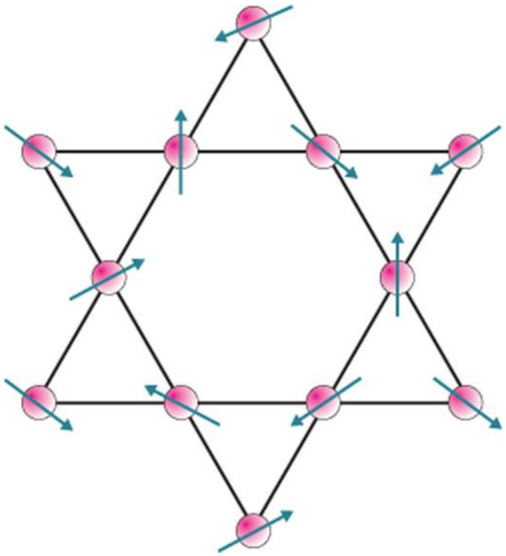
Gapless Spin Liquid Ground State in the S=1/2 Kagome Antiferromagnet



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Acknowledgment

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


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Haijun Liao


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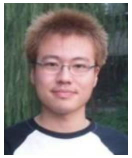
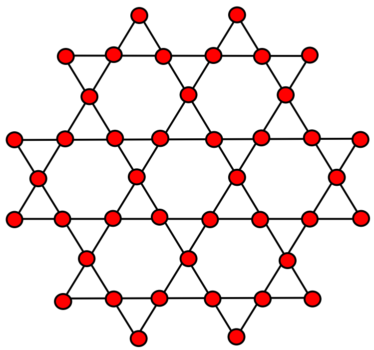
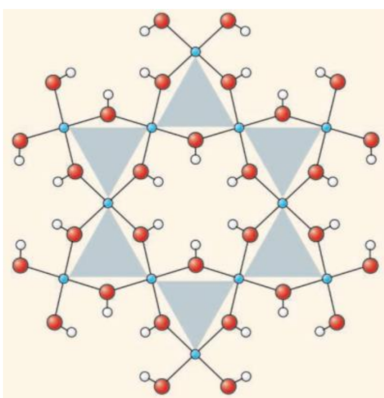

Jing Chen


Haidong Xie


Ruizhen Huang

Questions to Address





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. **a quantum spin liquid?**

Kagome Heisenberg: Possible Ground States

✓ **Valence bond crystal**

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

✓ **Gapped Z_2 spin liquid (Topological)**

Sachdev, PRB	1992	Schwinger boson
Gotze, et al, PRB	2011	coupled cluster
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
Nishimoto, Shibata, Hotta Nat. Commun.	2013	DMRG
Gong, Zhu & Sheng, Scientific Reports	2014	DMRG
Li, arXiv:1601.02165	2016	VMC
Mei, Chen, He & Wen, arXiv:1606.09639	2016	SU(2)-TNS

✓ **Gapless spin liquid (Algebra)**

Ran, Hermele, Lee, Wen, PRL	2007	VMC
Iqbal, Becca, Sorella, Poilblanc, PRB	2013	VMC+Lanczos
Iqbal, Poilblanc, Becca, PRB & 1606.02255	2015	VMC
Hu, Gong, Becca & Sheng, PRB	2015	VMC
Jiang, Kim, Han & Ran, arXiv:1610.02024	2016	SU(2)-PEPS
Liao et al, arXiv:1610.04727, PRL 2017	2016	PESS
He, Zaletel, Oshikawa, Pollmann, 1611.06238	2016	DMRG

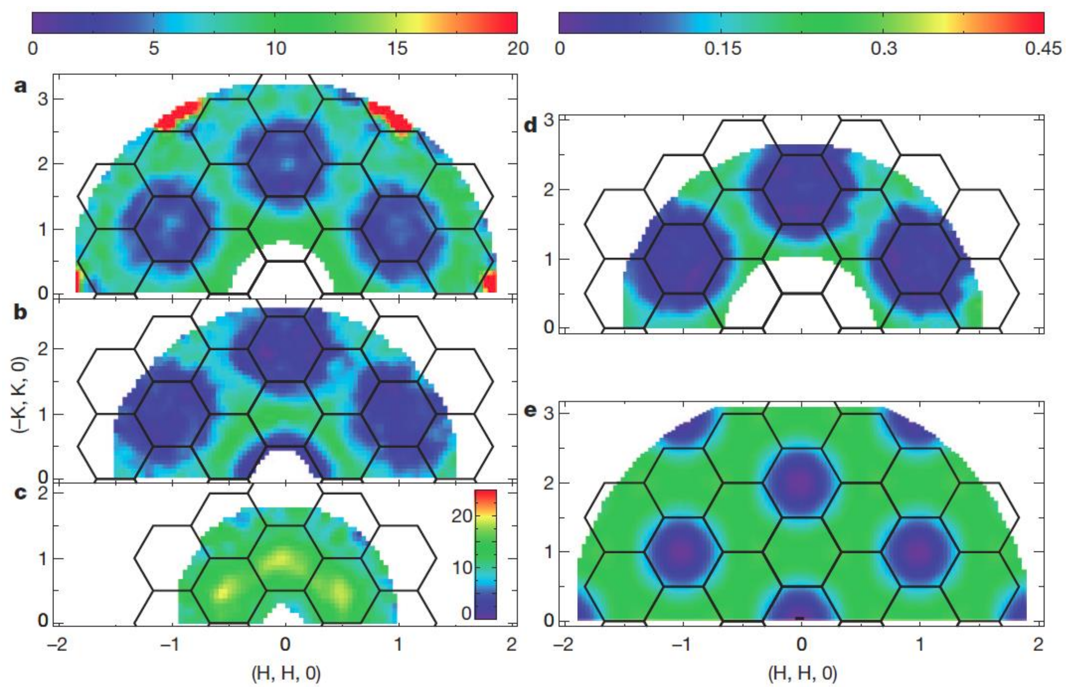
Hints from Experiments

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

Nature 492 (2012) 406

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]

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

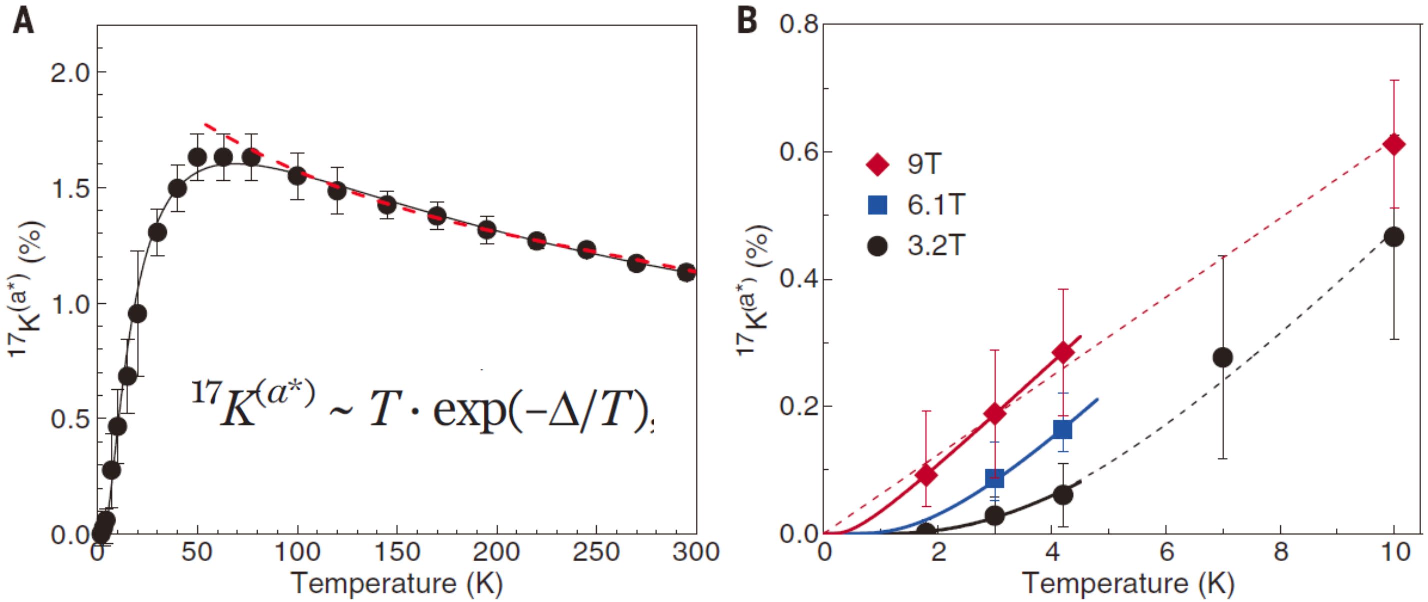
Hints from Experiments

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

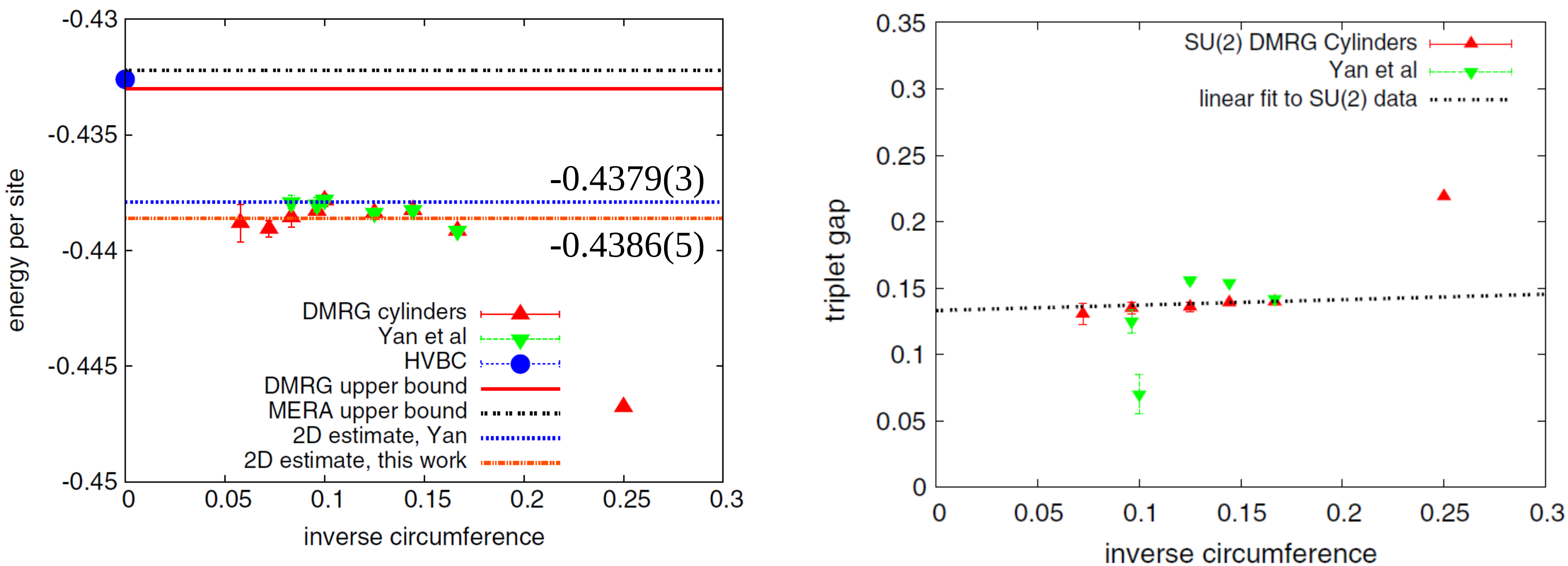
$$\Delta(0)/J = 0.03 \text{ to } 0.07$$

Problems in the theoretical studies

✓ Density Matrix Renormalization Group (DMRG):

strong finite size effect

error grows exponentially with the system size



Dependenbrock 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

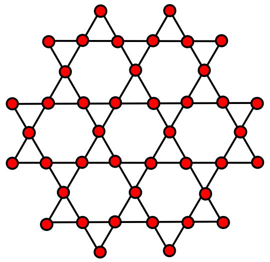
Tensor-Network States

1. **A variational wave function that satisfies the area law of entanglement entropy**

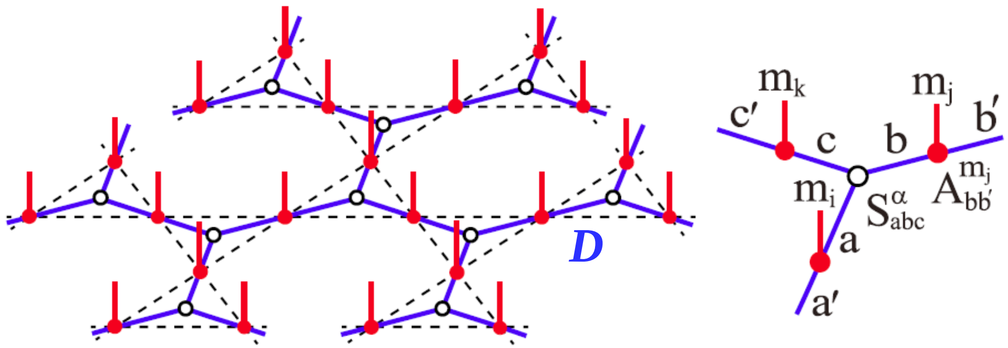
2. **Control parameter: bond dimension *D***

the wave function is exact in the $D \to \infty$ limit

Projected Entangled Simplex State (PESS)



Kagome
Frustrated lattice

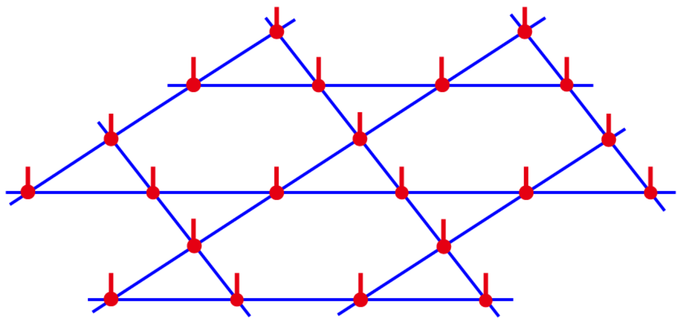


Local tensors defined on the honeycomb lattice
Rank-3 tensors, no frustration

Comparison between PEPS and PESS

Projected Entangled Pair State

(PEPS)



tensors defined on the original lattice

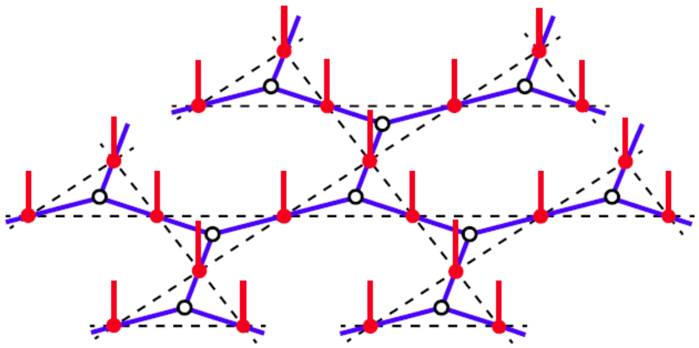
Rank-5 tensors

High cost

Virtual spins at two neighboring sites form a maximally entangled state

Projected Entangled Simplex State

(PESS)



tensors defined on honeycomb lattice

Rank-3 tensors

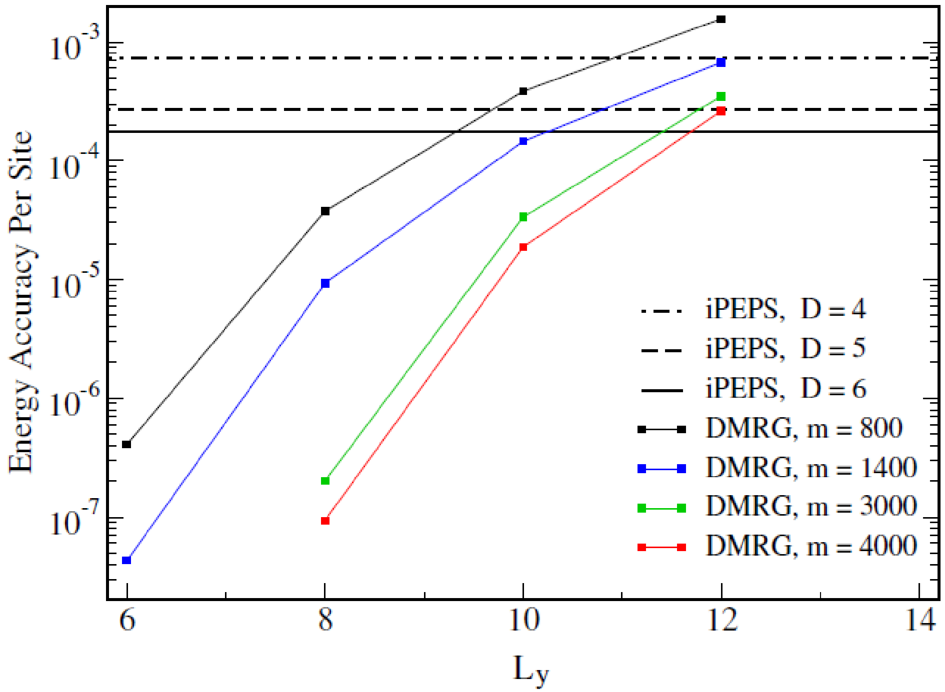
Low cost

Virtual spins at each simplex form a maximally entangled state

Advantage in using tensor-network states

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

2. Most accurate method for studying large lattice size systems



S=1/2 Heisenberg

model square lattice

Reference energy: VMC

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

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

Advantage in using tensor-network states

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

2. Most accurate method for studying large lattice size systems

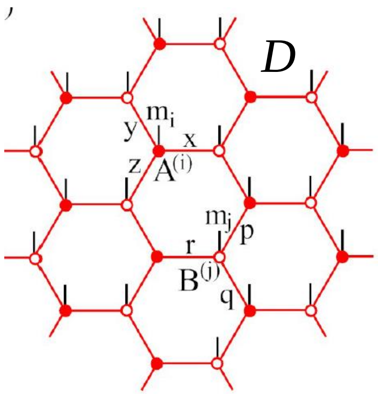
3. The ground state energy converges fast with the increase of the bond dimension ***D***

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

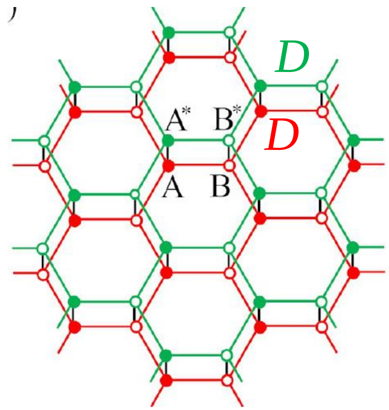
   We use this property to determine whether the ground state is gapped or gapless

Disadvantage: Cost is very high

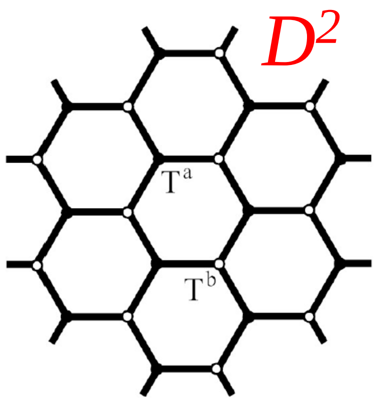
Double-Layer Approach



$|\Psi\rangle$



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

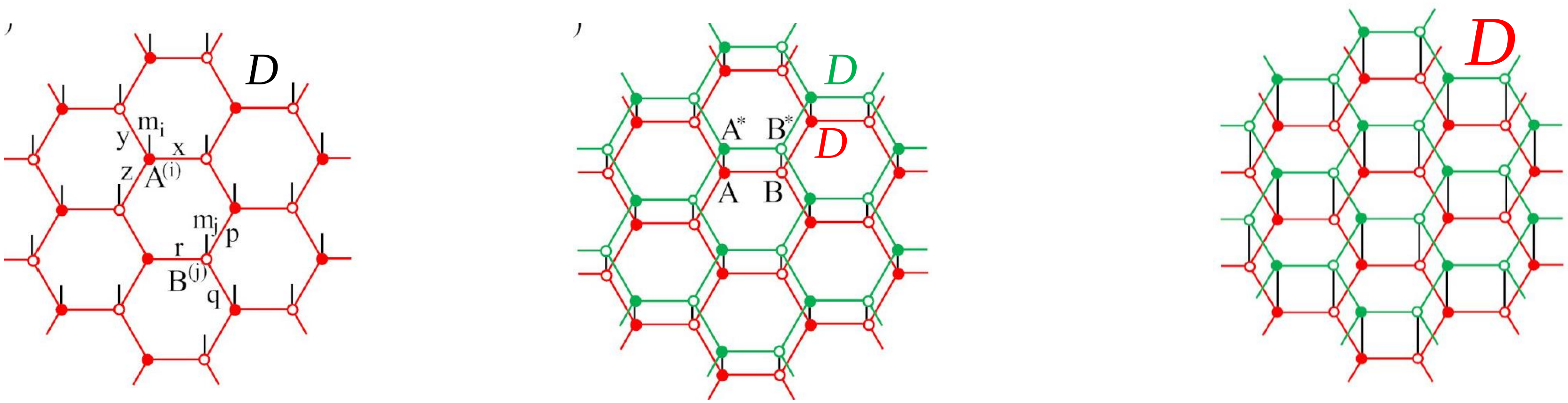


$\langle\Psi|\Psi\rangle$

	Double-layer
Computational Cost	$O(D^{12})$
Memory Cost	$O(D^{8})$
Limit of D	**13**

Reduce the Cost by Dimension Reduction

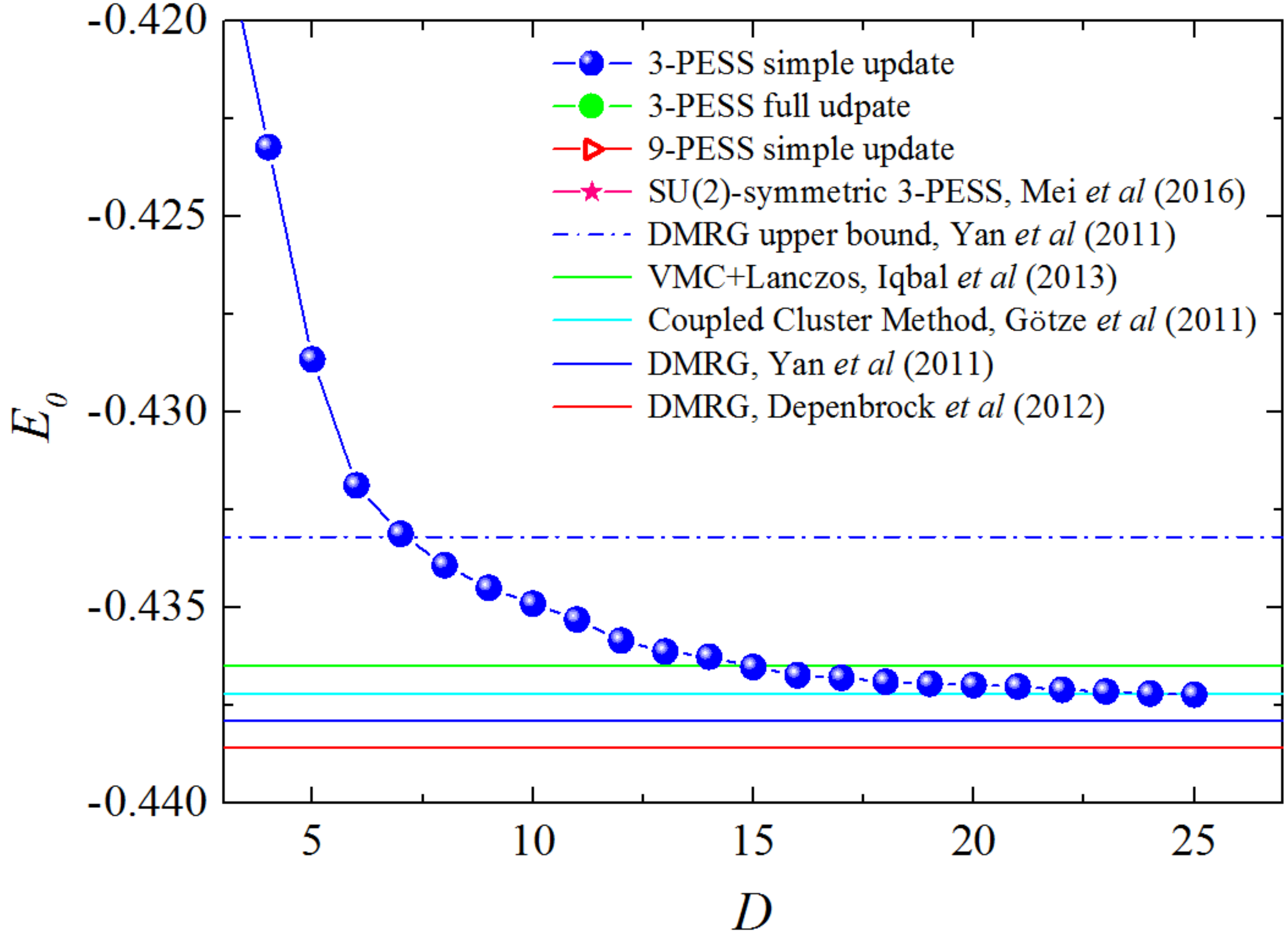
Shifted Single-Layer Approach



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

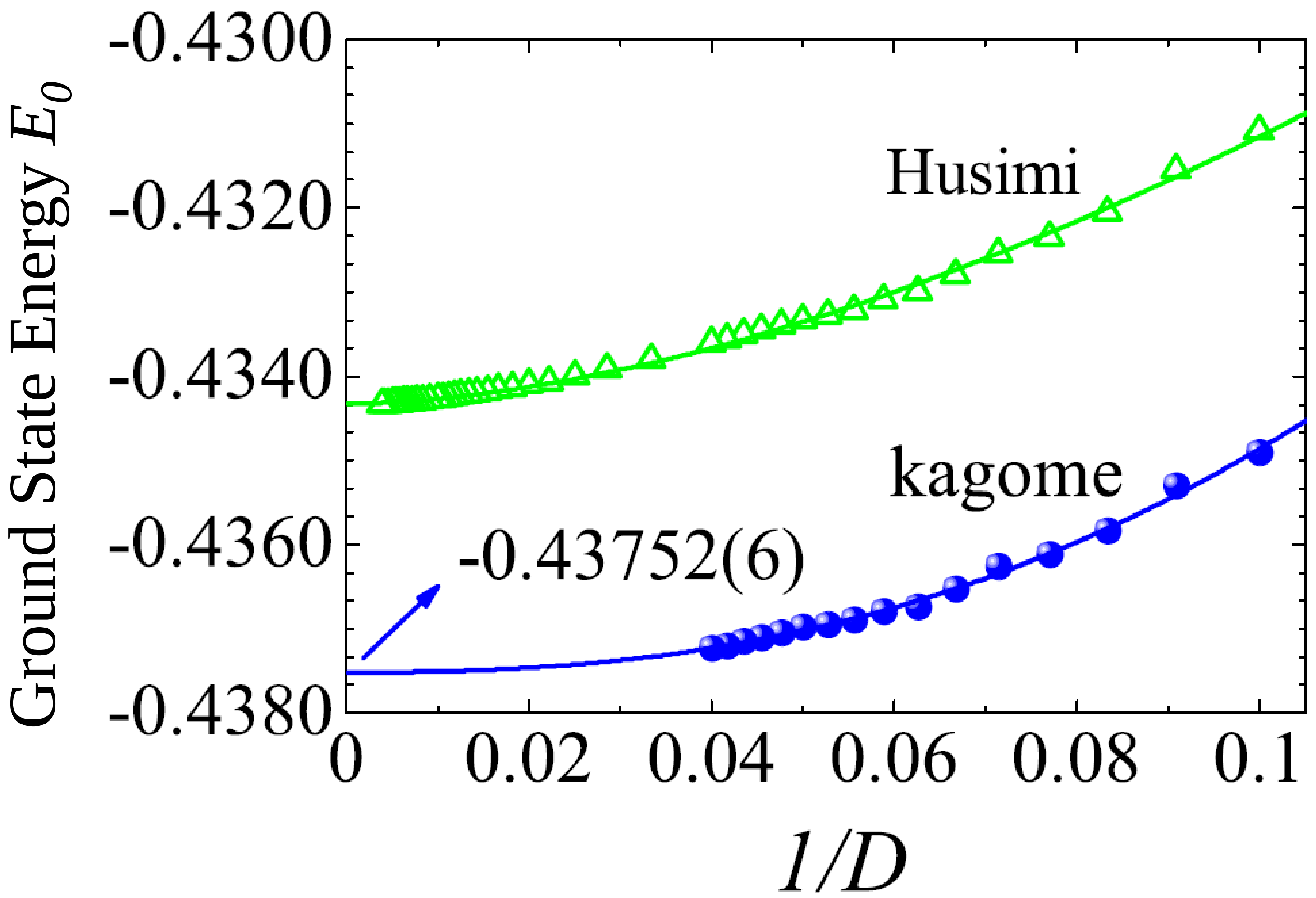
	Double-layer	Shifted single-layer
Computational Cost	$O(D^{12})$	$O(D^8)$
Memory Cost	$O(D^8)$	$O(D^6)$
Limit of D	**13**	**25 (not use symmetry)**

S=1/2 Kagome Heisenberg: Ground State Energy



Is this *D* large enough?

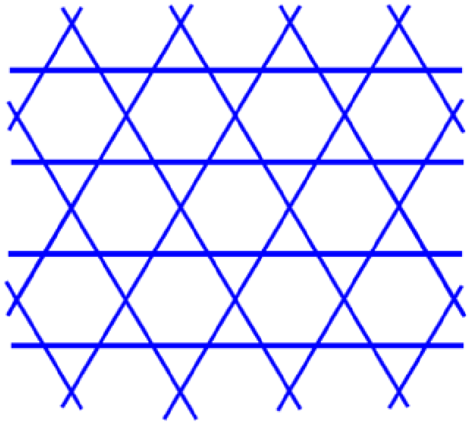
Kagome Heisenberg: Gapless



Energy converges algebraically with the bond dimension

Results obtained on the Husimi lattice provide good references

Make comparison between Kagome and Husimi results

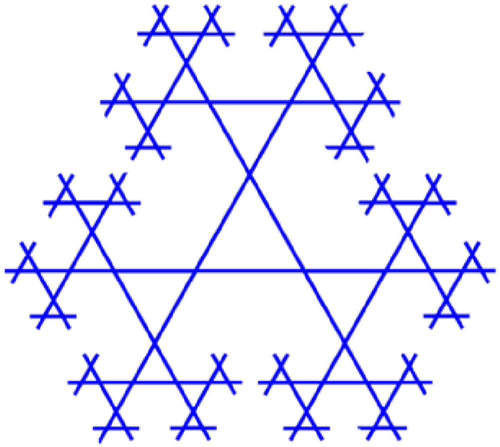


Kagome Lattice

Same local structure

←

Gain insight for the kagome system

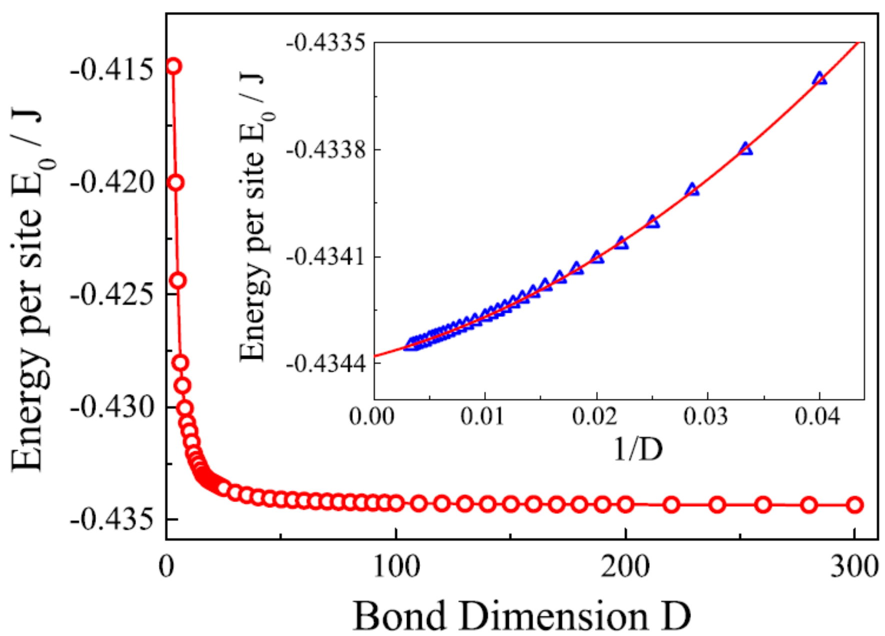


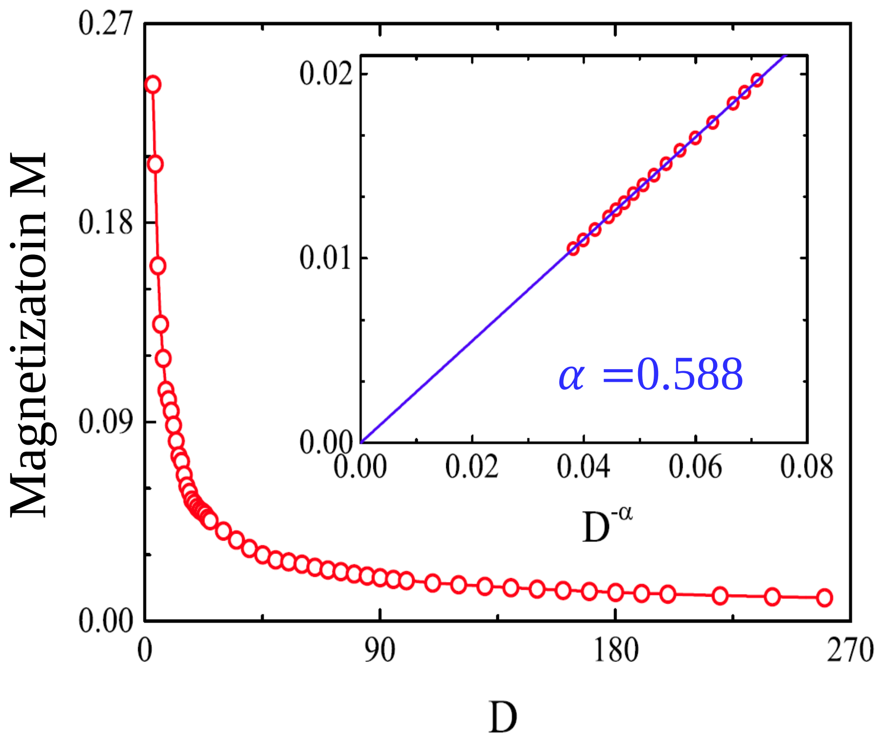
(b) Husimi Lattice

- ✓ Highly frustrated
- ✓ D is generally less than 20

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

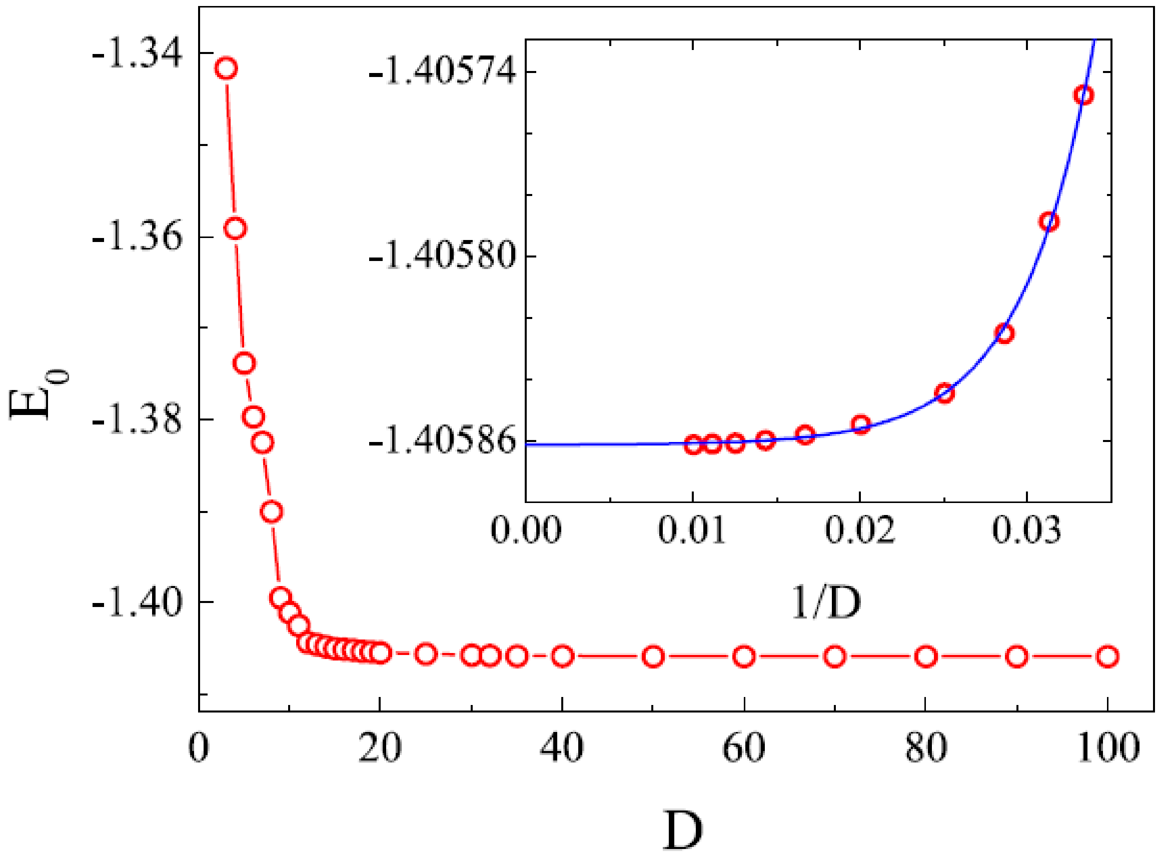
S=1/2 Husimi Lattice: Gapless Spin Liquid





Both energy and magnetization converge algebraically with D

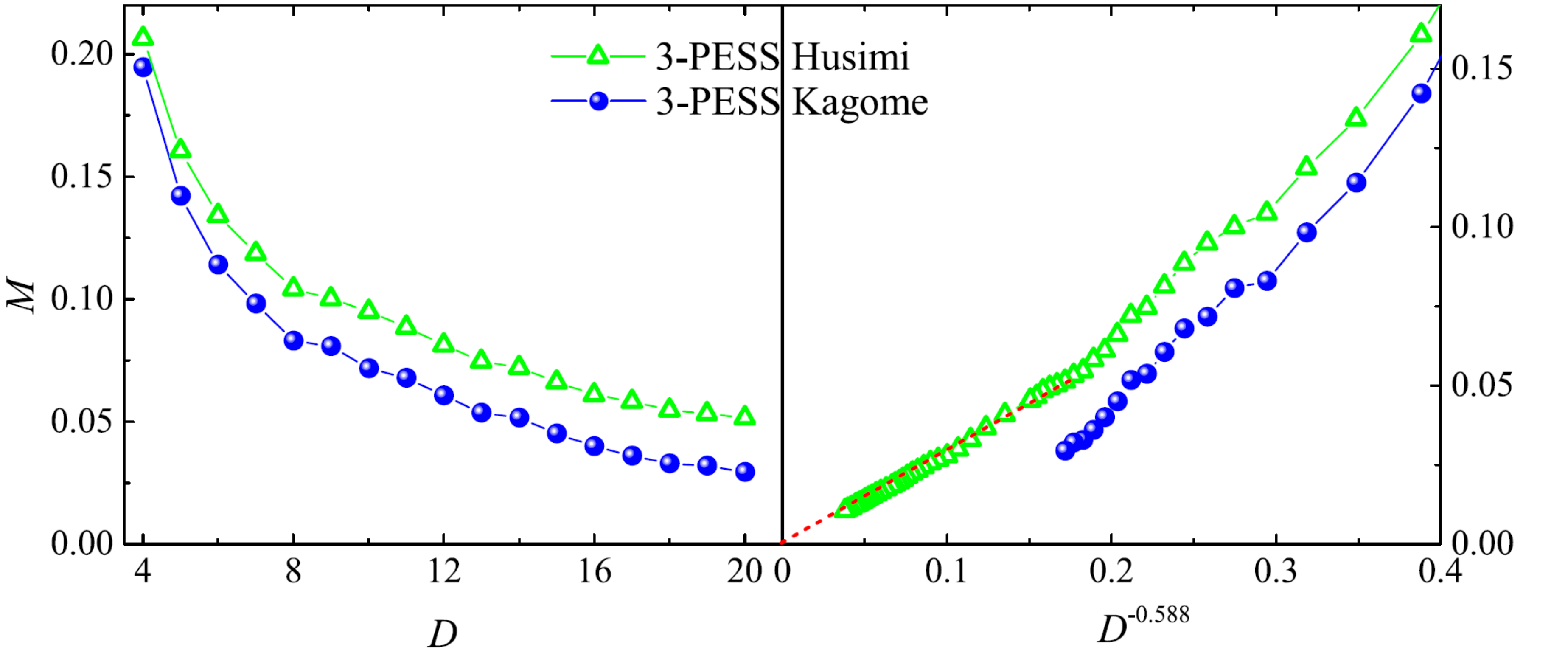
S=1 Husimi: Gapped Ground State



Energy converges exponentially with the bond dimension

Kagome Magnetization: magnetic order free

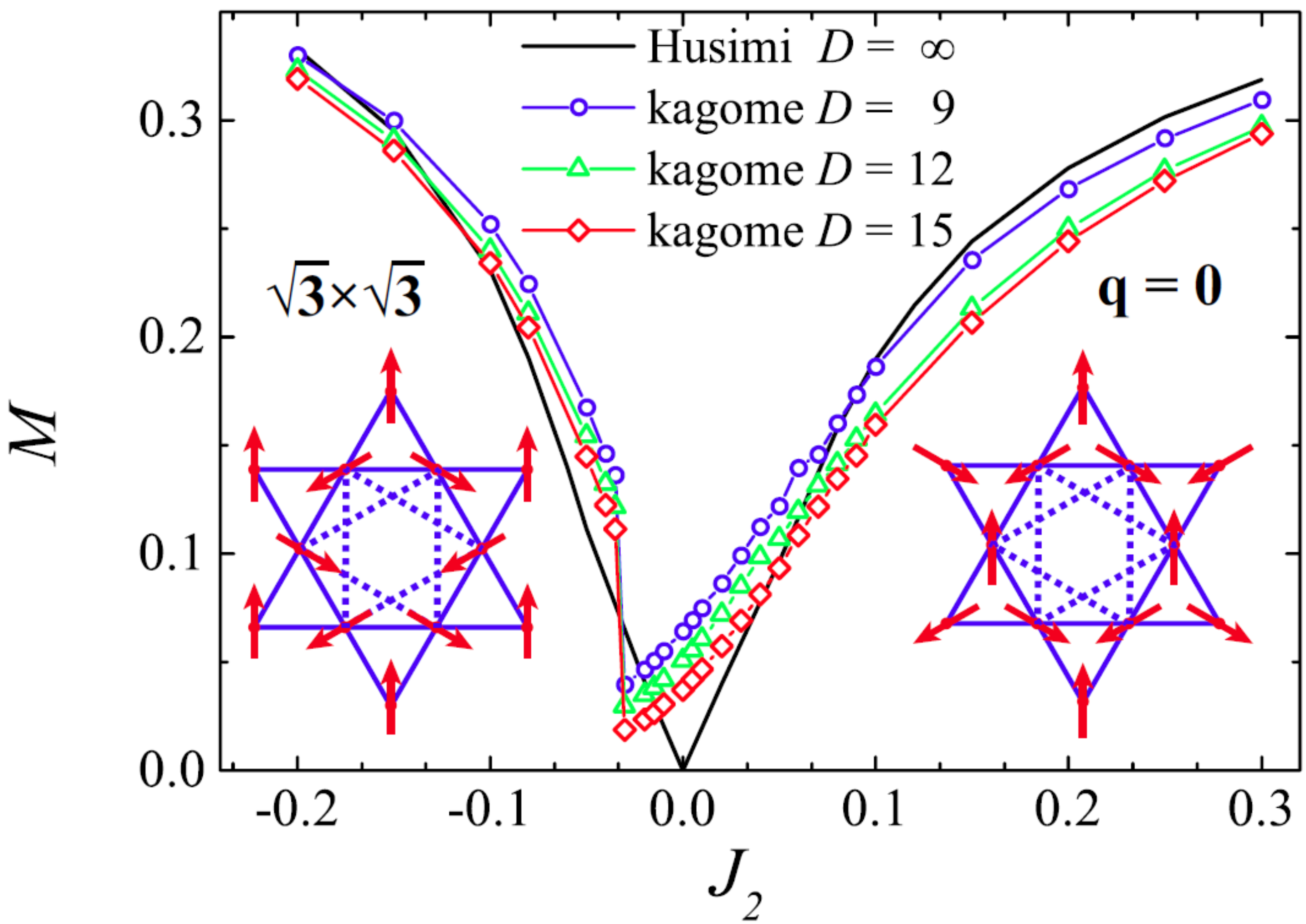
$$M_{Kagome} < M_{Husimi}$$



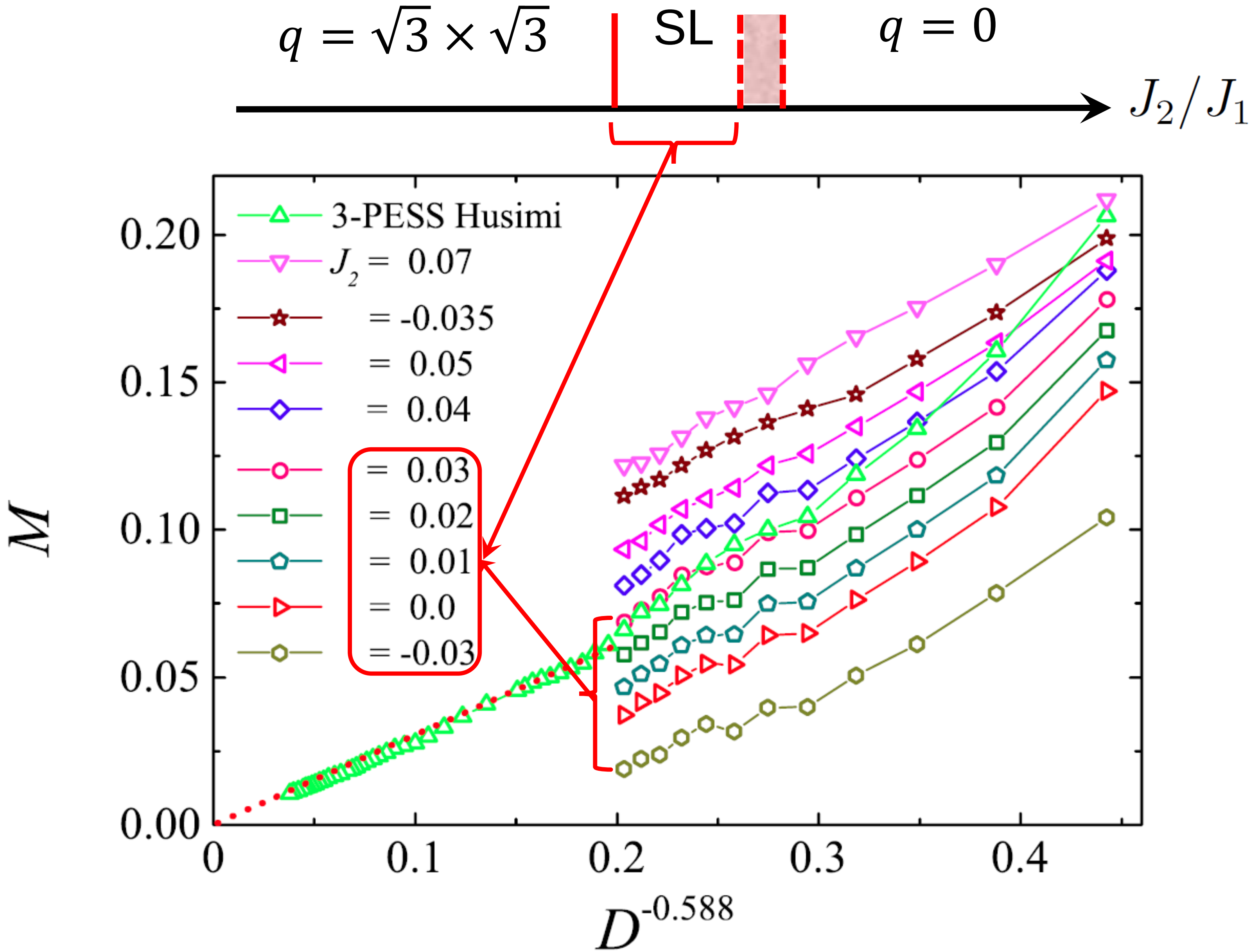
Magnetization: decays algebraically with *D*

Stability of the gapless spin-liquid state against other interactions

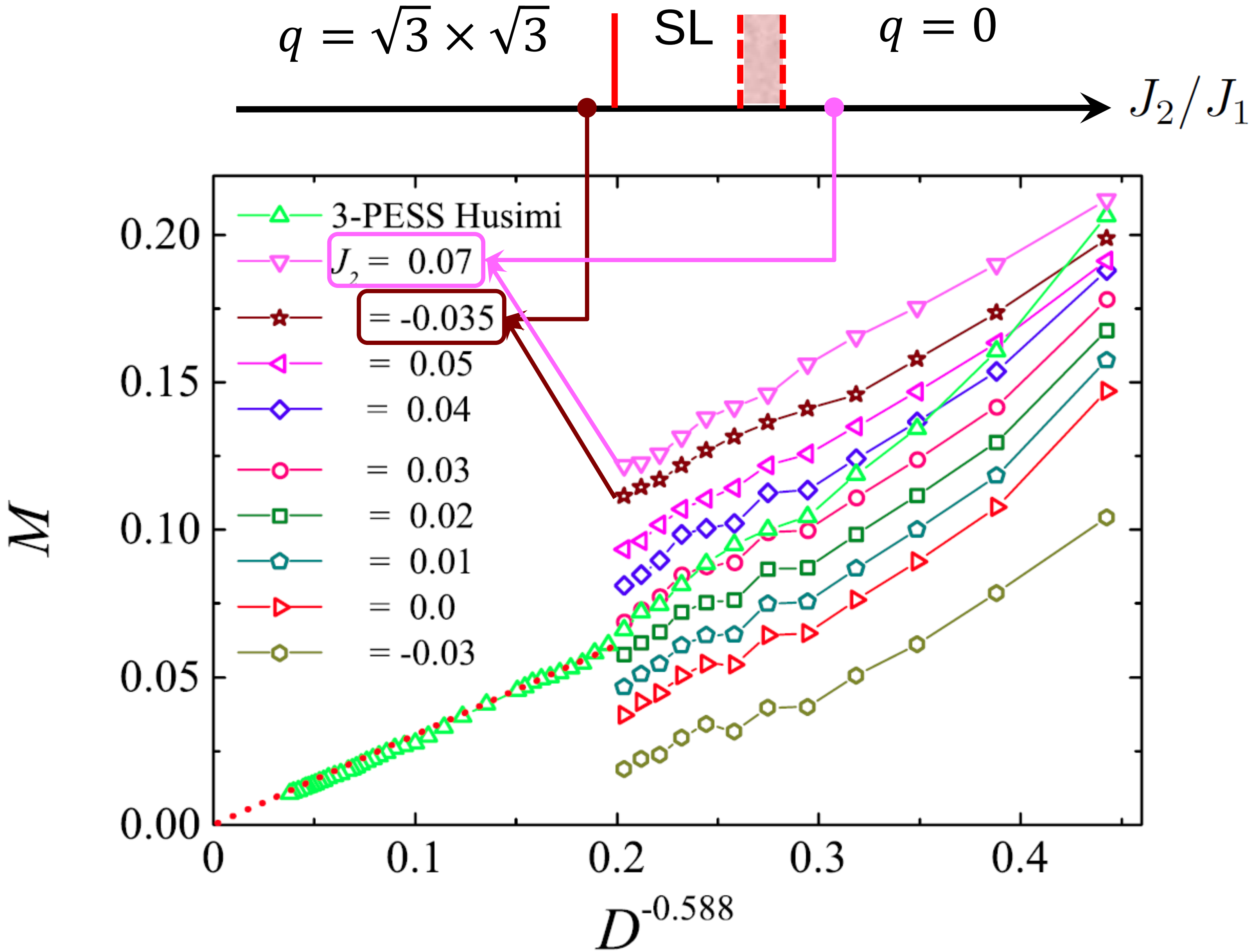
$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$



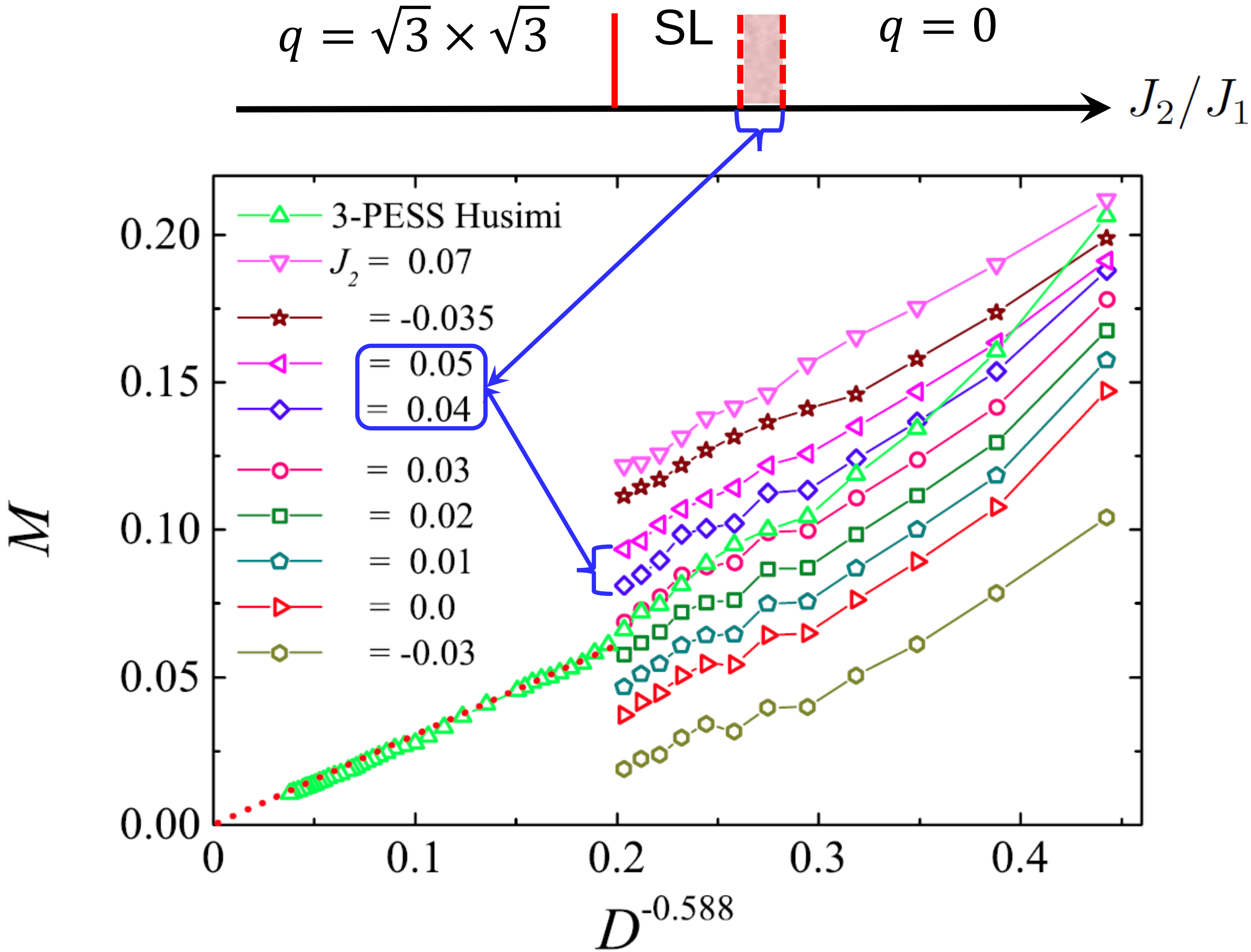
Bond dimension dependence of the magnetic order



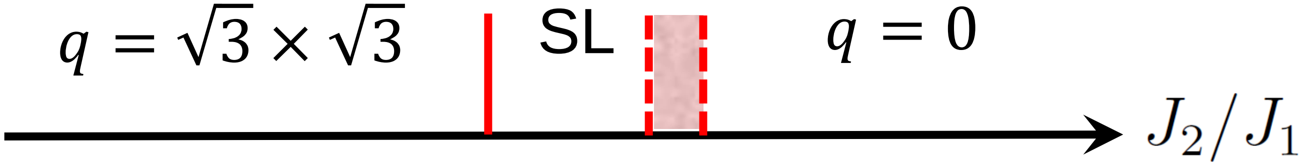
Bond dimension dependence of the magnetic order

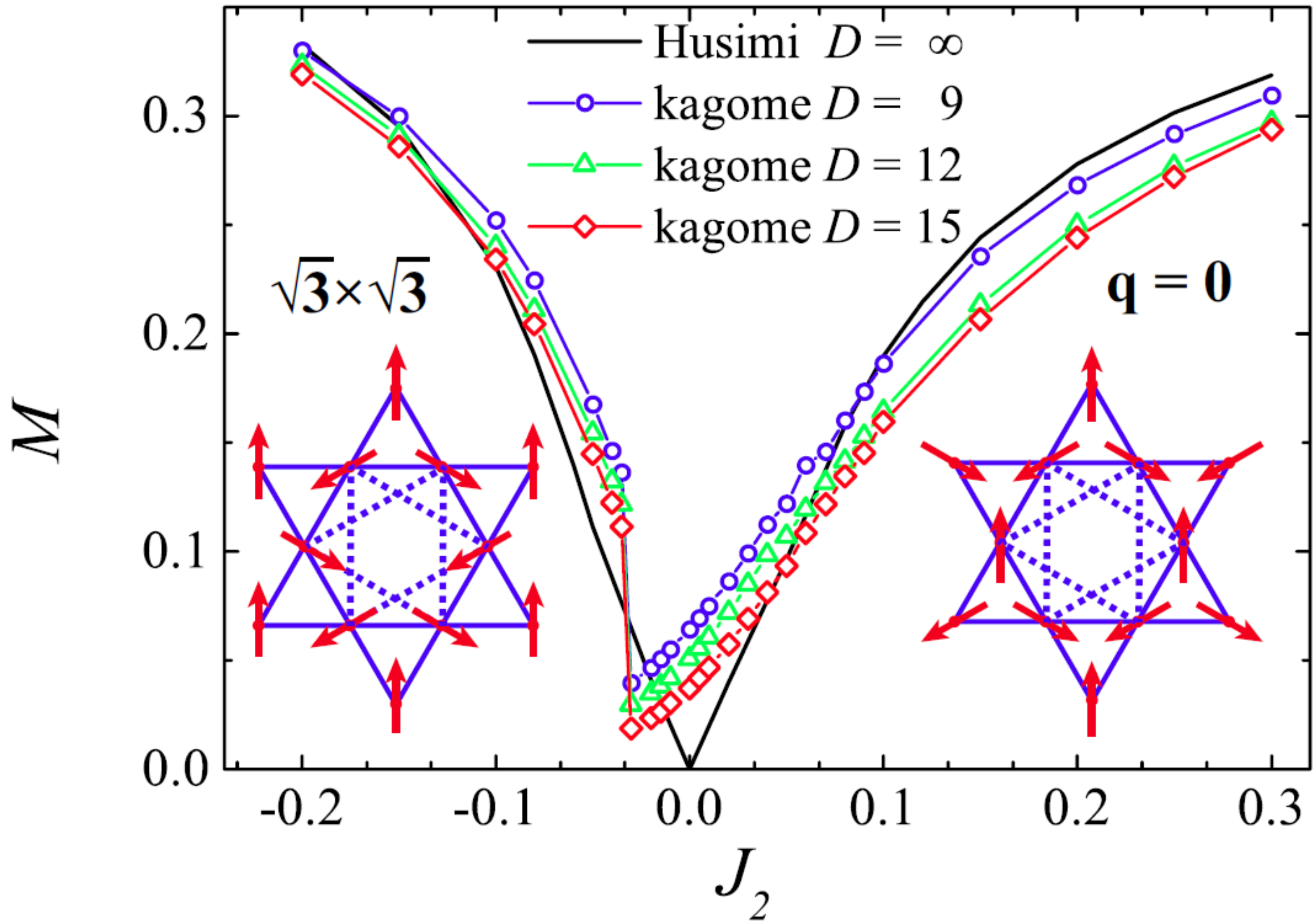


Bond dimension dependence of the magnetic order



Kagome $J_1 - J_2$ model: phase diagram of infinite D limit





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 of this system is a gapless quantum spin liquid**