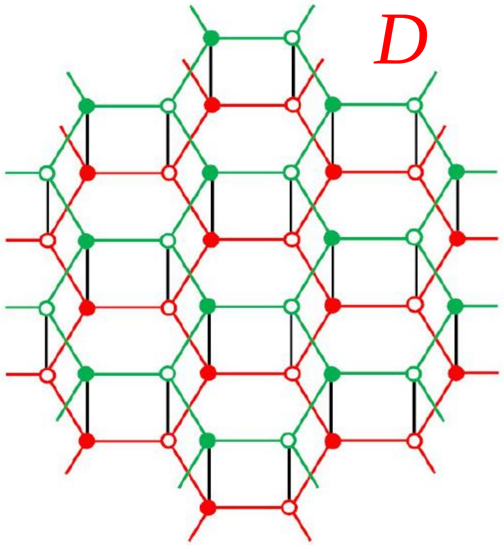
Shifted Single-Layer Approach



$|\Psi\rangle$



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

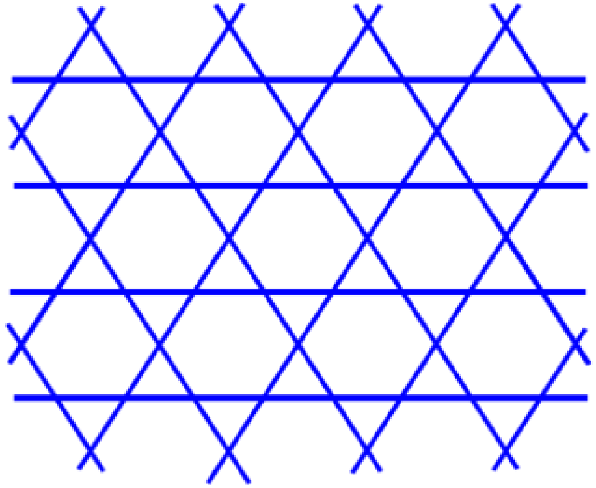


$\langle\Psi|\Psi\rangle$

Computational time scales as *D^8*   **Rise *D* to *25 or more***

Reference system: Husimi lattice

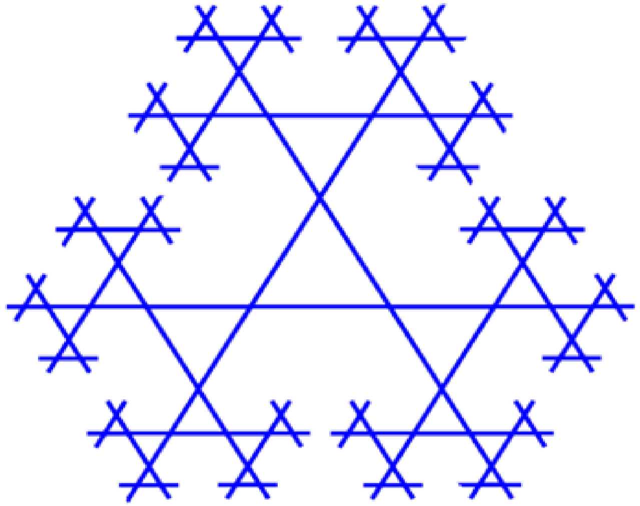
Make comparison between Kagome and Husimi results



Kagome Lattice

Same local structure

Gain insight for the kagome system

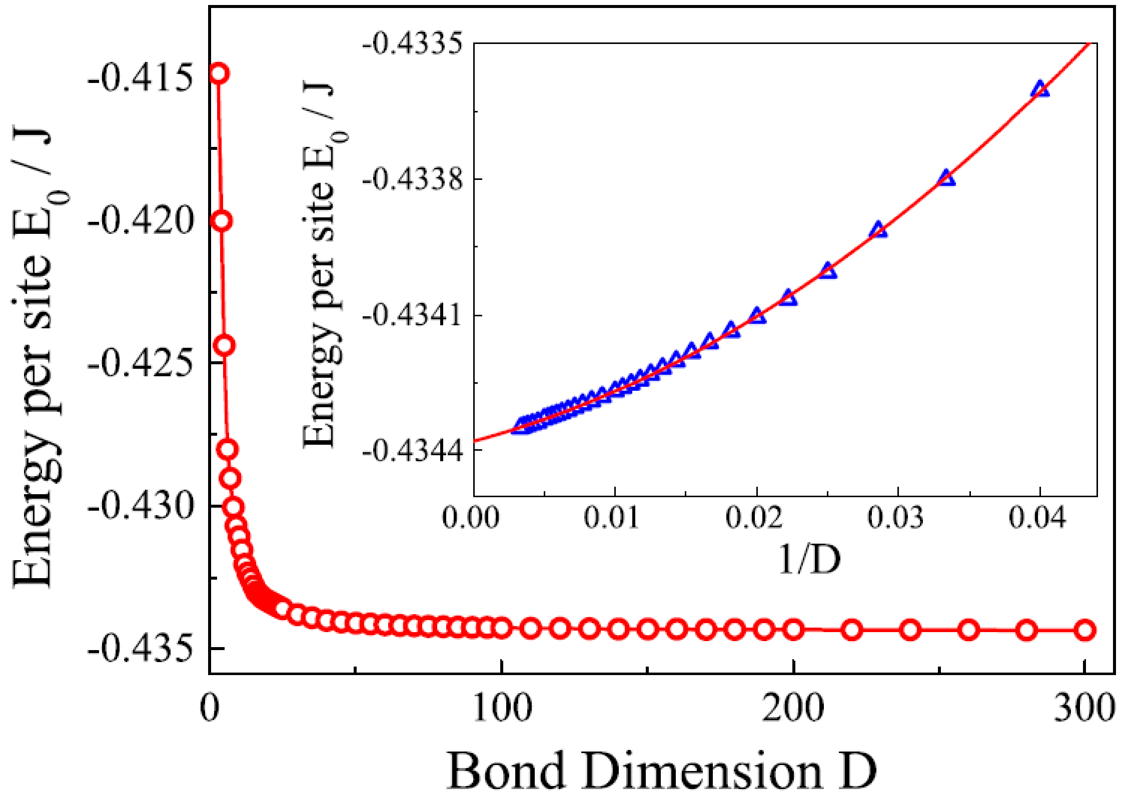


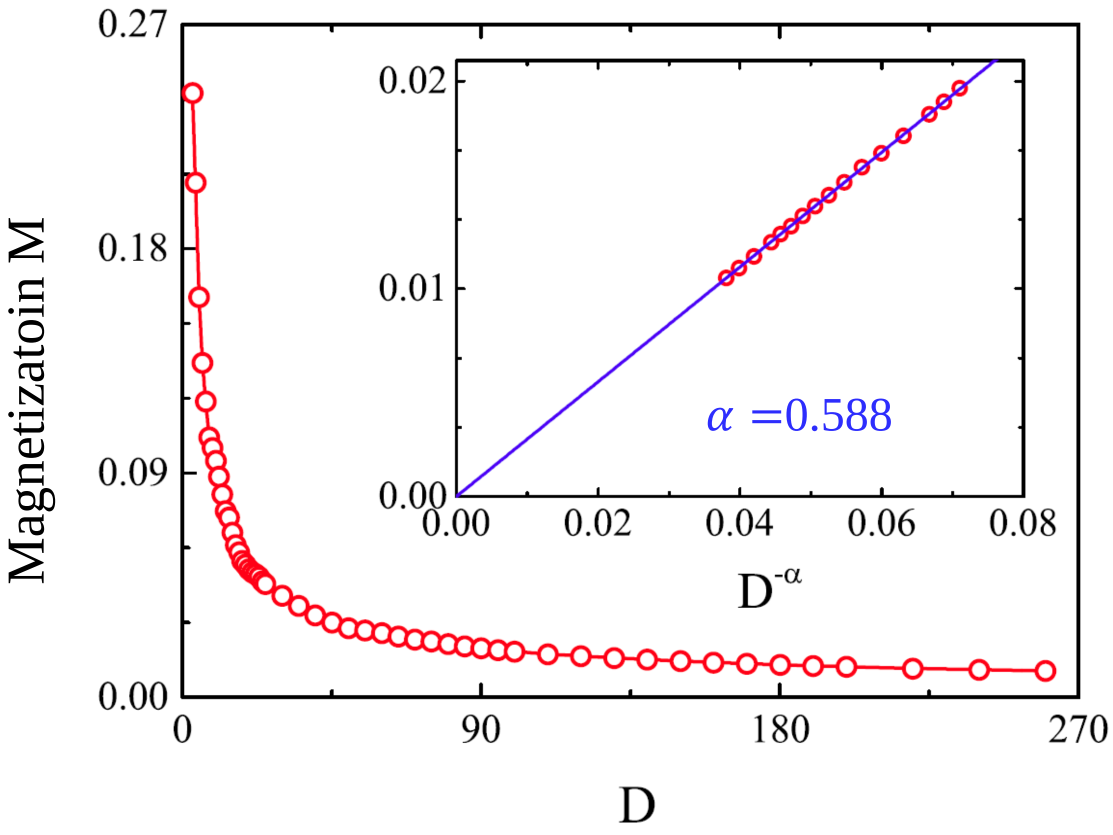
(b) Husimi Lattice

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

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

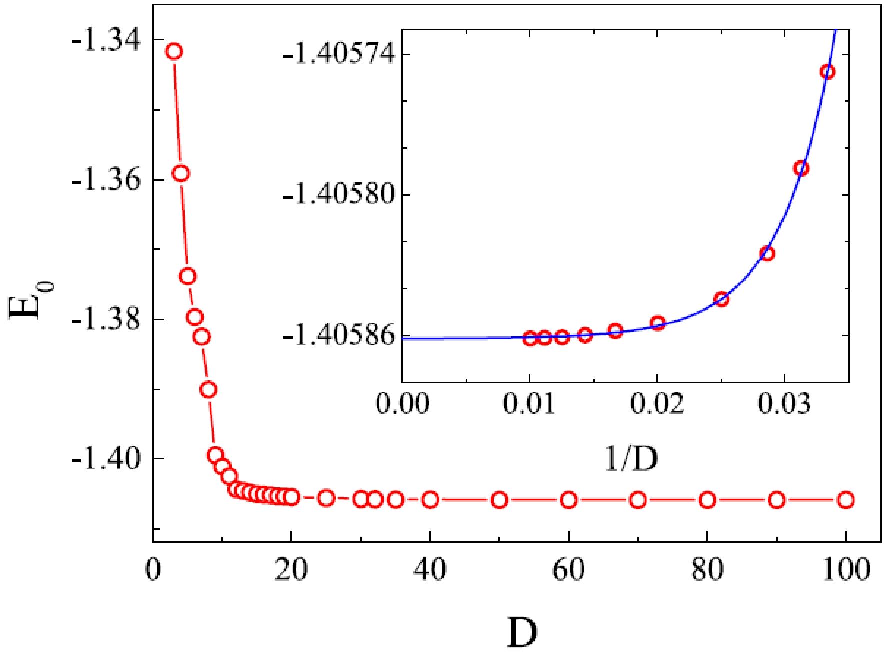
S=1/2 Husimi Lattice: Gapless Spin Liquid

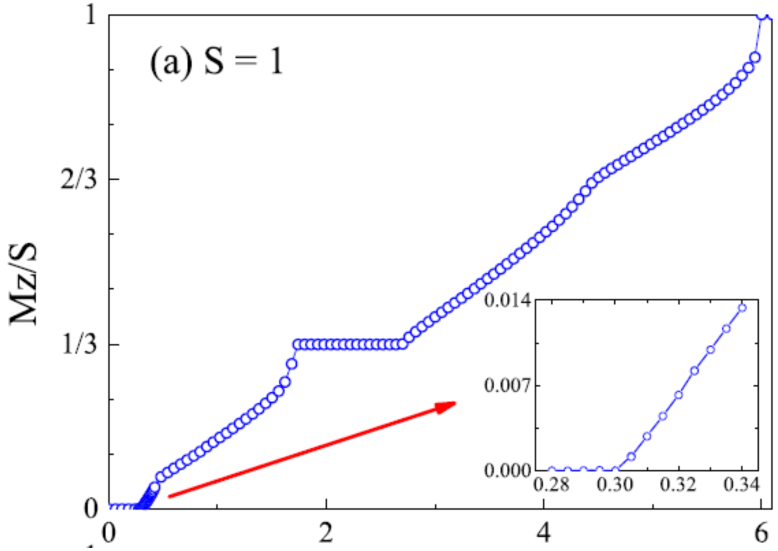


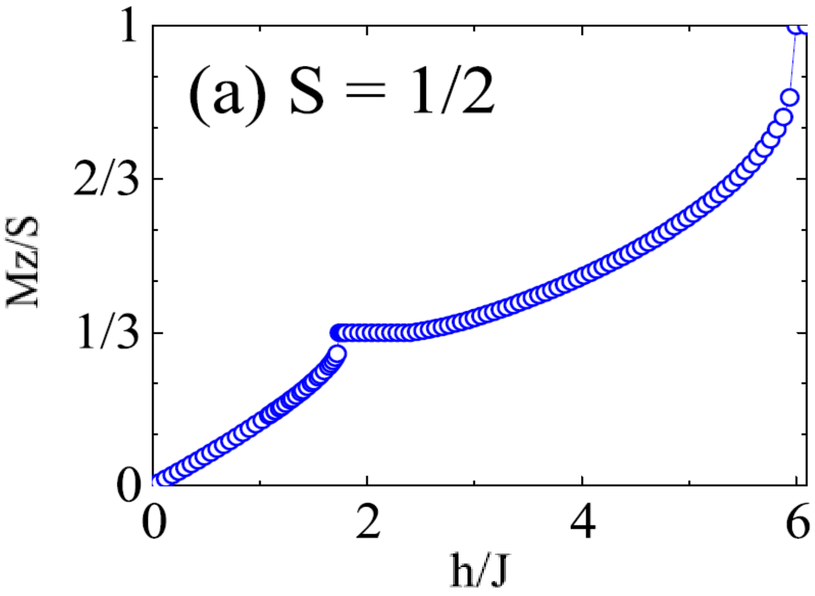


Both energy and magnetization converge algebraically with *D*

S=1 Husimi: Gapped Ground State

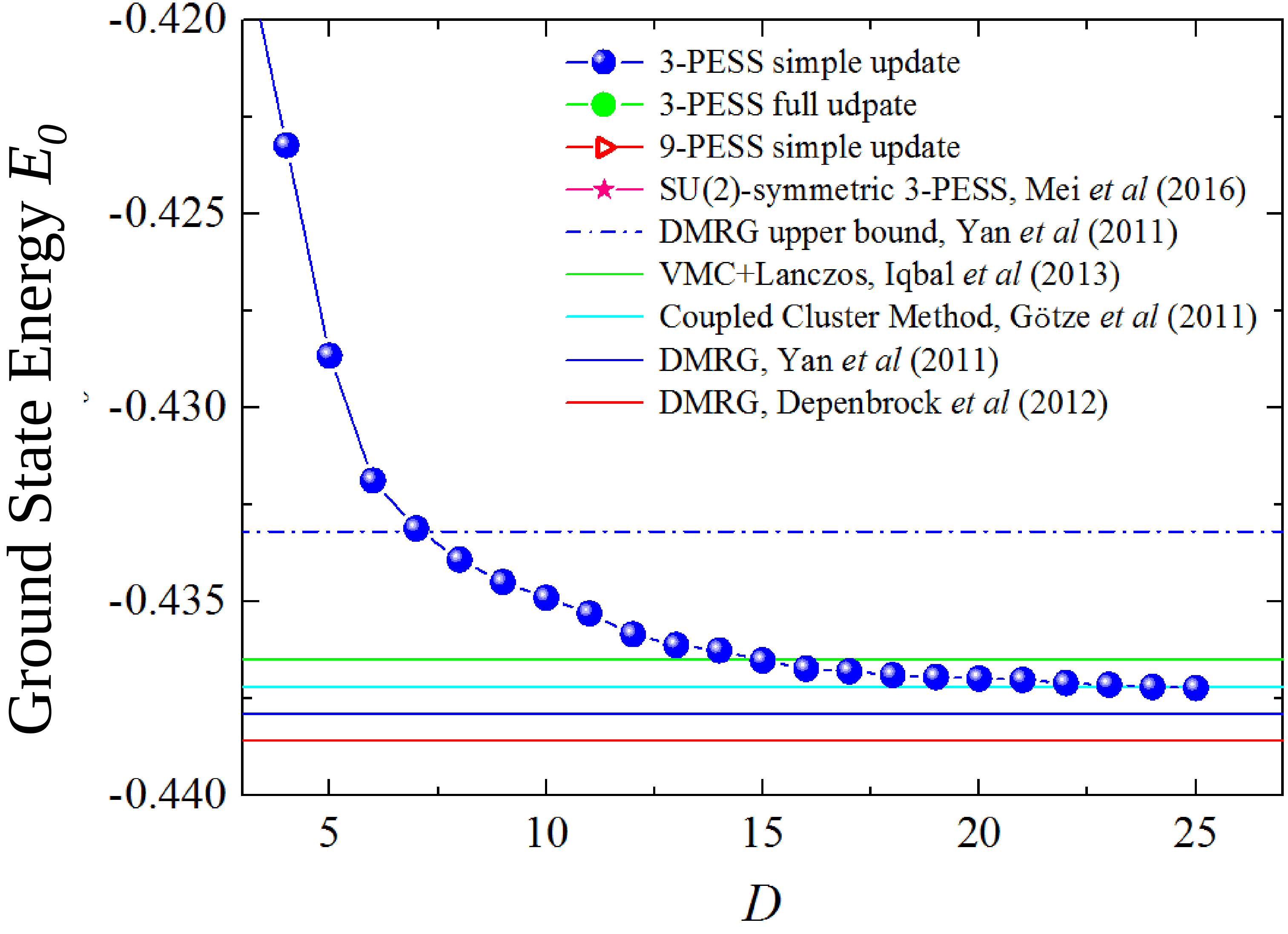






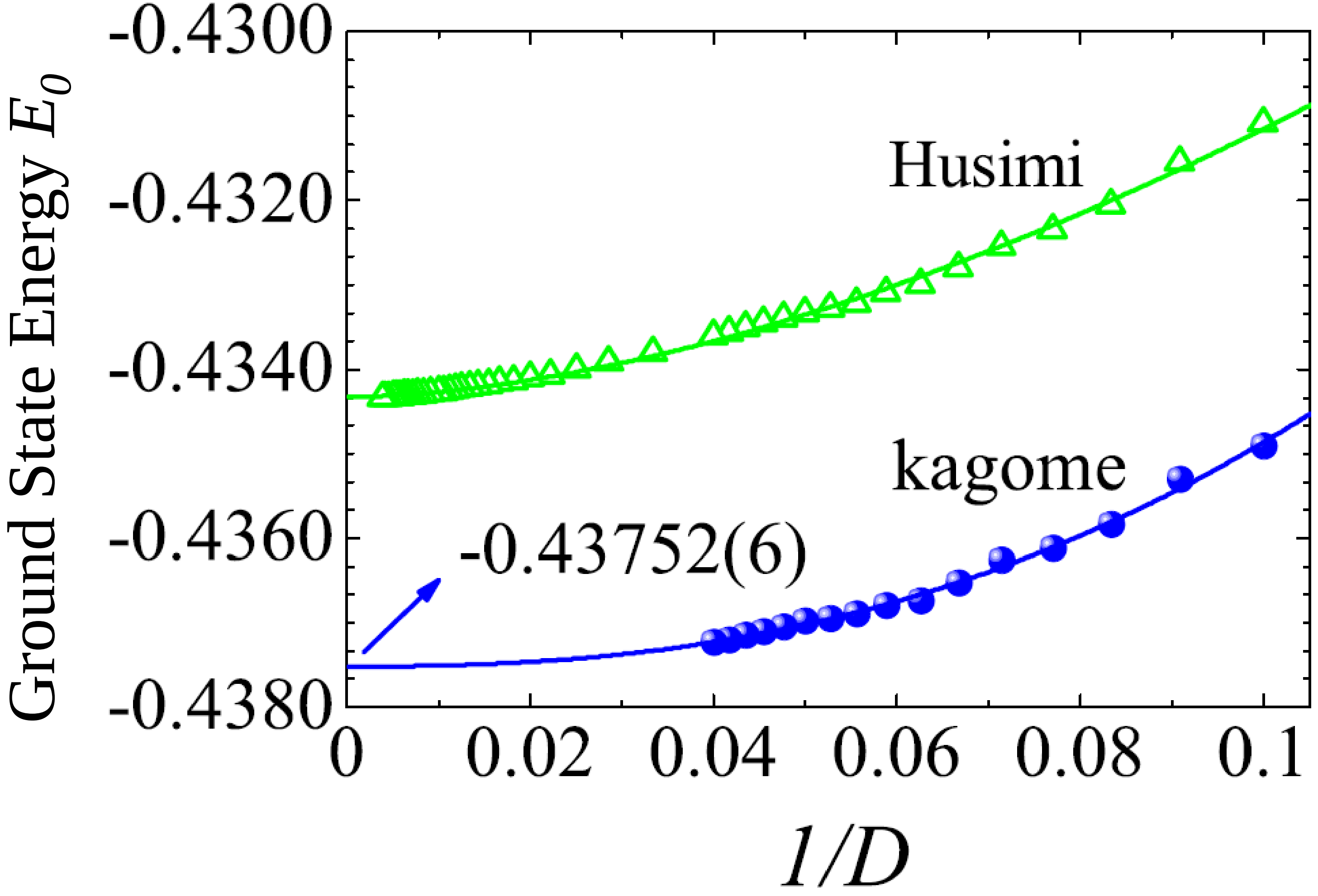
Energy converges exponentially with the bond dimension

Kagome Heisenberg: Ground State Energy



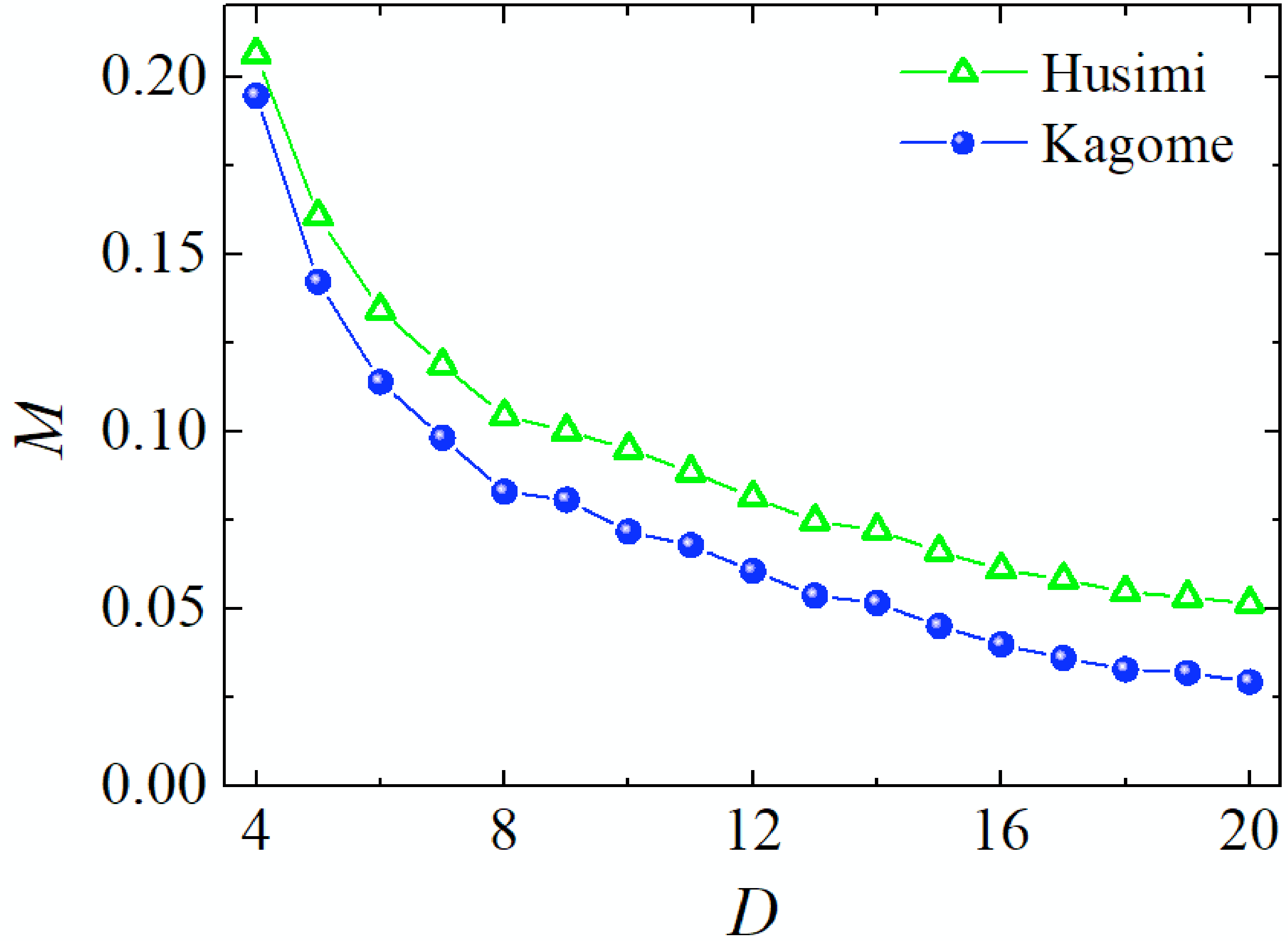
Ground state energy shows a power law behavior

Kagome Heisenberg: Gapless Ground State



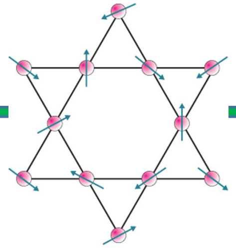
Energy converges algebraically with the bond dimension

Kagome Heisenberg: Magnetic Order Free

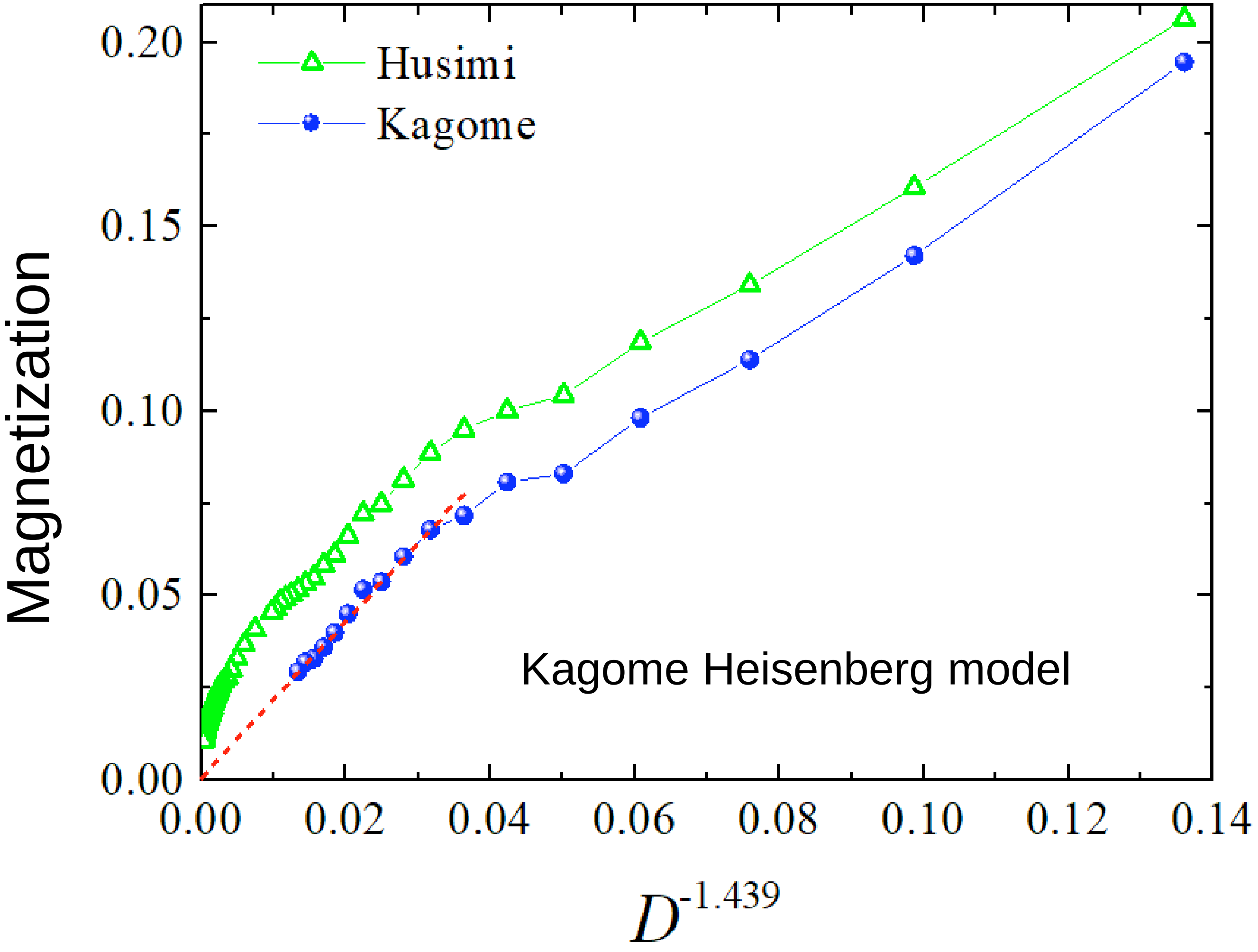


$$M_{Kagome} < M_{Husimi}$$

Magnetization: decays algebraically with *D*

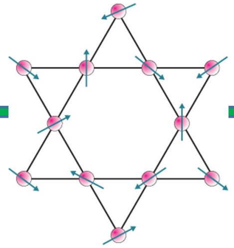


Kagome Heisenberg: Magnetic Order Free



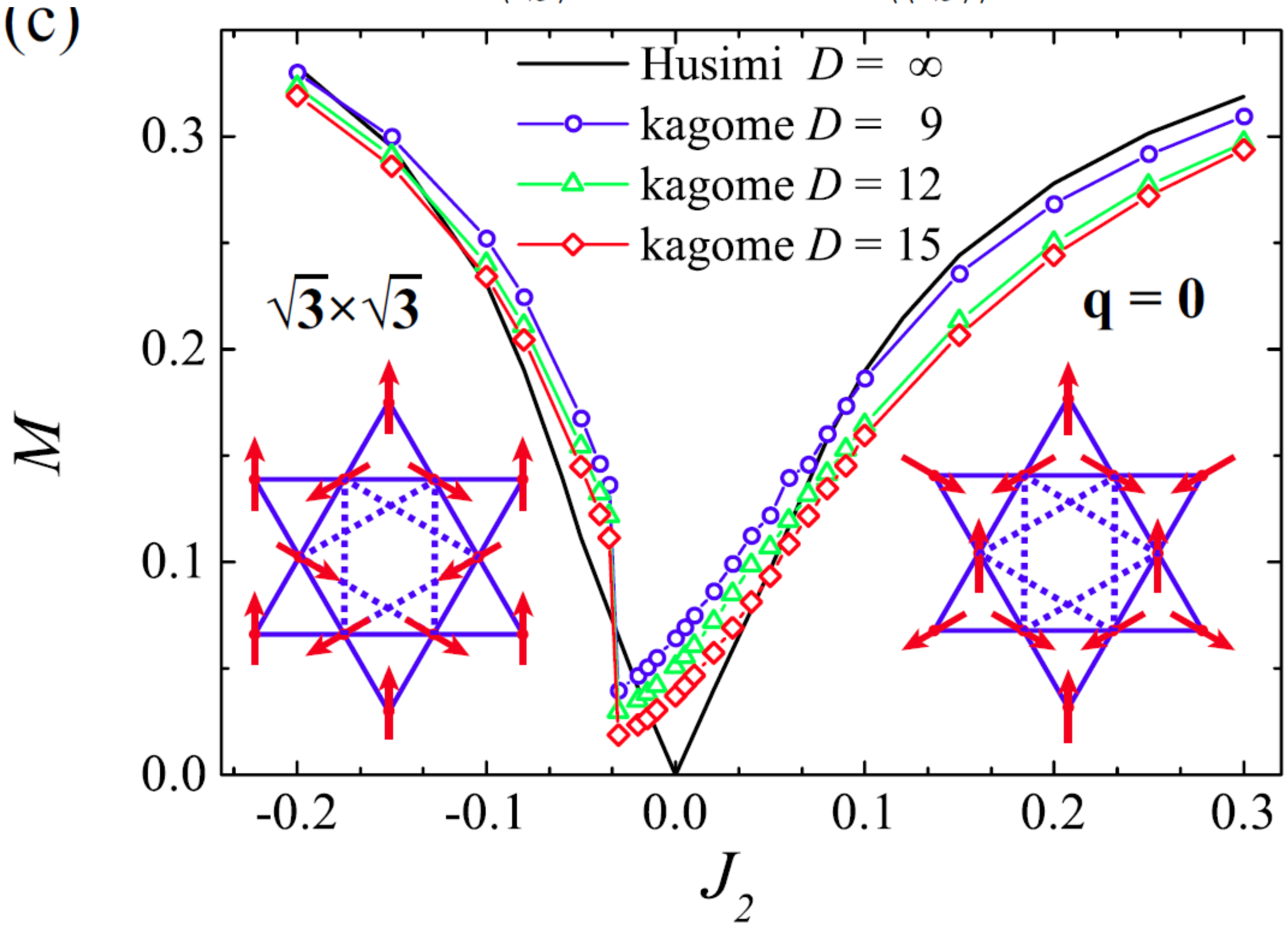
The magnetic long-range order vanishes in the infinite *D* limit

Ground state of the Kagome Heisenberg AFM is a spin liquid.

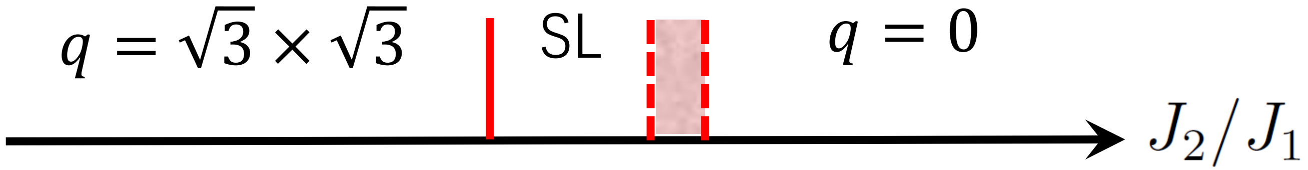


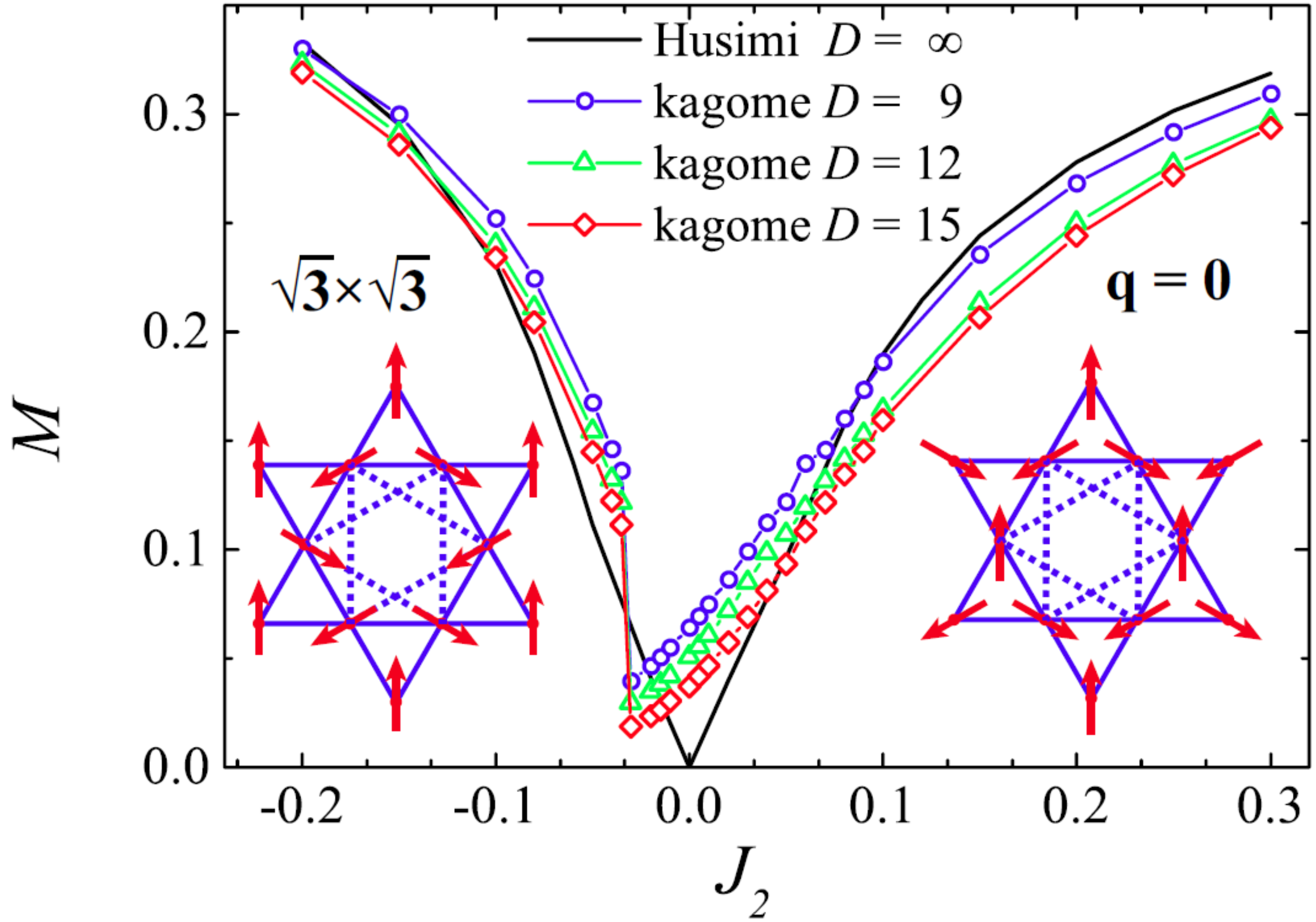
Stability against other interactions

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



Phase Diagram





Summary

- **We have performed a large scale tensor renormalization group calculation for the S=1/2 Kagome Heisenberg model**

- **Our result suggests that the ground state is a gapless quantum spin liquid**