# Renormalization of tensor network states

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# Outline

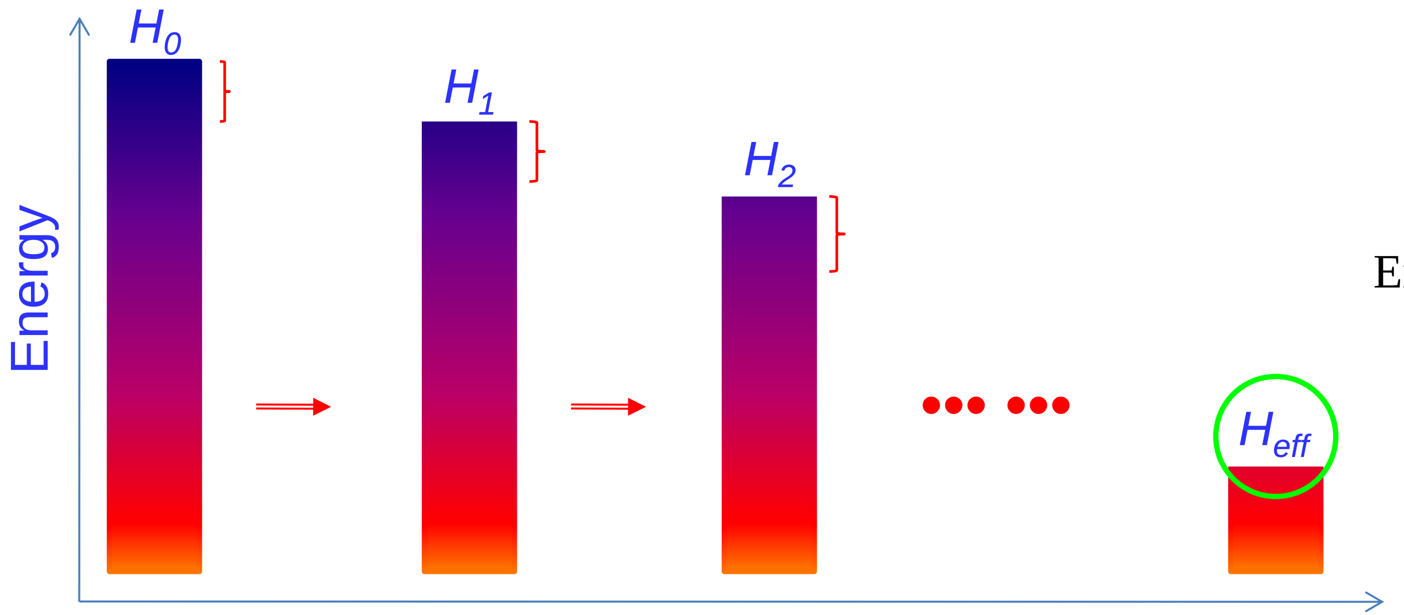
Issue to address: How to renormalize classical or quantum statistical models accurately and efficiently

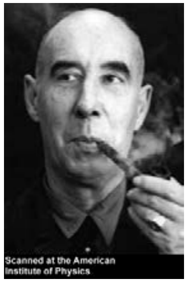
1. Brief introduction to the tensor renormalization

2. HOTRG: tensor renormalization based on the higher-order singular value decomposition

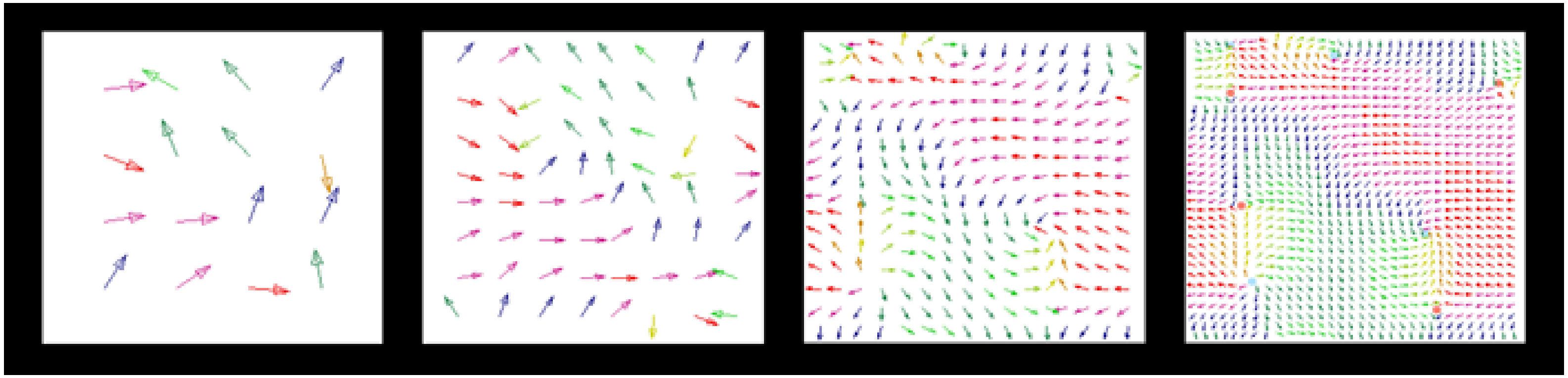
3. PESS: Projected Entangled Simplex State representation of quantum many-body wave function

# Idea of Renormalization Group




Ernst Stueckelberg



**coarse graining : refine the wavefunction by local unitary transformations**

# Idea of Numerical Renormalization Group

To represent a *targeted state*

$$|\psi_0\rangle = \sum_{l=1}^{\infty} f_l |n_l\rangle$$

by an approximate wavefunction using a limited number of many-body basis states

$$|\tilde{\psi}_0\rangle \approx \sum_{l=1}^{D} \tilde{f}_l |n_l\rangle$$

such that their overlap is maximized

$$\langle\tilde{\psi}_0|\psi_0\rangle = \sum_{l=1}^{D} \tilde{f}_l f_l$$

***Key issue:***

***How to determine these optimal basis states?***

# Evolution of Numerical Renormalization Group

## Stage I: Wilson NRG 1975 -

0 Dimensional problems (single impurity Kondo model)

**K. Wilson**

## Stage II: DMRG 1992 -

most accurate method for 1D quantum lattice models

**S R White**

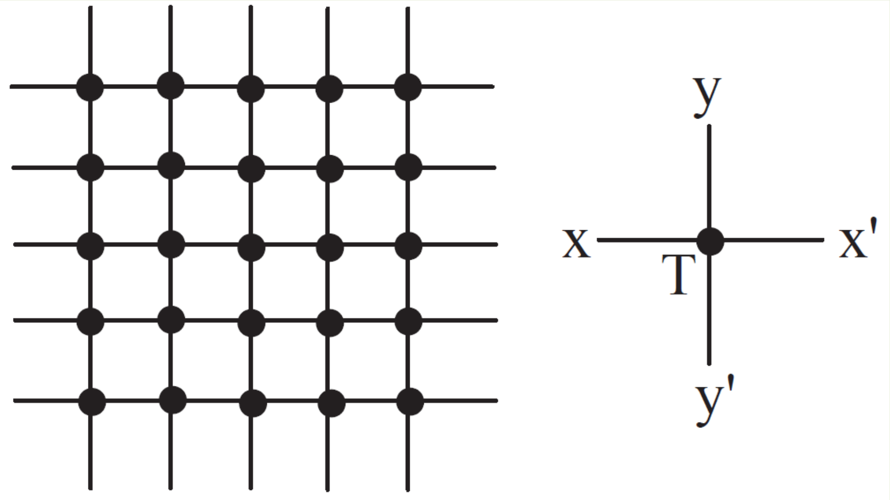
## Stage III: Renormalization of tensor network states

2D or higher dimensional quantum/classical models

# What are tensor-network states/models

- All classical and quantum lattice models are or can be represented as tensor network models

- Ground state wavefunctions of quantum lattice models can be represented as tensor-network states

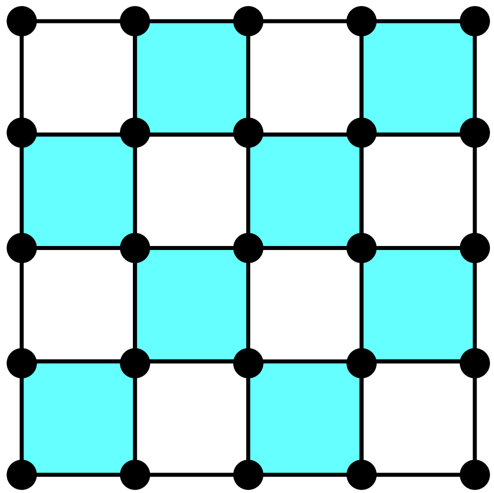



$$Z = Tr \prod_i T_{x_i x'_i y_i y'_i}$$

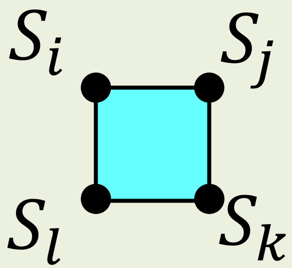
# Example: tensor-network representation of Ising model

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

$$H = \sum_{\blacksquare} H_{\blacksquare}$$



$$Z = \mathrm{Tr}\exp(-\beta H)$$
$$= \mathrm{Tr}\prod_{\blacksquare}\exp(-\beta H_{\blacksquare})$$
$$= \mathrm{Tr}\prod_{\{S\}} T_{S_i S_j S_k S_l}$$




$$= T_{S_i S_j S_k S_l} = \exp(-\beta H_{\blacksquare})$$

# Quantum lattice model

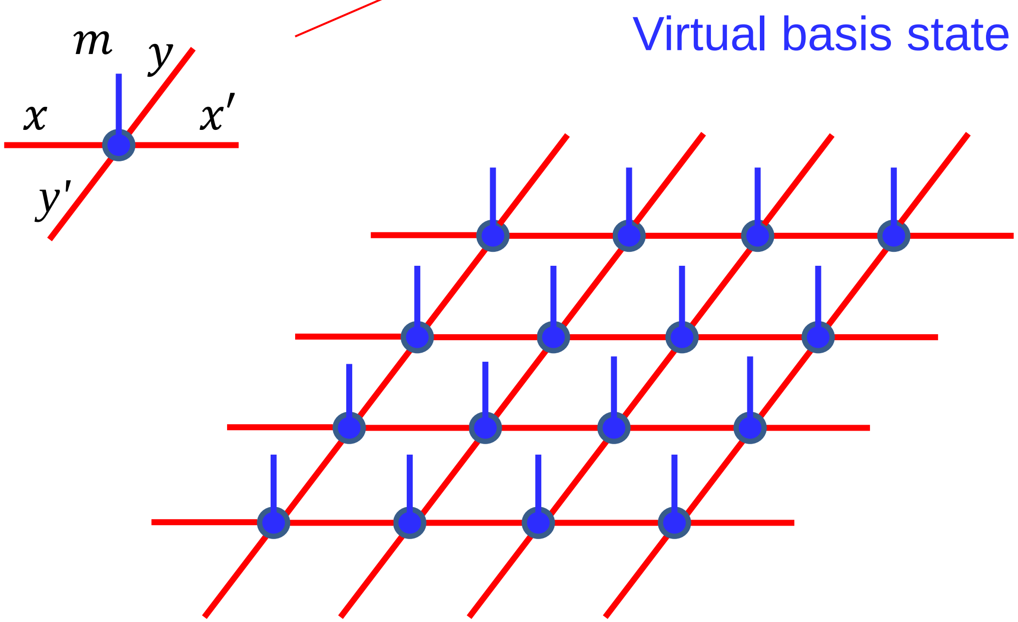
**d-dimensional quantum model = (d+1)-dimensional classical model**

under the framework of path integration

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

Virtual basis state

Physical state




Many-parameter variational wavefunction

the tensor elements are unknown and need to be determined

# Questions to be solved by the tensor renormalization group

**Classical statistical model**

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

How to trace out all tensor indices?

**Quantum lattice model**

1. How to determine all local tensor elements?

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

2. How to trace out all tensors to obtain the expectation values?

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

# How to renormalize tensor-network states?

HOTRG:

coarse graining tensor renormalization by the higher order singular value decomposition

**H.C. Jiang, et al, PRL 101, 090603 (2008)**

**Z. Y. Xie et al, PRL 103, 160601 (2009)**

**H. H. Zhao, et al, PRB 81, 174411 (2010)**

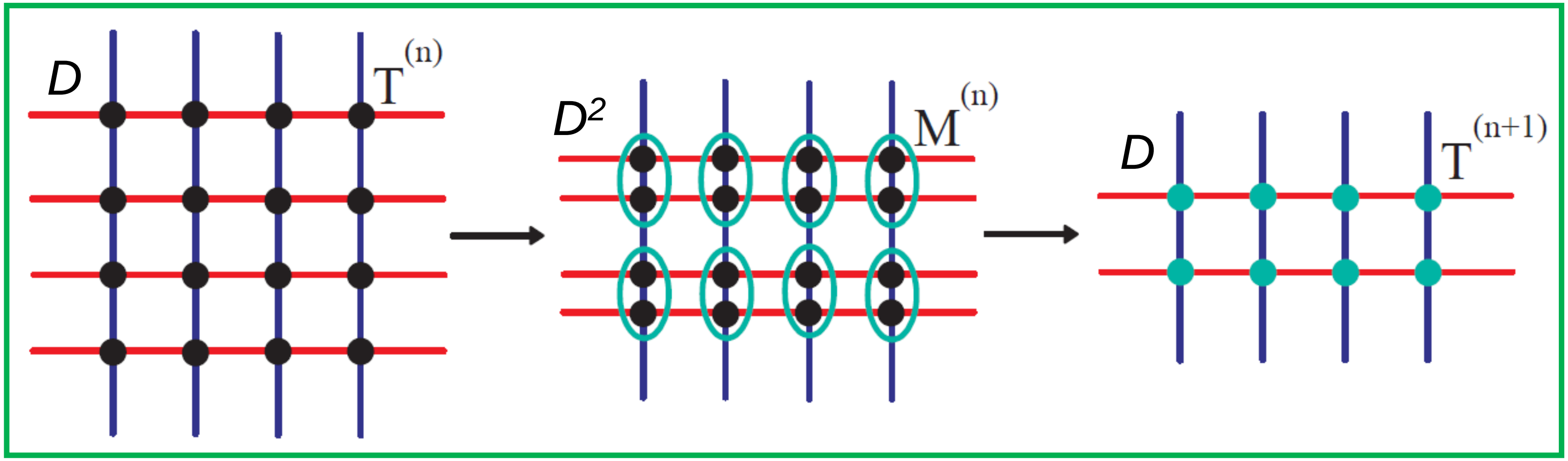
**Z. Y. Xie et al, PRB 86, 045139 (2012)**

# HOTRG: Coarse graining tensor renormalization based on HOSVD

Higher order singular value decompostion (HOSVD)

## Step 1: coarse graining

To contract two local tensors into one



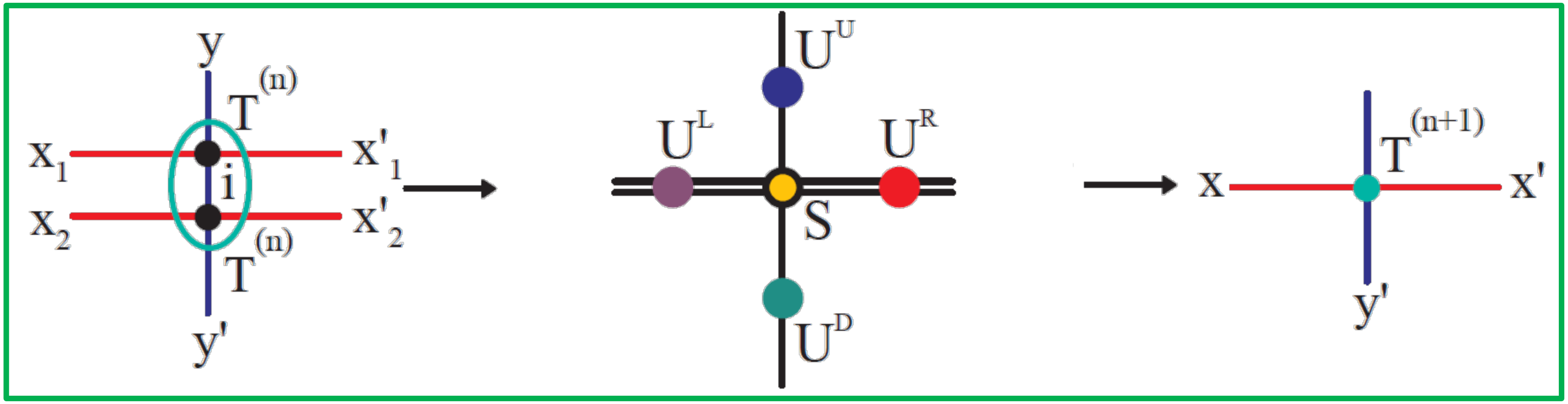

$$M^{(n)}_{xx'yy'} = \sum_i T^{(n)}_{x_1 x'_1 y i} T^{(n)}_{x_2 x'_2 i y'}$$

$$x = (x_1, x_2), \quad x' = (x'_1, x'_2)$$

# HOTRG: Coarse graining tensor renormalization based on HOSVD

## Step 2: determine the unitary transformation matrices

By the higher order singular value decomposition




$$\boxed{M^{(n)}_{xx'yy'} = \sum_{ijkl} S_{ijkl} U^L_{xi} U^R_{x'j} U^U_{yk} U^D_{y'l}}$$

# Singular value decomposition of matrix

**Singular value decomposition**

$$f_{ij} = \sum_{n=1}^{N} U_{i,n} \Lambda_n V_{j,n}$$

$$\approx \sum_{n=1}^{D} U_{i,n} \Lambda_n V_{j,n}$$

**Schmidt decomposition**

$$\boxed{|\psi\rangle = \sum_n \Lambda_n |n\rangle_{sys} |n\rangle_{env}}$$

**$\Lambda_n^2$ is the eigenvalue of reduced density matrix**

$|i\rangle_{sys}$ — $|j\rangle_{env}$

System Environment

$$\boxed{|\psi\rangle = \sum_{i,j} f_{ij} |i\rangle_{sys} |j\rangle_{env}}$$

# Higher order singular value decompostion (HOSVD)

Generalization of the singular value decomposition of matrixs to tensors

$$\boxed{M^{(n)}_{xx'yy'} = \sum_{ijkl} S_{ijkl} U^{L}_{xi} U^{R}_{x'j} U^{U}_{yk} U^{D}_{y'l}}$$

**Core tensor**

- **all-orthogonal:**

$$\langle S_{:,j,:,:} \mid S_{:,j',:,:} \rangle = 0, \qquad \text{if } j \neq j'$$

- **pseudo-diagonal / ordering:**

$$|S_{:,j,:,:}| \geq |S_{:,j',:,:}|, \qquad \text{if } j < j'$$

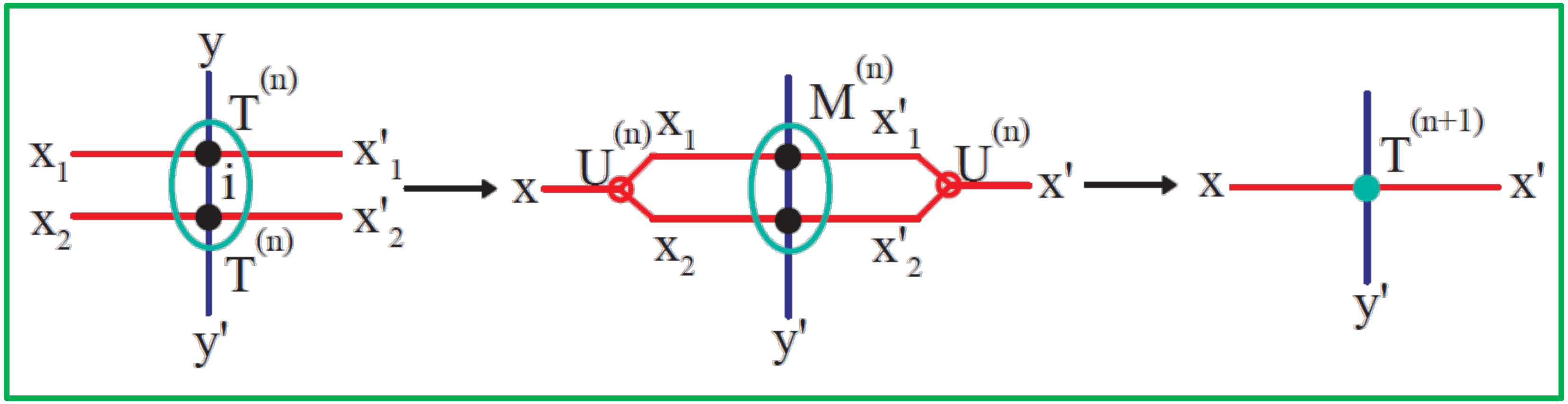
low-rank approximation for tensors

L. de Latheauwer, B. de Moor, and J. Vandewalle, SIAM, J. Matrix Anal. Appl, 21, 1253 (2000).

# HOTRG: Coarse graining tensor renormalization based on HOSVD

## Step 3: renormalize the tensor

cut the tensor dimension according to the norm of the core tensor




$$\boxed{T^{(n+1)}_{xx'yy'} = \sum_{ij} U^{(n)}_{ix} M^{(n)}_{ijyy'} U^{(n)}_{jx'}}$$

$$\varepsilon_1 = \sum_{i>D} |S(i,:,:,:)|^2$$

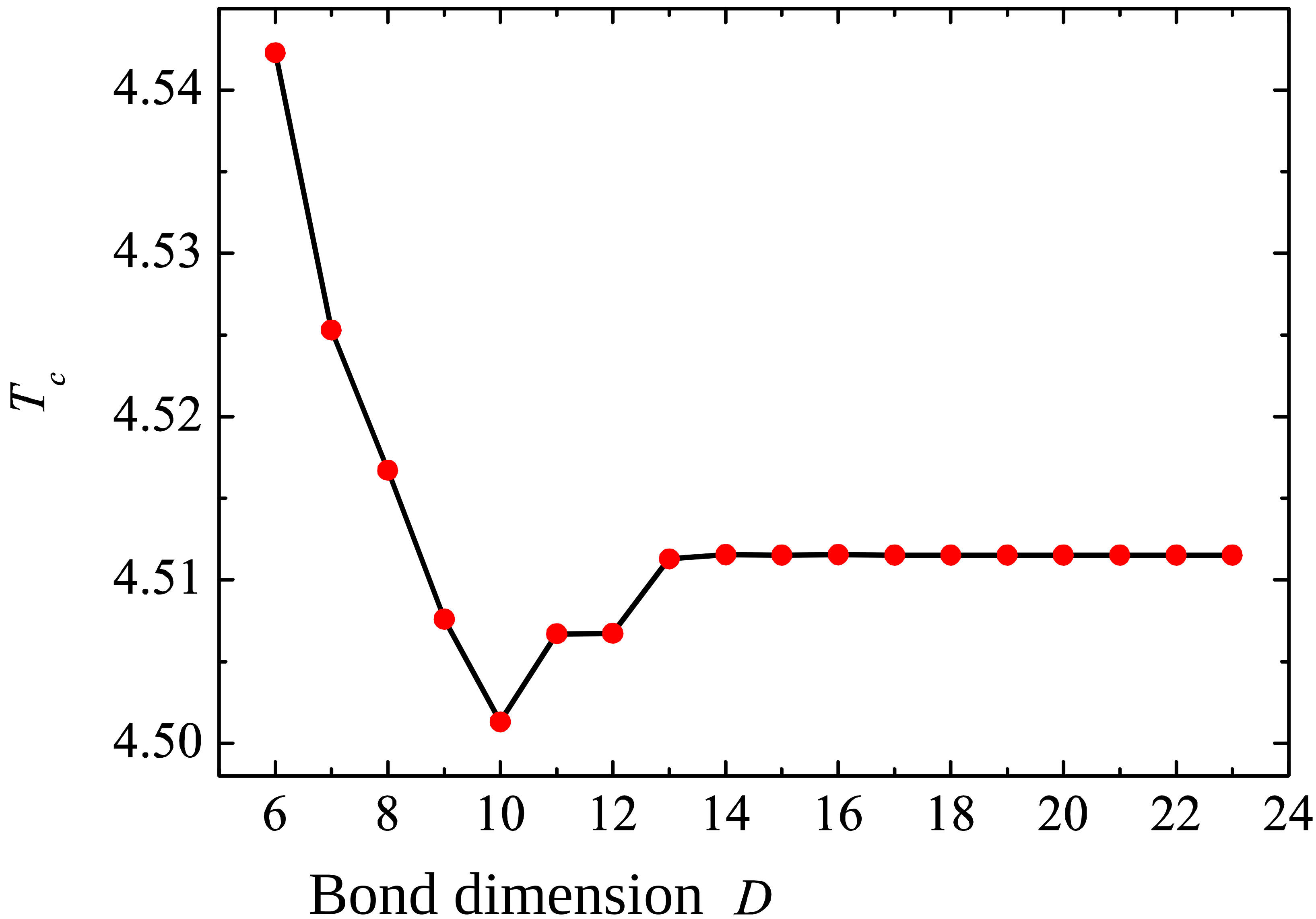
$$\varepsilon_2 = \sum_{j>D} |S(:,j,:,:)|^2$$

**truncation error = min($\varepsilon_1$, $\varepsilon_2$)**

**if $\varepsilon_1 < \varepsilon_2$, $U^{(n)} = U^L$**

**if $\varepsilon_1 > \varepsilon_2$, $U^{(n)} = U^R$**

# Critical Temperature of 3D Ising model



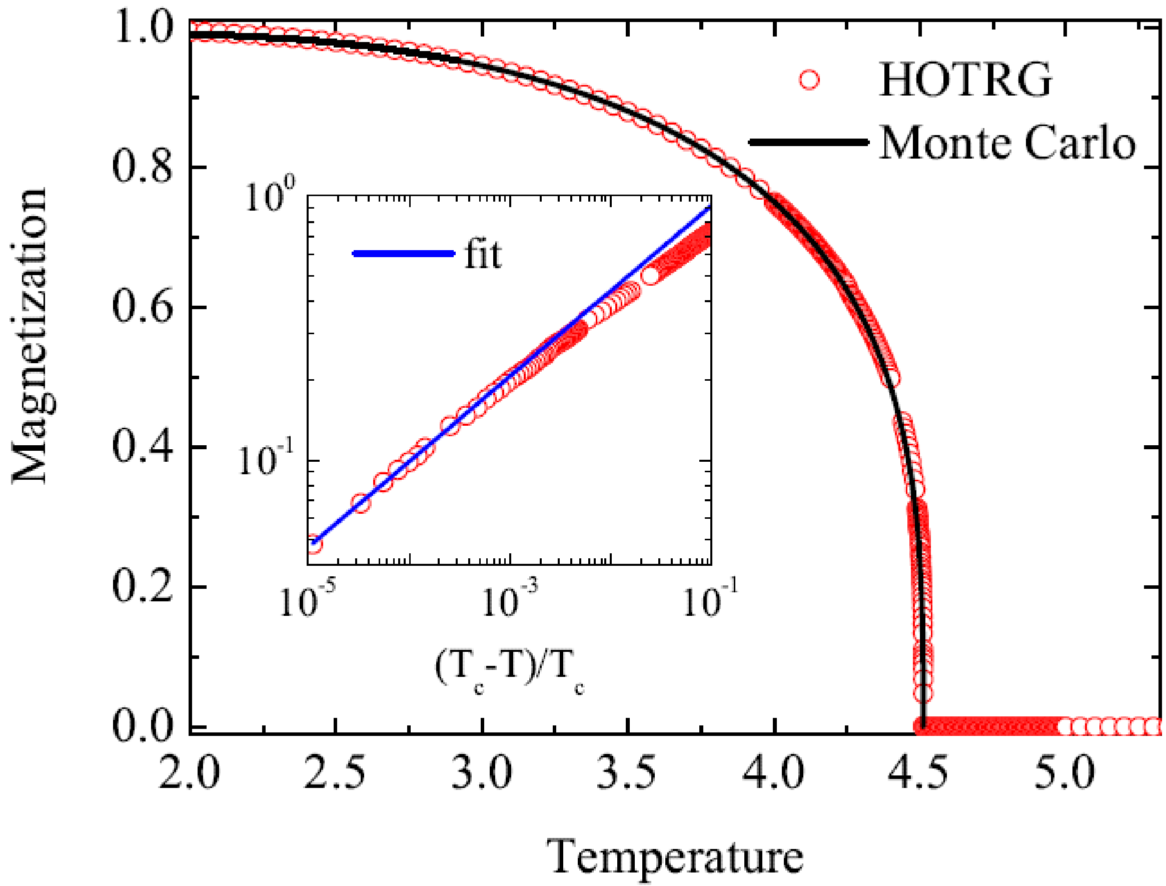
# Critical Temperature of 3D Ising model

| method | $T_c$ |
|---|---|
| HOTRG D = 23 | 4.51152469(1) |
| Monte Carlo[37] | 4.511523 |
| Monte Carlo[38] | 4.511525 |
| Monte Carlo[39] | 4.511516 |
| Monte Carlo[35] | 4.511528 |
| Series expansion[40] | 4.511536 |
| CTMRG[12] | 4.5788 |
| TPVA[13] | 4.5704 |
| CTMRG[14] | 4.5393 |
| TPVA[16] | 4.554 |
| Algebraic variation[41] | 4.547 |

Other RG methods

# Magnetization of 3D Ising model

Xie et al, PRB 86,045139 (2012)




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

**HOTRG (D=14): 0.3295**

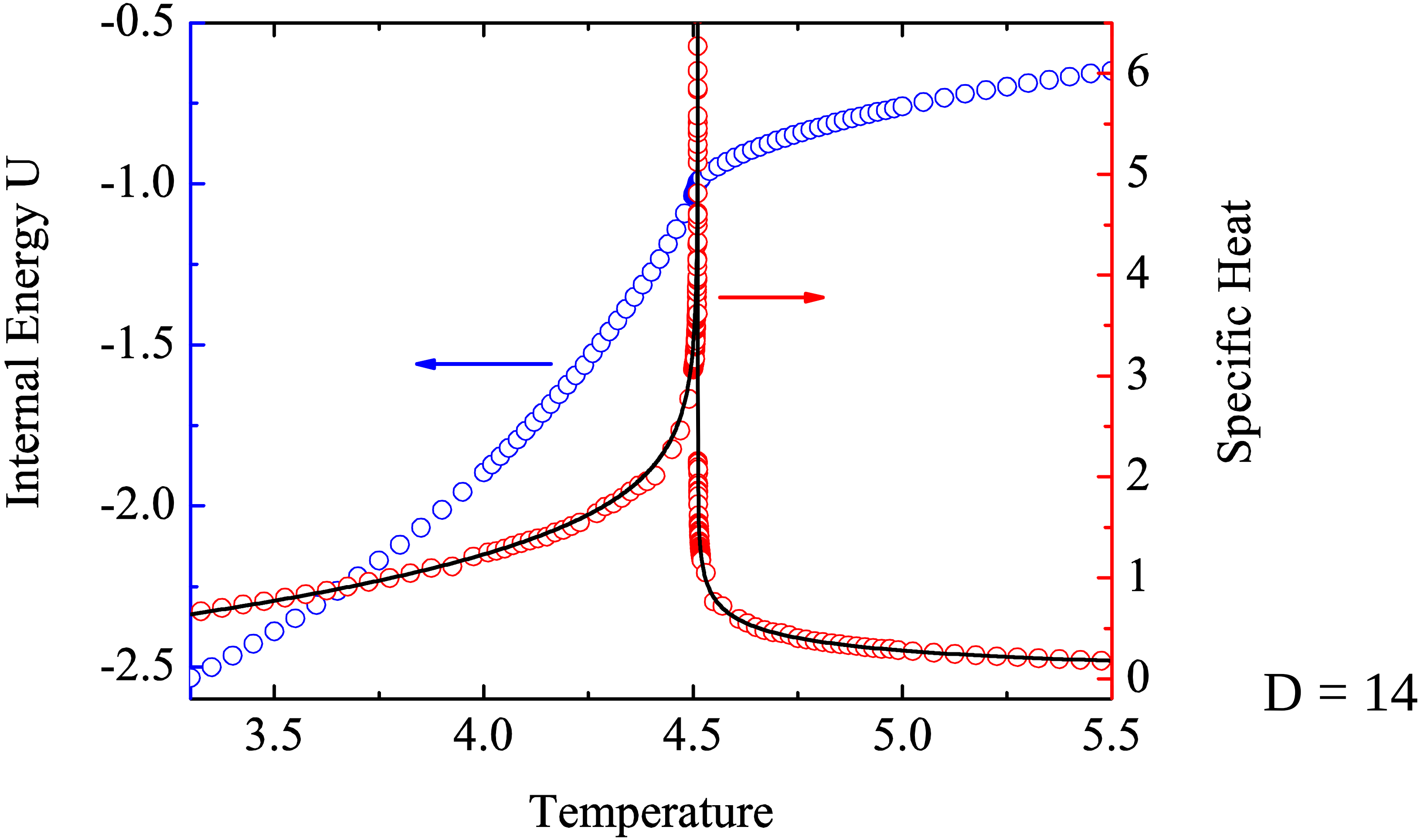
**Monte Carlo: 0.3262**

**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).

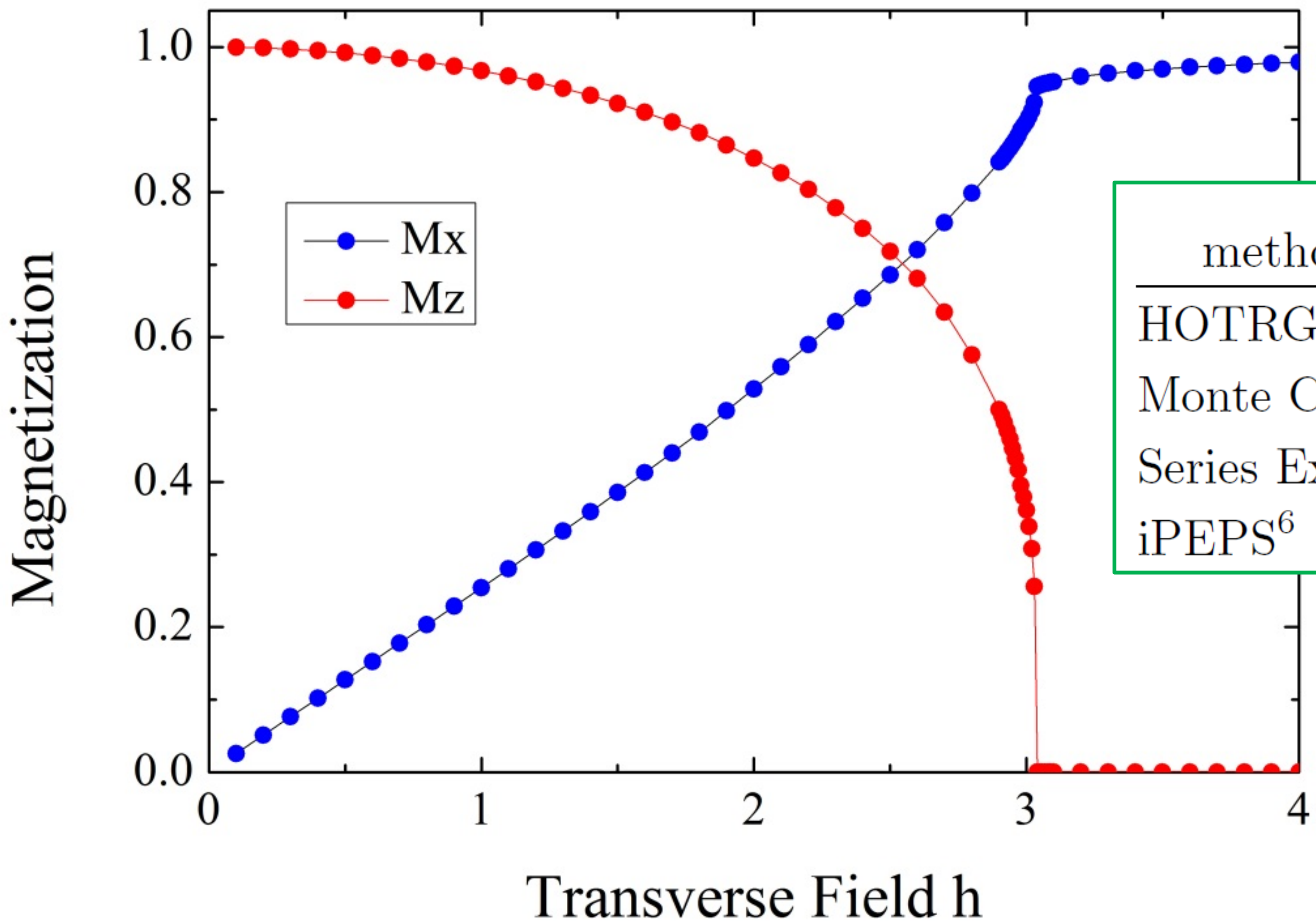
# Specific Heat of 3D Ising model




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

# 2D Quantum Ising model

2D QuantumTransverse Ising Model at T = 0K




| method | $h_c$ |
|---|---|
| HOTRG(D=14) | 3.0439 |
| Monte Carlo[42] | 3.044 |
| Series Expansion[43] | 3.044 |
| iPEPS[6] | 3.06 |

# Novel Tensor-Network States

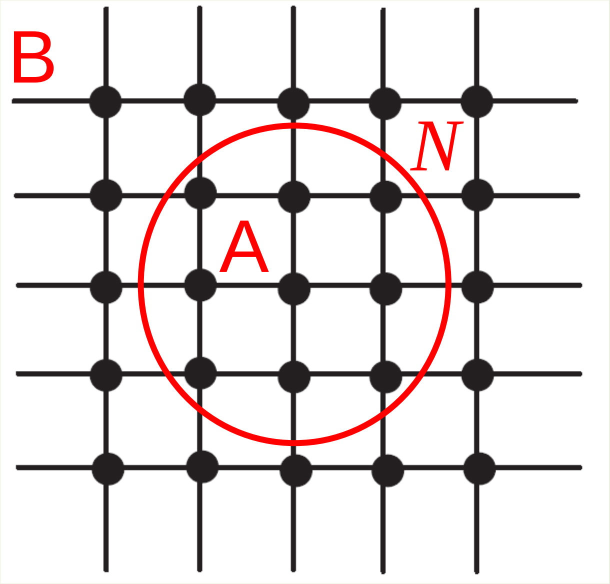
Projected Entangled Simplex State (PESS)

arXiv:1307.5696

# Basic properties of quantum many-body wavefunction

|

## Area Law of Entanglement Entropy




**Entanglement Entropy between A and B**

$$\boldsymbol{S_{ent} \sim N \sim \ln \chi}$$

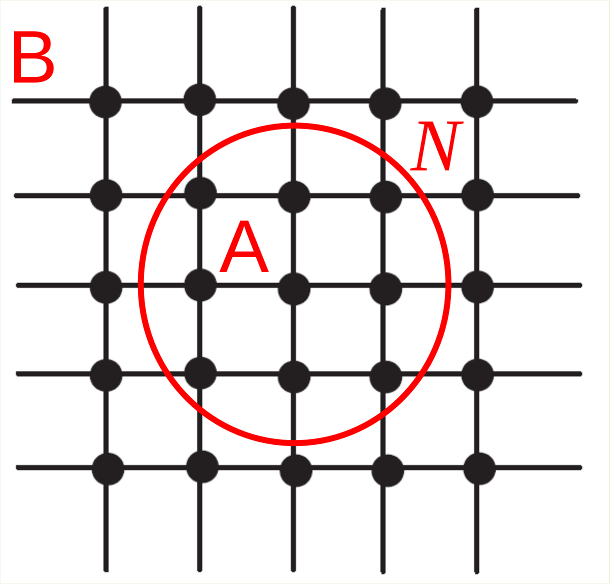
$$\boldsymbol{\chi \sim e^{N}}$$

**minimal number of basis states needed grows exponentially with system size**

# Basic properties of quantum many-body wavefunction

What kind of wavefunctions satisfy the entanglement area law?

## Area Law of Entanglement Entropy




**Entanglement Entropy between A and B**

$$\boxed{\begin{gathered} S_{ent} \sim N \sim \ln \chi \\ \chi \sim e^{N} \end{gathered}}$$

**minimal number of basis states needed grows exponentially with system size**

# The Answer: tensor-network states

- 1 dimension

  Matrix product state (MPS)

  Multi-scale entanglement renormalization ansatz (MERA)

- 2 or higher dimensions

  Projected entangled pair state (PEPS)

  = tensor product state

  ……

  Projected Entangled Simplex State (PESS)

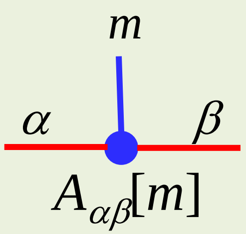
# 1D: Matrix product state

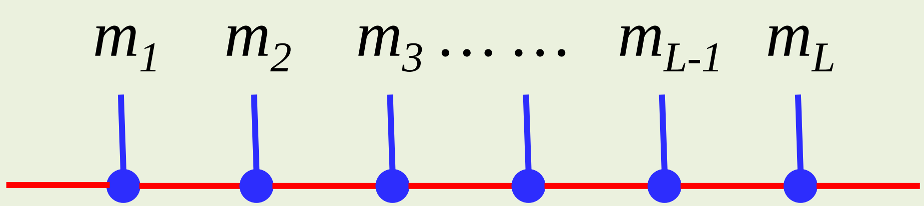
|

Matrix product state (MPS)

$dD^2L$ parameters

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



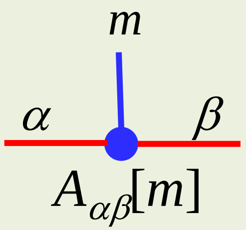
# 1D: Matrix product state

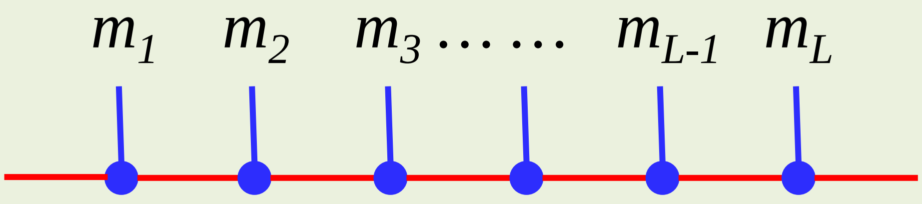
Ostlund and Rommer, PRL **75**, 3537 (1995)

- ✓ It is the wavefunction generated by the DMRG
- ✓ Can be taken as an efficient trial wave function in 1D

## Matrix product state (MPS)

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

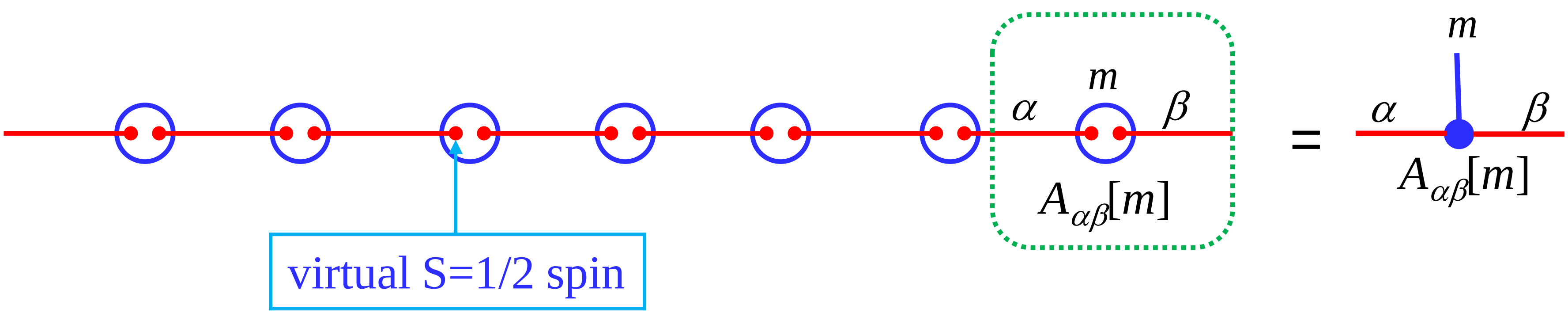


# Example AKLT valence bond solid state

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

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




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

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

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

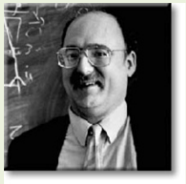
To project two virtual S=1/2 states, $\alpha$ and $\beta$, onto a S=1 state $m$


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

# Matrix Product State and Haldane Conjecture

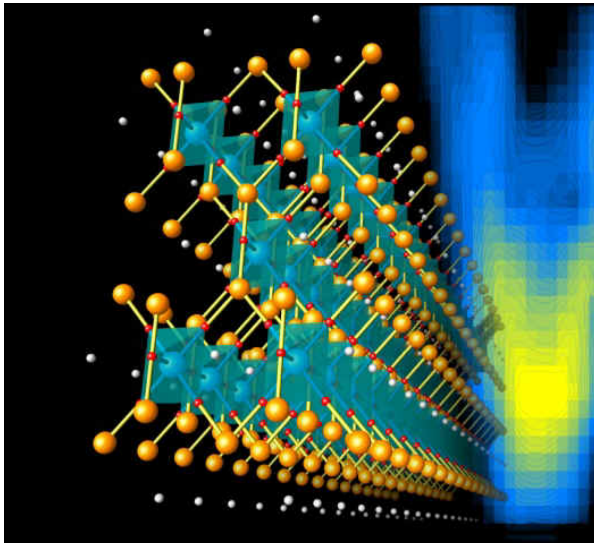
$$H = \sum_i S_i \cdot S_{i+1}$$

Integer antiferromagnetic Heisenberg spin system has a finite excitation gap

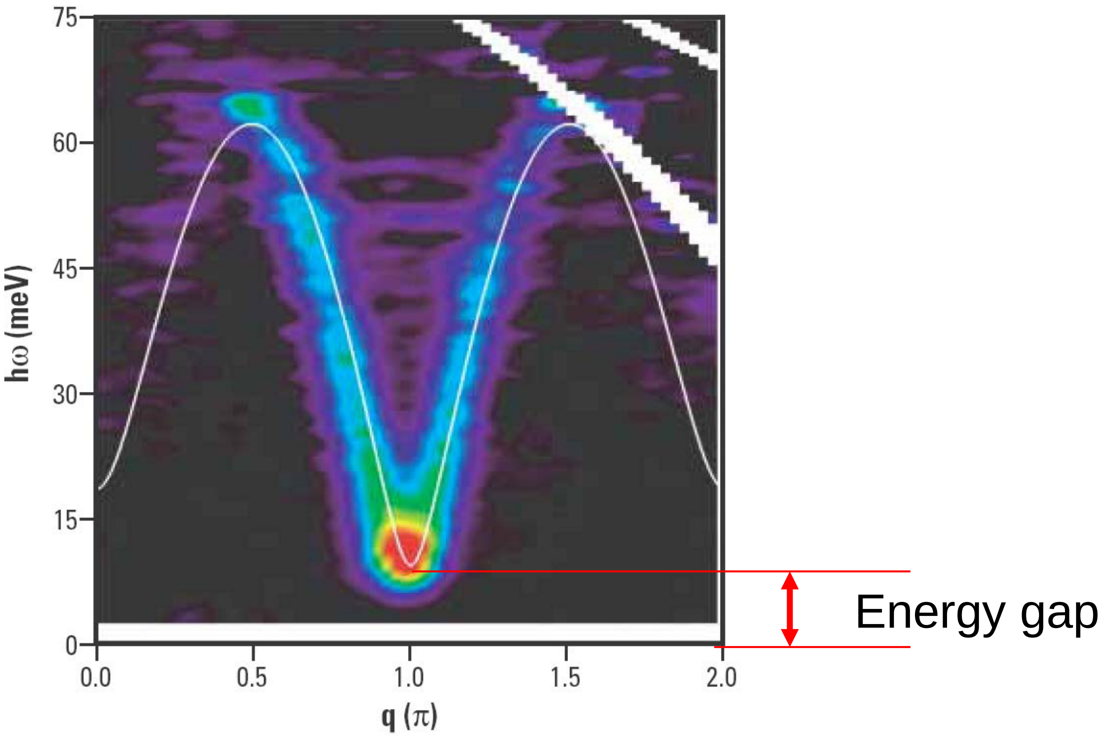


Haldane

$Ni^{2+}$ $S = 1$



$Y_2BaNiO_5$



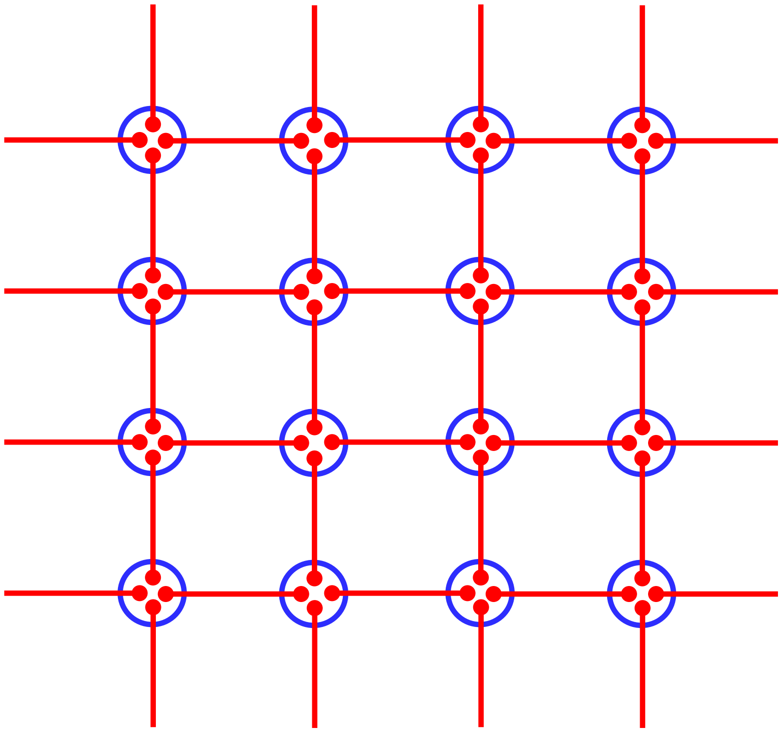
# AKLT valence bond solid state in 2D

S = 2

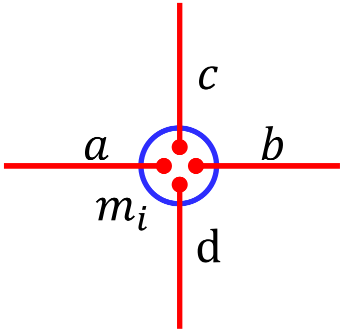
$$|\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'}[m_i] |m_i\rangle$$

Virtual basis state

Physical state



$$T_{abcd}[m_i] =$$



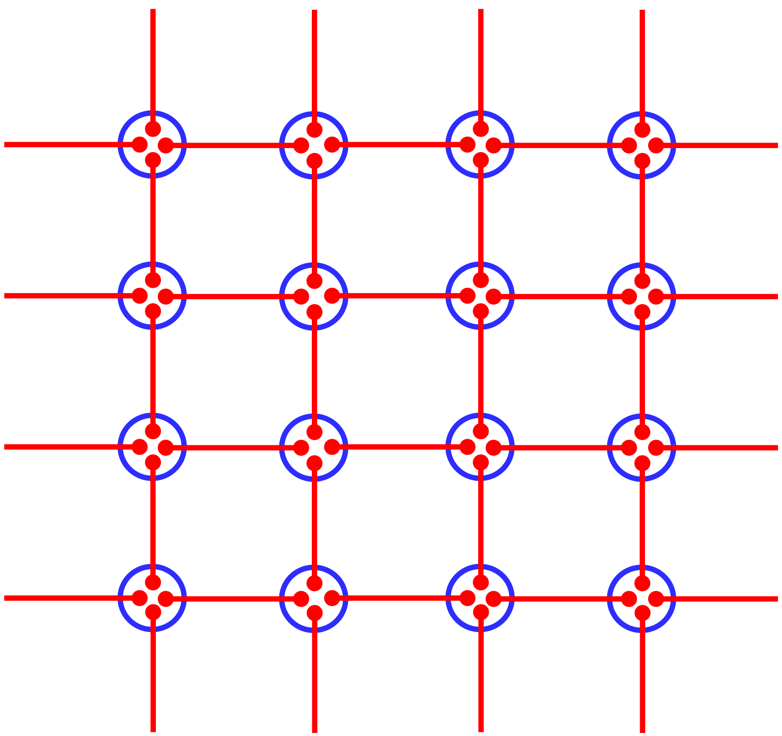

$$H = \sum_{\langle ij \rangle} P_4(i,j)$$

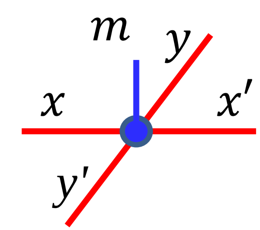
**To project two S=2 spins on sites *i* and *j* onto a total spin S=4 state**

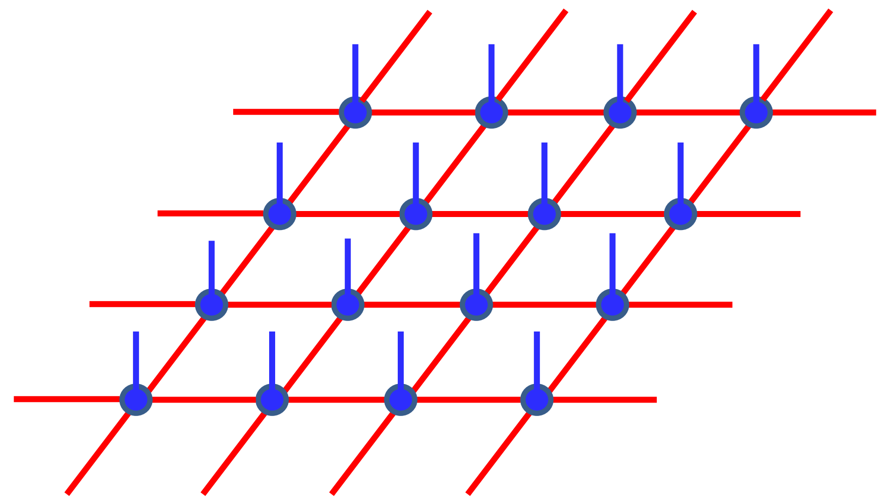
# 2D tensor network state: Projected Entangled Pair State (PEPS)

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

Virtual basis state    Physical state



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

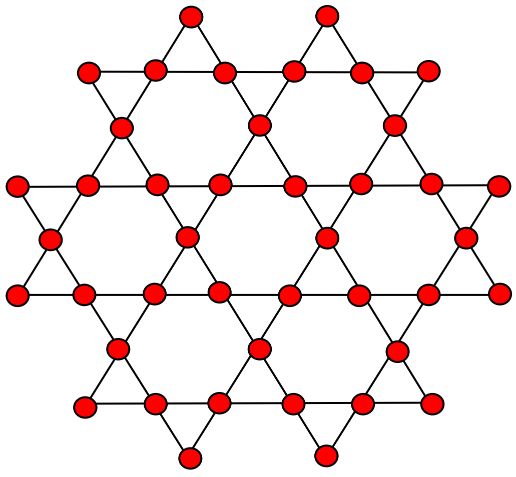
Verstraete, Cirac, arXiv:0407066

# Projected Entangled Pair State (PEPS)

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

Virtual basis state　　　Physical state

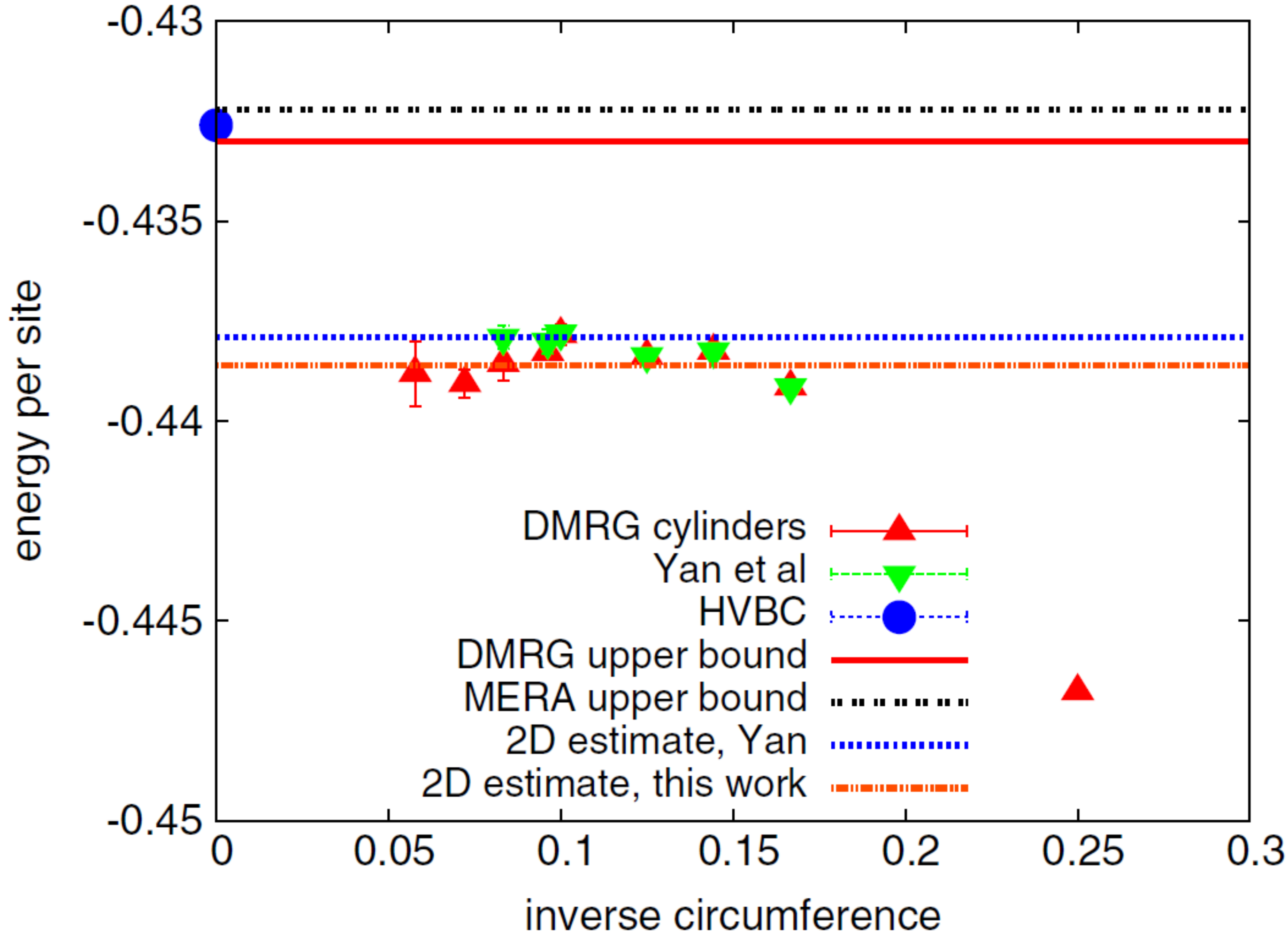
- Successfully applied to the quantum spin models on honeycomb and square lattices
- But, difficult to obtain a converged result if applied to the AFM Heisenberg or other models on the Kagome or other frustrated lattices

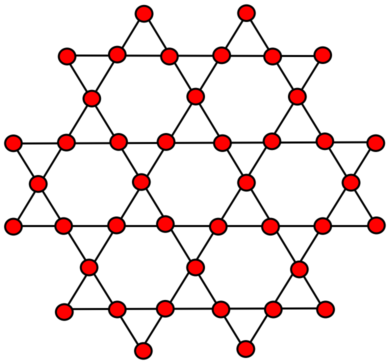


Kagome Lattice

# S=1/2 Kagome Heisenberg model: $Z_2$ spin liquid

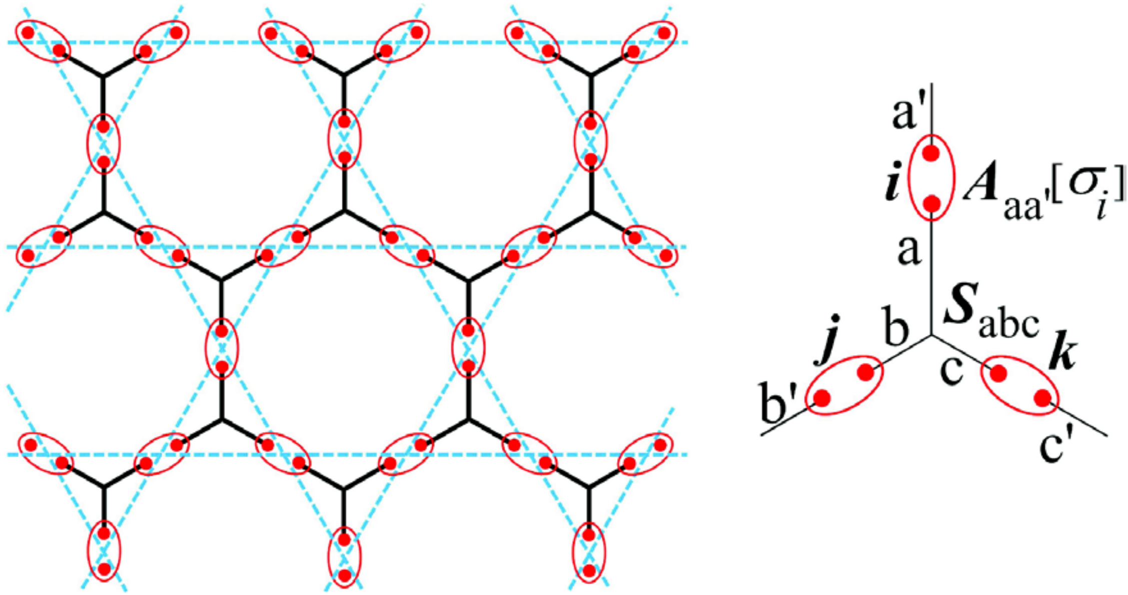
Depenbrock,McCulloch,Schollwock, PRL 109, 067201 (2012)



Ground state energy obtained with different methods

# Projected Entangled Simplex States (PESS)




Projection tensor

Simplex tensor

- Virtual spins at each simplex (here triangle), instead of at each pair, form a maximally entangled state
- Remove the geometry frustration: The PESS wavefunction on the Kagome lattice is defined on the decorated honeycomb lattice (no frustration)

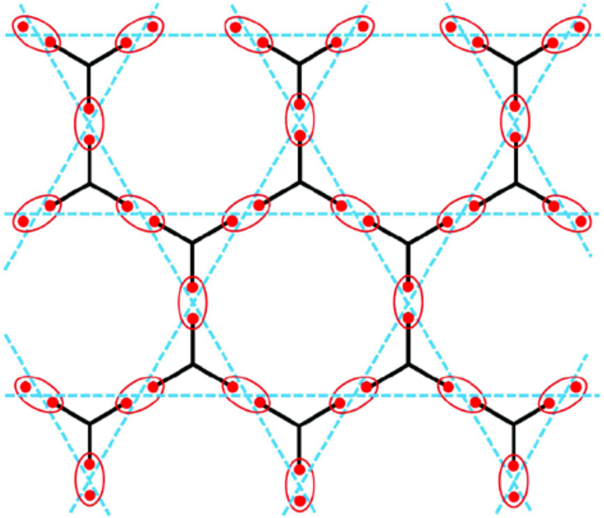
# Simplex Solid States

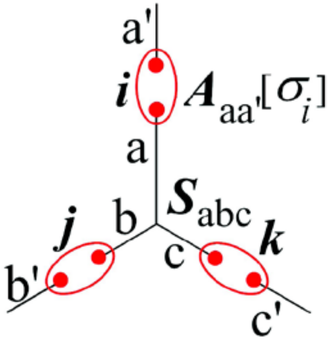
D. P. Arovas, Phys. Rev. B **77**, 104404 (2008)

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 on the Kagome Lattice

## 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

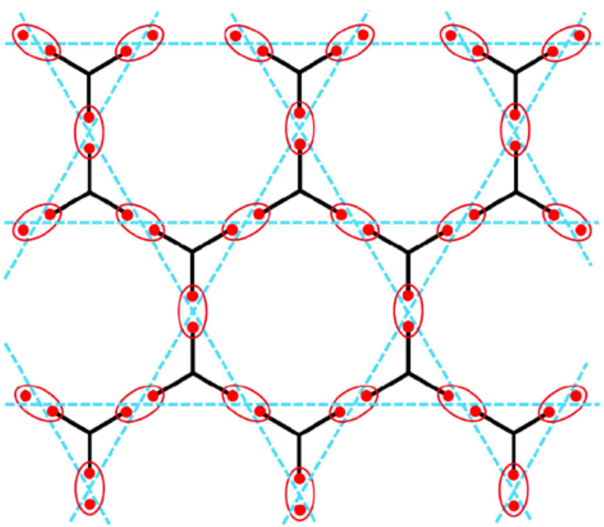
## Parent Hamiltonians

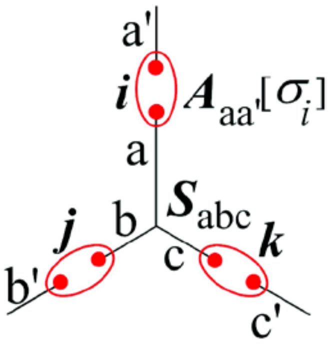
$$H = \sum_{\langle ij \rangle} P_4(ij)$$

or

$$H = \sum_{ijk \in \nabla} \sum_{n=4,5,6} J_n P_n(ijk)$$

$P_n$ : projection operator





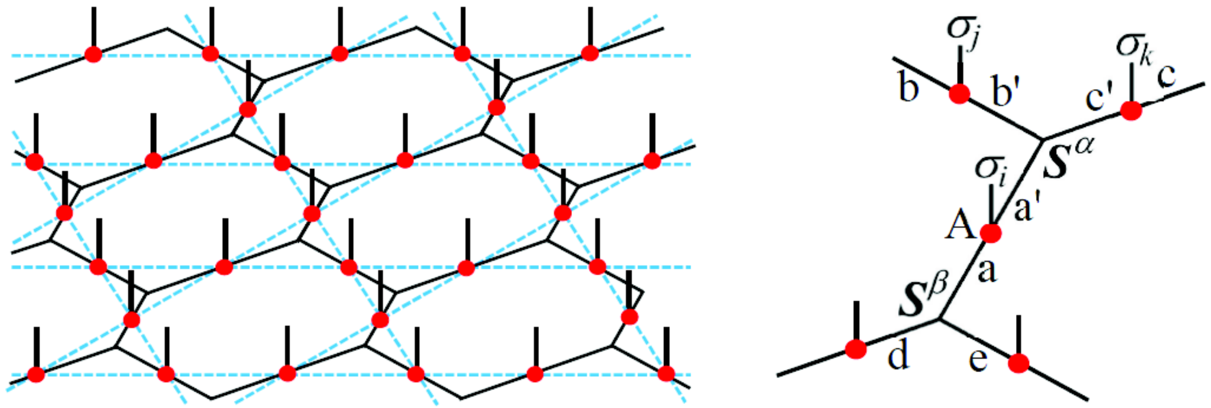

Projection tensor

Simplex tensor

# Projected Entangled Simplex State (PESS)

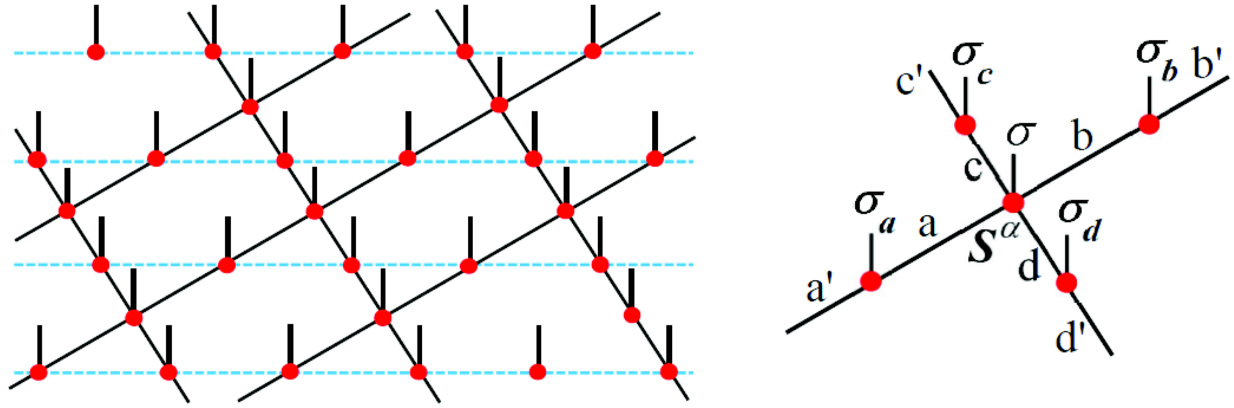
Kagome Lattice

3-PESS form a decorated honeycomb lattice




(a) 3-PESS

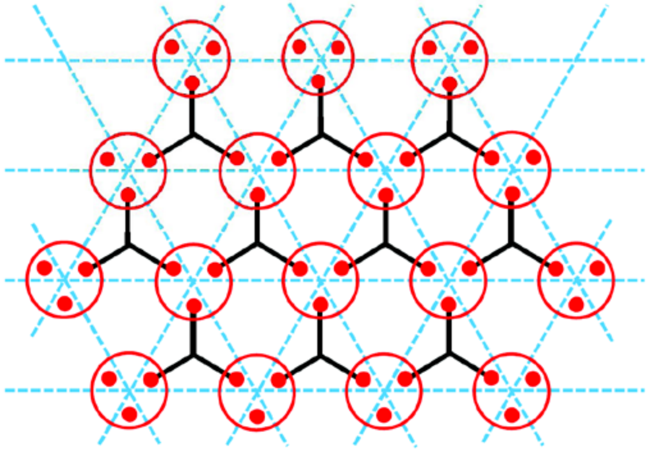
5-PESS form a decorated square lattice




(b) 5-PESS

# PESS on other lattices

Triangular Lattice



Order of local tensors:

Simplex tensor: $D^3$

Projection tensor: $dD^3$

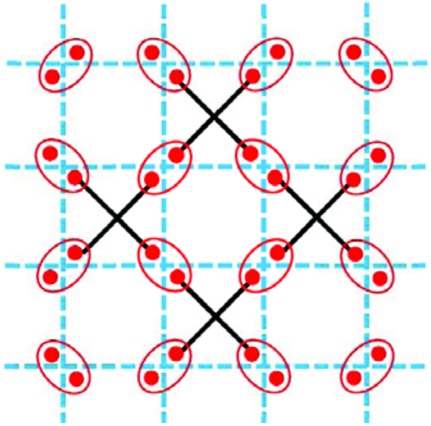
Order of local tensor in PEPS: $dD^6$

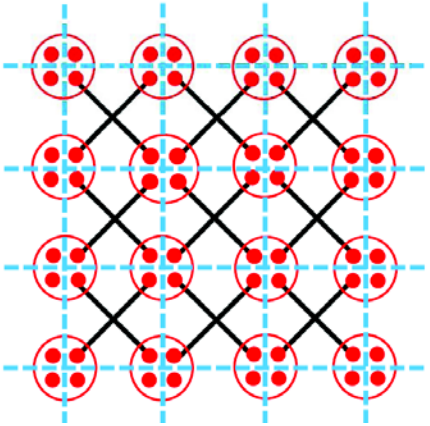
Square Lattice

Two kinds of simplex solid states

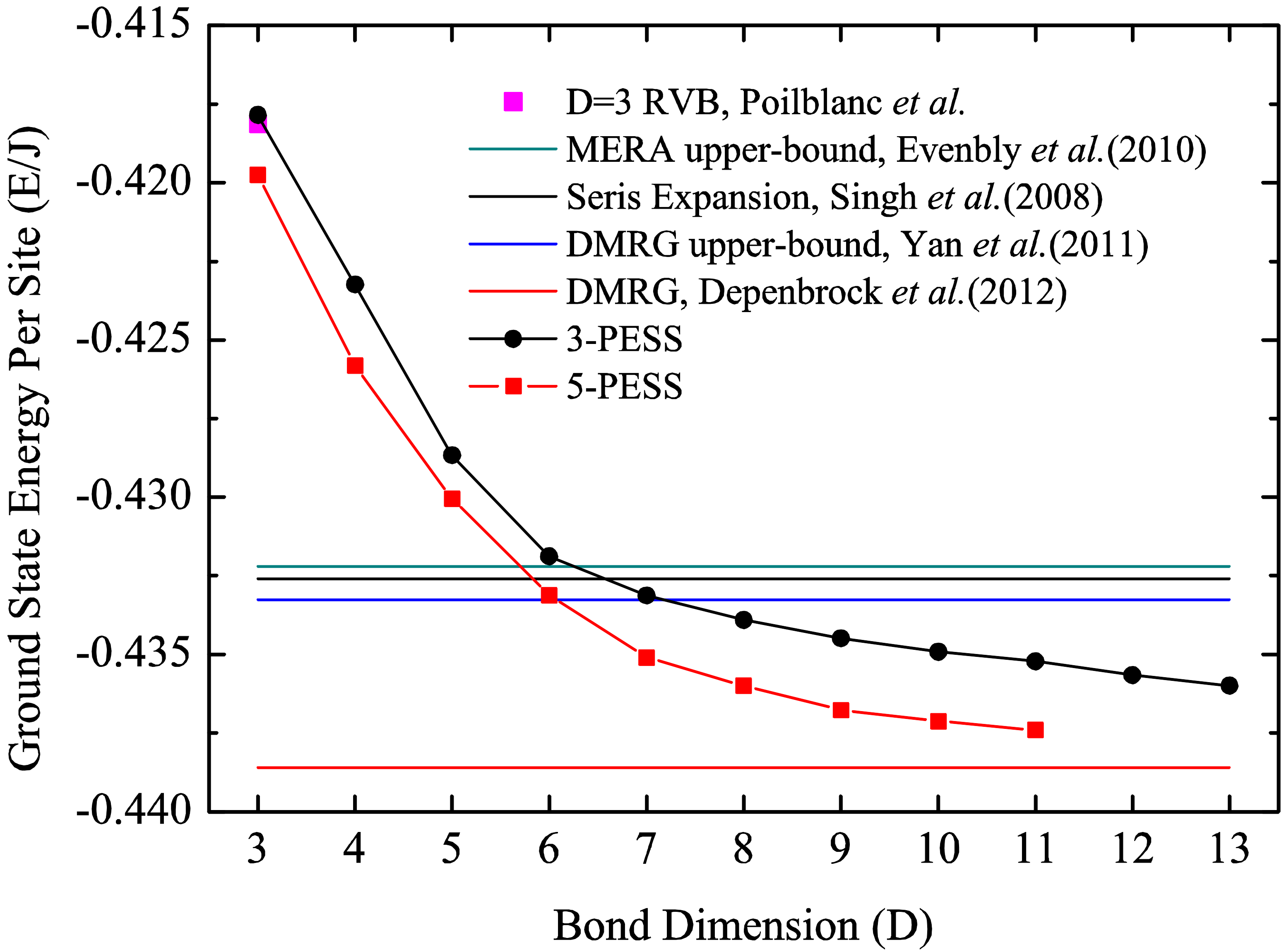
Vertex-sharing

Edge-sharing





# Ground state energy of the S=1/2 Kagome Heisenberg model



# Summary

- HOTRG provides an accurate numerical method for studying thermodynamic quantities of classical/quantum statistical models

- Projected Entangled Simplex State (PESS) is a good representation for solving the frustrated quantum lattice models

# Simple Update based on the HOSVD