Tensor networks and its applications to quantum frustrated systems

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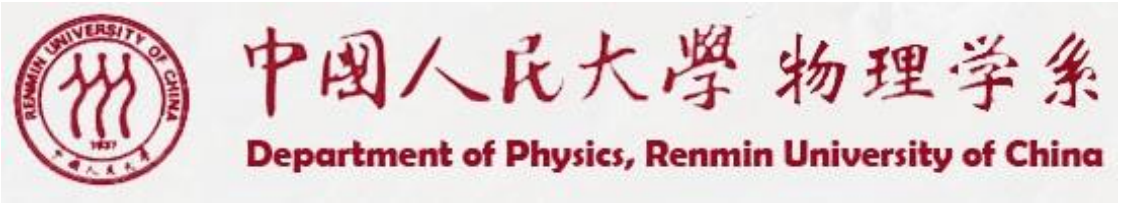


Outline

- **Some basics of Tensor Network States**
  - Matrix Product State (MPS)
  - Projected Entangled Pair State (PEPS)
- **Determination of the Ground State Representation**
  - Imaginary-time evolution
  - Simple update, canonicalization
  - Projected Entangled Simplex State (PESS)
- **Expectation value calculation**
  - Corner Transfer Matrix Renormalization (CTMRG)
  - Nested technique
- **Application in quantum frustrated spin systems**

1. Some basics of Tensor Network States

The Goal of numerical renormalizaion: To challenge strongly correlated systems

- Non-perturbative: no obvious small parameters
- Exponential wall: degree of freedom grows exponentially with system size

- Dirac: Chemistry is over due to the powerful Schrodinger equation!
- Kohn: In general the many-electron wf for a system of N electrons is not a legitimate scientific concept, when N ~ 1000

P. A. M. Dirac
1933 物理奖

Walter Kohn
1998 化学奖

Weak Coupling Approach: Suitable for weak-coupling systems

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

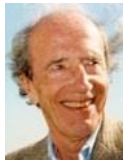
Strong Coupling Approach:

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

数值的重正化群（RG）：变分，可控

- 数值RG：在标度变换中，把高能Hilbert空间(不相关自由度)给积掉，最终得到有效场论(模型/表示)。
- RG在量子场论：

Stueckelberg, Petermann 1951-1953

Gell-Mann(1969物理) Low, RG-flow, 1954



Feynman, Schwinger, Tomonaga, QED(1965物理)


t'Hooft,Veltman, 1971,规范场可RG (1999物理)



Gross, Politzer,Wilczek 1973年,QCD渐进自由 (2004物理)

1950 1960 1970 1980

- RG在统计物理与凝聚态物理：

Kadanoff 标度变换，变分计算（1975）

Wilson 相变与临界系统，数值RG (Kondo问题) (1982物理)

Anderson 1979，局域化的标度理论（1977物理）

White 1992，密度矩阵RG

张量重正化群
（张量网络态，
张量网络模型，
粗粒化重正化群，
类转移矩阵重正化群）

1960 1970 1980 1990 2000

0D 1D 2D

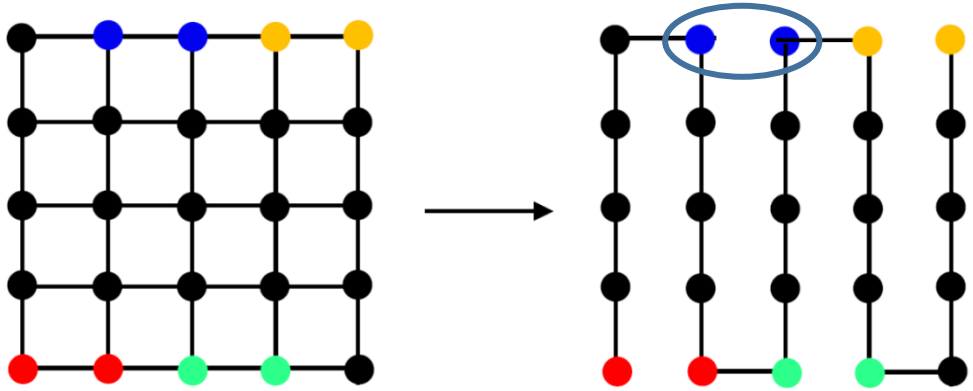
Why do we need tensor renormalization?

✓ Density Matrix Renormalization Group

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

✓ Quantum Monte Carlo

- No dimension consideration
- Generally suffer from the "minus-sign" problem for fermion and frustrated spin system



A possible direction: Tensor Renormalization (TNS, TNM)

Why renormalization is possible?

An illusion about Hilbert space

PRL 106, 170501 (2011)

- Boundary area law

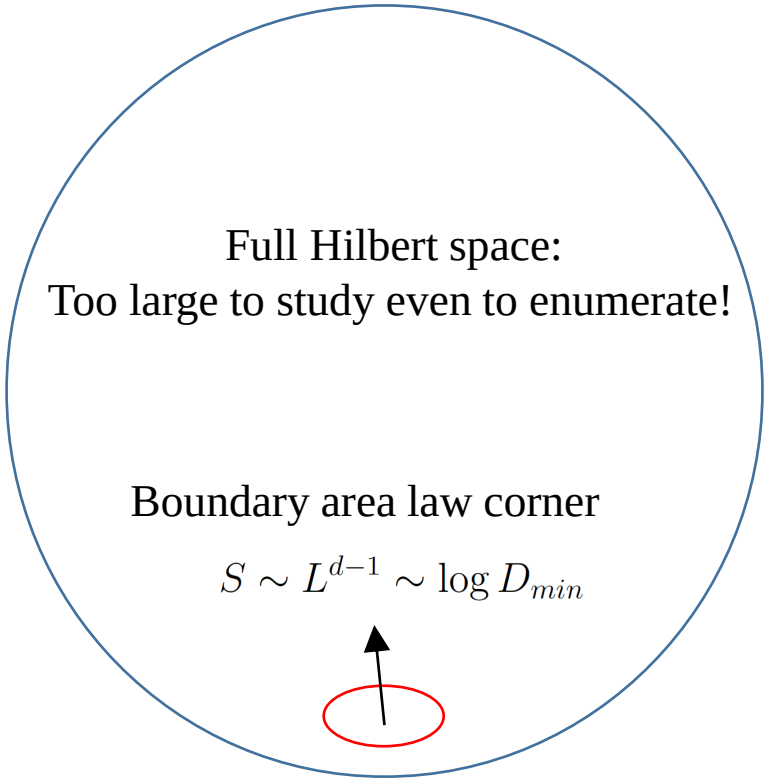
Rev. Mod. Phys. 82, 277 (2010)

- Tensor Network State (TNS)

Nat. Rev. Phys. 1, 538 (2019)

  - Can satisfy the area law: 2D thermodynamic limit
  - Variational ansatz: grdst/low-excited wf. of a quantum lattice model
  - No obvious sign problem: frustration, fermionic

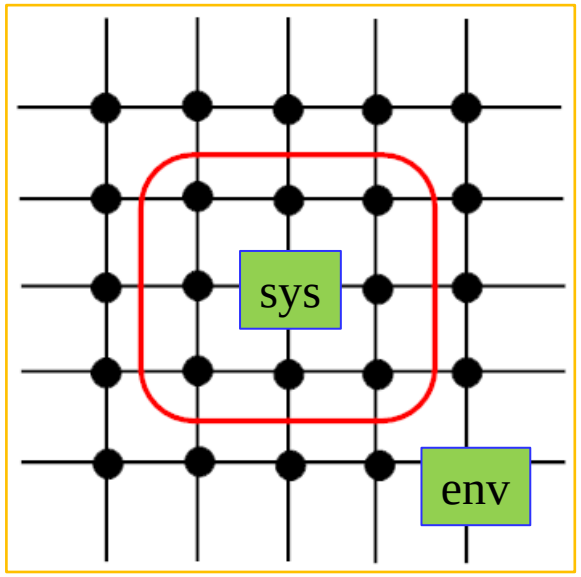
- Success: str-el-sys, frustrated spin, statistical, QFT, TO, ML, quan-circuit, …



Rev. Mod. Phys. 94, 025005 (2022)

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.

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

- 1D: local gapped Hamiltonian with only constant degeneracy of ground state
- Quasi-free (i.e., quadratic terms only) boson and fermion gapped local-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<=2 in isotropic case, h=2 in anisotropic case)
- **General expectation**: ground state of local gapped Hamiltonian obeys.

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

Partial history about tensor network state

✓ AKLT authors: 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'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

- Verstraete: in name of Projected Entangled Pair State (PEPS), general variational ansatz, variational method
- Vidal: Multi-scale Entanglement Renormalization Ansatz (MERA)
- Garnet: Correlator Product State (CPS)
- Our Group: Projected Entangled Simplex State (PESS)
- Continuous TNS, fermionic TNS, tangent space / single-mode approximation ……

✓ Note: One can choose any suitable wavefunction ansatz according to the problem at hand.

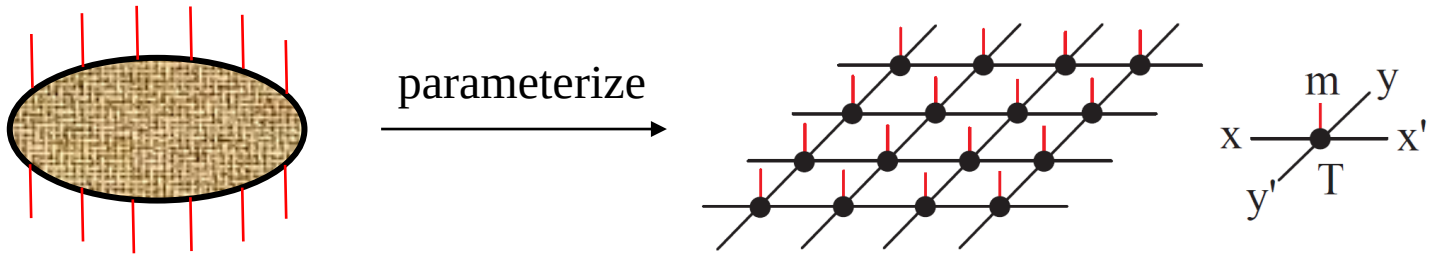
✓ It doesn't matter whether the cat is black or white, as long as it catches mice!

Quantum lattice system: Tensor Network State (TNS)

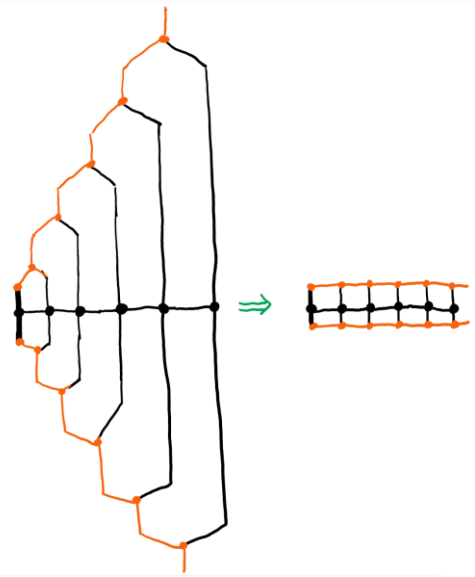
- *Tensor network state* provides a faithful representation[1] of the ground state wavefunction of a quantum lattice model that satisfies the area law of the entanglement entropy.

Ref: arXiv:0407066; F Verstraete, *et al*, PRA81, 052338(2010)

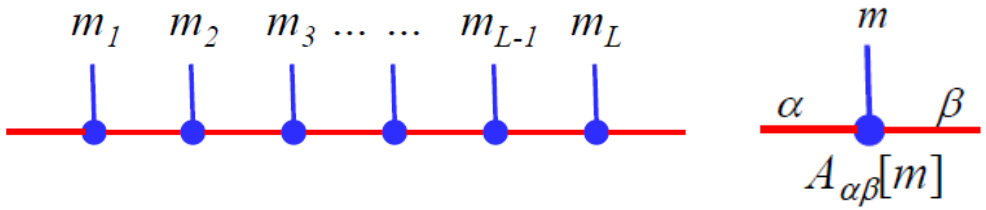
- Parameters: $d^N \rightarrow ND^4d$



$$|\Psi\rangle = \sum_{\{m\}} C_{m_1 m_2 \ldots} |m_1 m_2 \ldots\rangle \qquad |\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'} [m_i] |m_i\rangle$$



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



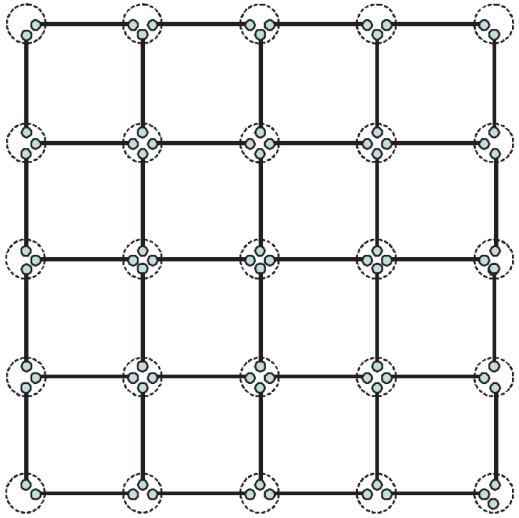
$$|\Psi\rangle = \sum_{m_1 \cdots m_L} Tr\left(A[m_1] \ldots A[m_L]\right) |m_1 \ldots m_L\rangle$$

DMRG and (isometric/canonical) MPS

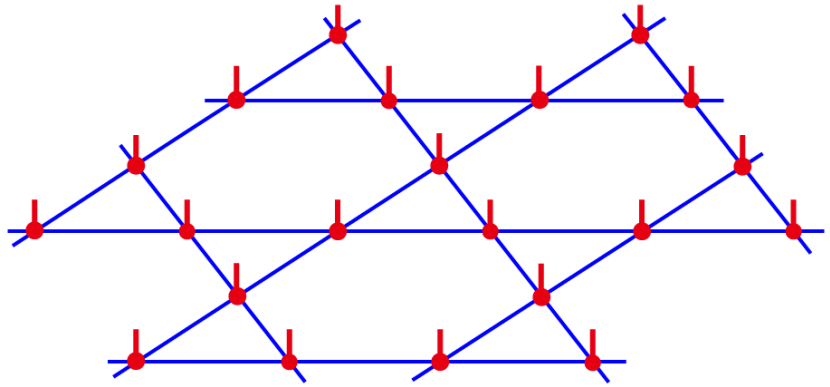
Ref: M. Fannes, *et al*, Comm. Math. Phys. 144, 443 (1992).

Tensor Network State (TNS) as wavefunction ansatz

- Projected entangled ***pair*** states(PEPS) on kagome lattice:



Circle: Projector
Lines: entangled pair



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

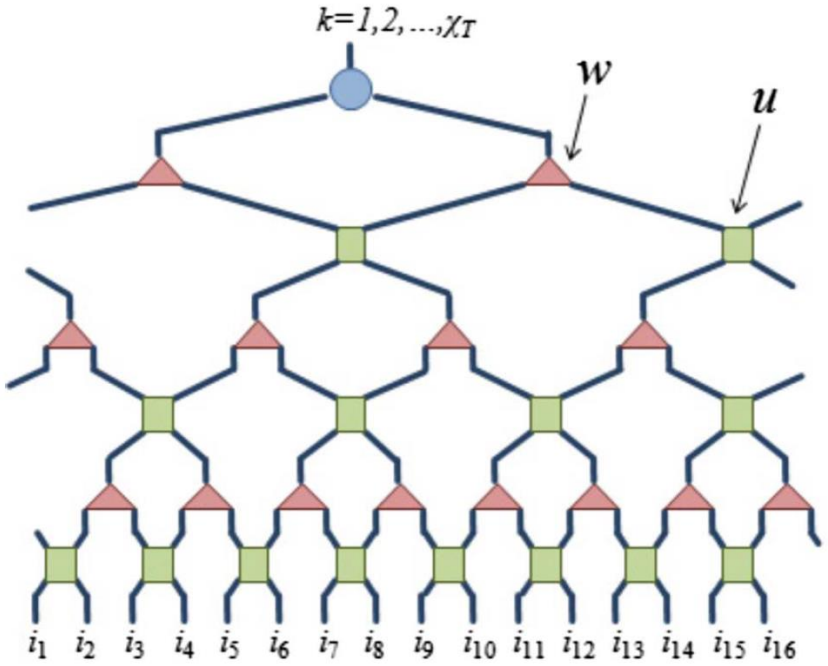
Virtual auxiliary state
Bond dimension (D)

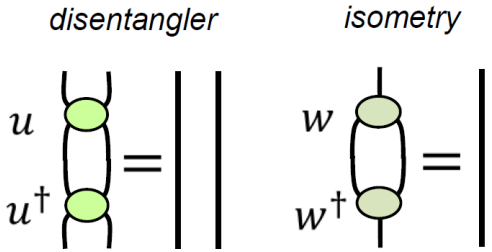
Real physical state

- ✓ 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
- ✓ Probably the most popular TNS used in practice.

arXiv:0407066; F Verstraete, et al, PRA81, 052338(2010)

➢ Multi-scale Entangled Renormalization Ansatz (MERA): 1D binary example

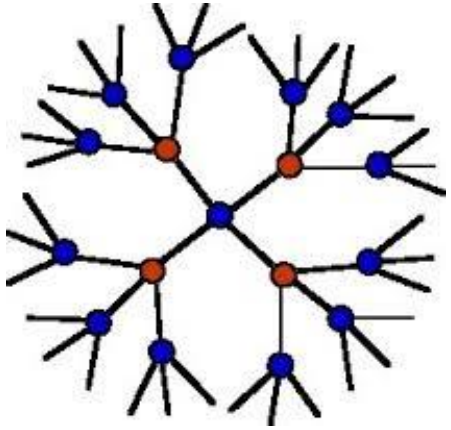




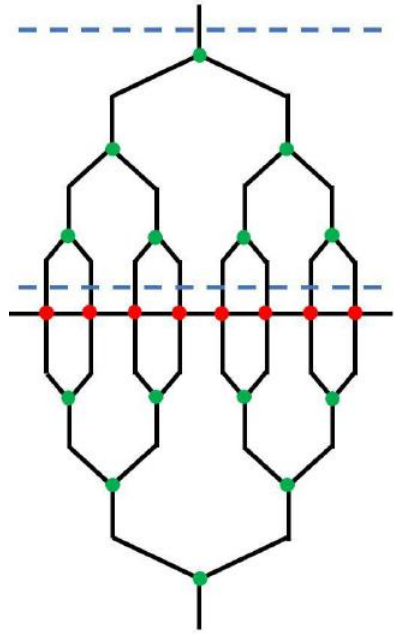
- ✓ disentangler is to disentangle the local entanglement between constituents.
- ✓ isometry is to renormalize the DOF.
- ✓ Layers of scale: ~ log(N)
- ✓ The upmost index k is the rank of MERA should be summed over when exp. Cal.
- ✓ Transfer matrix, or (D+1)-dim wave function.
- ✓ In 1D, can have log correction of area law
- ✓ In 2D, branching MERA can go beyond area-law

G. Vidal, PRL 99, 220405 (2007)
G. Evenbly and G. Vidal, PRL 112, 240502 (2014)

➢ Tree Tensor network (TTN): or Hierarchical Tensor Train in App-Math



1. Defining feature: No loop or closed circuit
2. Actually MPS is such kind of wavefunction in 1D.
3. Violate area law in higher dimension, and the problem is similar as that in DMRG.
4. Bethe lattice is an example, see left.
5. Can be evaluated exactly, canonical form



NRG and (isometric) Tree TN

Correlator Product State (CPS):

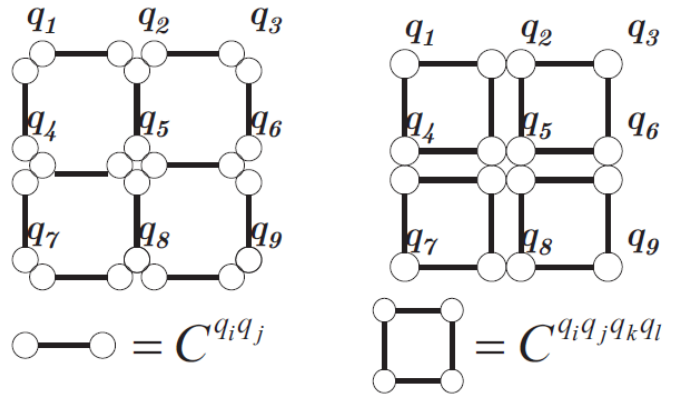
Given a configuration, its coefficient can be written as the dot product of some group coefficient

E.g., C^{ij} is a group coefficient with 2 members, i.e., two neighbours

$$|\Psi\rangle = \sum_{\{q\}} \prod_{\langle ij\rangle} C^{q_i q_j} |q_1, \ldots, q_L\rangle$$

or written explicitly as: Q means given a configuration

$$\Psi(Q) = C^{q_1 q_2} C^{q_2 q_3} C^{q_3 q_4} \ldots C^{q_{L-1} q_L}.$$



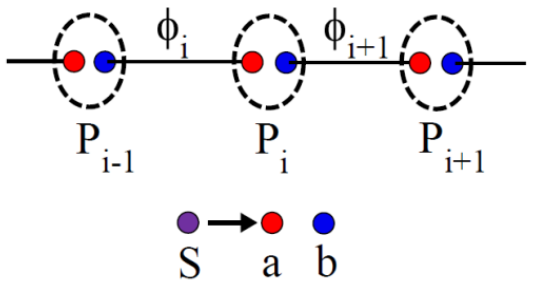
H. J. Changlani, et al, PRB 80, 245116 (2009)

Note:

- Physical DOF correlated with each other explicitly, instead of through virtual DOF as in PEPS.
- In general, C can be long distance covered, or has more members, or has more overlap
- The coefficient can only be obtained by variation
- Can violate/satisfy/exceed area law: depends on the group structure.

Some exact representation in terms of MPS

- AKLT state construction: Spin-1



$|\phi^i\rangle = \frac{|12\rangle - |21\rangle}{\sqrt{2}}$，这里设定$|1\rangle \equiv |\uparrow\rangle$, $|2\rangle \equiv |\downarrow\rangle$.

$|\phi^i\rangle = \sum_{\alpha\beta} B_{\alpha\beta}|\alpha\beta\rangle, \quad \alpha, \beta = 1, 2,$

$$B = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$\sigma = \pm, 0$

$$P = \sum_{\sigma} |\sigma\rangle\langle\sigma| = \sum_{\alpha\beta\sigma} A^{\sigma}_{\alpha\beta}|\sigma\rangle\langle\alpha\beta|$$

$$A^{+} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A^{-} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad A^{0} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$|\Psi\rangle = (\prod_i P^i)(\prod |\phi^i\rangle) = (\prod_i \sum_{\alpha_i\beta_i\sigma_i} A^{\sigma_i}_{\alpha_i\beta_i}|\sigma_i\rangle\langle\alpha_i\beta_i|)(\prod_j \sum_{\alpha_{j+1}\beta_j} B_{\beta_j\alpha_{j+1}}|\beta_j\alpha_{j+1}\rangle)$$

$$= \prod_i \sum_{\alpha,\beta} A^{\sigma_i}_{\alpha_i,\beta_i} B_{\beta_i\alpha_{i+1}}|\sigma_i\rangle$$

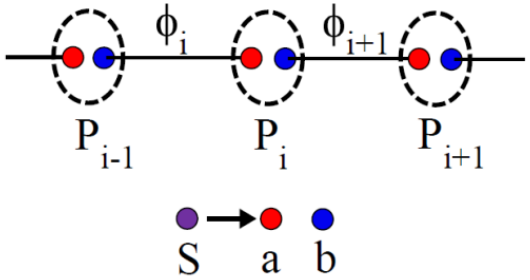
$$= Tr \prod_i T_{\alpha_i,\alpha_{i+1}}[\sigma_i]|\sigma_i\rangle$$

$T^{\pm} = \pm\frac{1}{\sqrt{2}}\sigma^{\pm}, \quad T^{0} = -\frac{1}{2}\sigma^{z}$. (normalization: $\times\sqrt{4/3}$)

AKLT, PRL 59, 799 (1987)
AKLT, Commun. Math. Phys. 115, 477 (1988)

Some exact representation in terms of MPS

- AKLT model (Spin-1): parent Hamiltonian (gapped)



Introduce $T_{ij} \equiv (S_i + S_j)^2$, S : total spin AMO

$|0\rangle$, $|1\rangle$, $|2\rangle$: eigenstate of total spin (without z component)

Satisfying : $T|0\rangle = 0$, $T|1\rangle = 2|1\rangle$, $T|2\rangle = 6|2\rangle$

$P^{(2)} \equiv |2\rangle\langle 2|$, Semi-positive operator

Construct $H = \sum_{\langle ij \rangle} P_{ij}^{(2)} \Rightarrow H|AKLT\rangle = 0$

Expand $P_{ij}^{(2)}$ in terms of T_{ij} as : $(n+1)-$dimension

$P^{(2)} = C_0 + C_1 T + C_2 T^2$ (complete set; Cayley-Hamiton)

$T_{ij} = S_i^2 + S_j^2 + 2S_iS_j = 4 + 2S_iS_j$

$P^{(2)}|0\rangle = 0 \Rightarrow C_0|0\rangle + 0 + 0 = 0$

$P^{(2)}|1\rangle = 0 \Rightarrow C_1|1\rangle + 2C_1|1\rangle + 4C_2|1\rangle = 0$

$P^{(2)}|2\rangle = |2\rangle \Rightarrow C_1|2\rangle + 6C_1|2\rangle + 36C_2|2\rangle = |2\rangle$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 2 & 4 \\ 1 & 6 & 36 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{matrix} 0 \\ 0 \\ 1 \end{matrix} \Rightarrow \begin{cases} C_0 = 0 \\ C_1 = -\frac{1}{12} \\ C_2 = \frac{1}{24} \end{cases}$$

$$\Rightarrow P_{ij}^{(2)} = -\frac{1}{12} T_{ij} + \frac{1}{24} T_{ij}^2 ,$$
$$= \frac{1}{6}\left[2 + 3S_iS_j + (S_iS_j)^2\right]$$

Injective (PBC), non-injective (OBC)

Ground state of Toric code

R. Orus, Annals of Physics 349, 117 (2014)

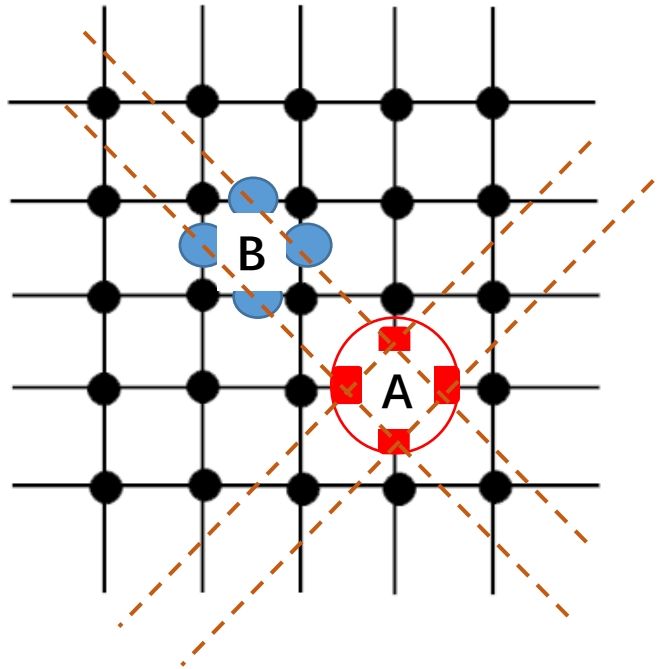
$$H = -J_a \sum_s A_s - J_b \sum_p B_p \qquad A_s = \prod_{\vec{r}\in s} \sigma_x^{[\vec{r}]}, \qquad B_p = \prod_{\vec{r}\in p} \sigma_z^{[\vec{r}]}.$$

where s/p denotes star/plaquette: spins are only defined on bonds!

- [Ai, Bj] = 0 for any site and plaquette.

  Ai and Bj have 2 relative pos: (X,Z) and (X,Z) overlap; no overlap

- Both A and B are projectors in the sense that $A^2 = B^2 = 1$: since $S^2 = 1$

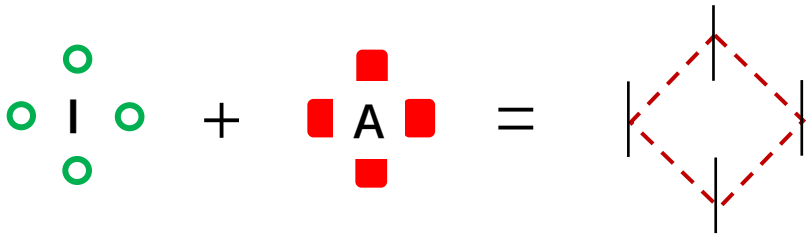


The below state are simultaneous eigenstate of all A and B with (+1)

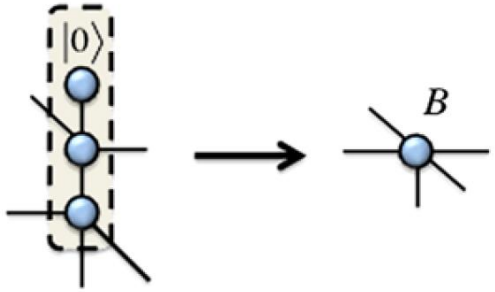
$$|\Psi_{TC}\rangle = \prod_s \frac{(\mathbb{I}+A_s)}{2} \prod_p \frac{(\mathbb{I}+B_p)}{2} |0\rangle^{\otimes N\to\infty} = \prod_s \frac{(\mathbb{I}+A_s)}{2} |0\rangle^{\otimes N\to\infty}$$

- note |0=↑↑↑…> is the eigenstate of B, by definition, therefore omitted.

Similarly, write 1 + A as the following PEPO:



Definition on dashed squares:
the virtual link can only chosen as (1,1,1,1) and (2,2,2,2)
One: identity operator, the other: A



Each site is evolved in 2 PEPOs: D = 2 (double-sublattice)

2. Determination of Ground State Representation

Determination of the ground state representation

- Mapped to a 3D classical model, and study the 3D tensor network as for classical statistical model
- Choose a wavefunction ansatz/form of the targeted state.
- Determine the unknown parameters in the wavefunction form.

➢ 1. global variational extremum problem

find a PEPS $|\Psi\rangle$ which minimize the energy: $\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$

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

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

H^e : (D^4d, D^4d), the effective environment of X-pair in the acted network with H
N: (D^4d, D^4d), the effective environment of X-pair in the norm network, positive definite in principle

➢ Probably much more unstable than time evolution.

Determination of the ground state representation

➢ 2. imaginary time evolution

$$e^{-\beta H}|\Psi\rangle = \sum_i e^{-\beta E_i}|\phi_i\rangle \xrightarrow{\beta\to\inf} e^{-\beta E_0}|\phi_0\rangle$$

- Starting from arbitrary (non-orthogonal) state, then do evolution.
- But we do not know how to represent the full exponent.

➢ Trotter-Suzuki idea: fortunately we do know how to represent the local term!

$$e^{-\tau H} = e^{-\tau H_\nabla} e^{-\tau H_\Delta} + O(\tau^2)$$

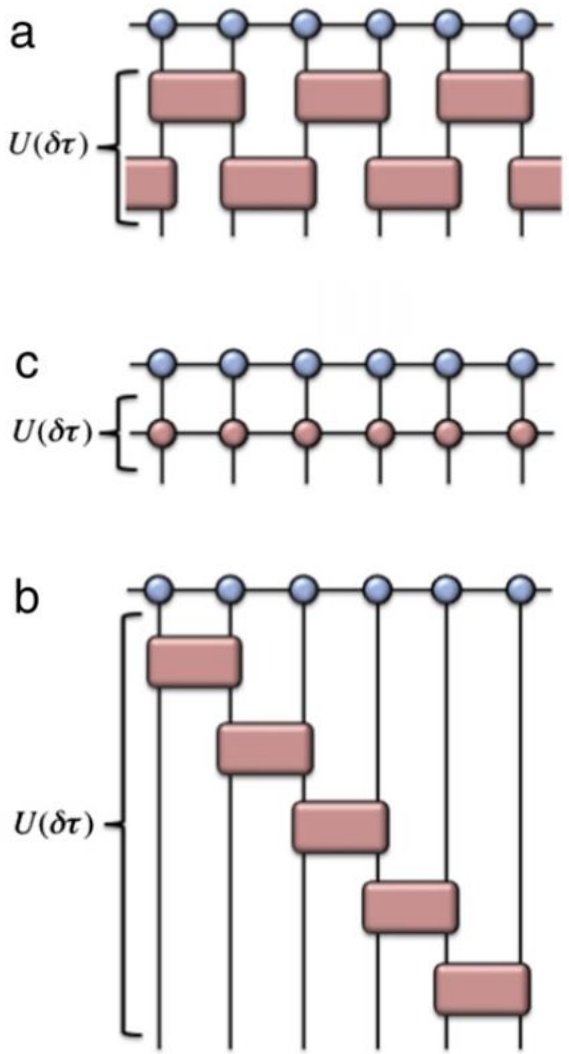
$$e^{-\tau H} = e^{-\frac{\tau}{2} H_\nabla} e^{-\tau H_\Delta} e^{-\frac{\tau}{2} H_\nabla} + O(\tau^3)$$

- We express the full exponent in terms of very small imaginary-time slices

$$e^{-\beta H} = [e^{-\tau H}]^M \qquad \tau M = \beta$$

- And then expand each slice in terms of local terms by the Trotter formula

$$e^{-\tau H} = e^{-\tau \sum_i h_i} \simeq \prod_i e^{-\tau h_i} + O(\tau^2)$$

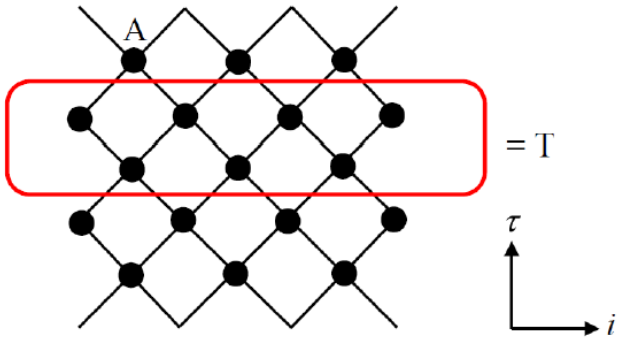


R. Orus, AOP 349, 117 (2014)

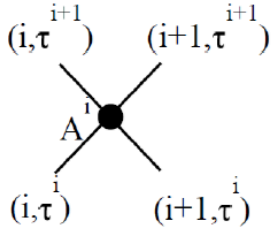
Actually it maps n-dim quantum to (n+1)-dim classic: 1D example

$$
\begin{aligned}
H &= H_o + H_e \\
H_o &= \sum_{i\in odd} H_{i,i+1} \\
H_e &= \sum_{i\in even} H_{i,i+1}
\end{aligned}
$$

$$
\begin{aligned}
Z = Tre^{-\beta H} = Tr(e^{-\tau H})^M &\approx Tr(e^{-\tau H_o}e^{-\tau H_e})^M \\
&= \sum_{s^1}\langle s^1|(e^{-\tau H_o}e^{-\tau H_e})^M|s^1\rangle \\
&= \sum_{s}\langle s^1|e^{-\tau H_o}|s^2\rangle\langle s^2|e^{-\tau H_e}|s^3\rangle\ldots \\
&\quad \ldots\langle s^{2M-1}|e^{-\tau H_o}|s^{2M}\rangle\langle s^{2M}|e^{-\tau H_e}|s^1\rangle \\
&= Tr\prod_i A^i
\end{aligned}
$$

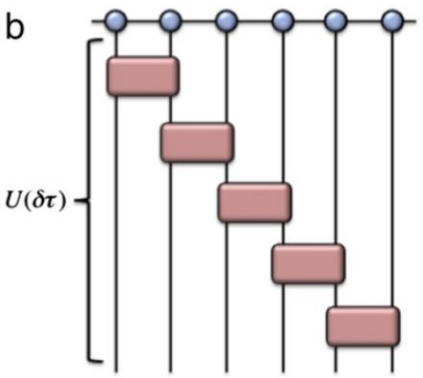


(a)



(b)

- Note: In time evolution, each equivalent terms in a single h(i), can be done either simultaneously or sequentially
- In principle, the simultaneous action is more accurate but more costly: *still highly suggested*!
- We can also combine several h(i) into a single MPO: Gate decomposition!



Determination of the ground state representation

➢ After Trotter-Suzuki expansion,

- In practice the central problem is how to update/renormalize the wavefunction after a small evolution step

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

G. Vidal, PRL **91**, 147902 (2003)

G. Vidal, Phys. Rev. Lett. 98, 070201 (2007).

H. C. Jiang, PRL 101, 090603 (2008)

There are 3 ways to deal with this:

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

✓ Use the local entanglement spectra (bond vector/field) as the environment

✓ Then update can be reduced to a local tree approximation which can be solved by SVD/HOSVD

◆ **A small trick:** to get SVD of A*B, we can firstly do SVD/QR of A and B separately,

$$\begin{aligned} AB &= (U_a \Lambda_a V_a^\dagger)(U_b \Lambda_b V_b^\dagger) \\ &= U_a(\Lambda_a V_a^\dagger U_b \Lambda_b) V_b^\dagger \end{aligned}$$

and then do SVD of the middle product,

$$\begin{aligned} &= U_a(U_c \Lambda_c V_c^\dagger) V_b^\dagger \\ &= (U_a U_c)\Lambda_c (V_b V_c)^\dagger \end{aligned}$$

This is nothing but the SVD of A*B!

Determination of the ground state representation

(2). Full update (Global variation)

find a PEPS which minimize the difference globally: $||\Psi_f\rangle - e^{-\tau H}|\Psi_i\rangle|$

$$f(|\Psi_f\rangle) = ||\Psi_f\rangle - |\Psi_i\rangle|^2 = \langle\Psi_f|\Psi_f\rangle + \langle\Psi_i\Psi_i\rangle - 2\langle\Psi_f|\Psi_i\rangle$$

$$NX = M^e$$

FU:
J. Jordan, et al, PRL 101, 250602 (2008)
M. Lubasch, et al., PRB 90, 064425 (2014)

Fast FU: (sequential picture)
H. N. Phien, et al, PRB 92, 035142 (2015)

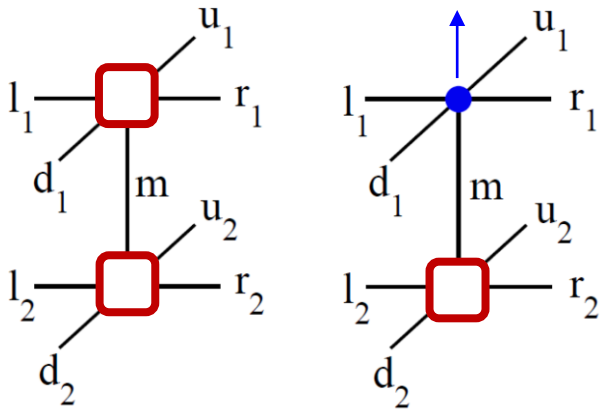
M^e : (D^4d, 1), the effective environment of X in the Mixed overlap network
N: (D^4d, D^4d), the effective environment of X-pair in the Norm network, in principal, positive definite

- The equation can be written equivalently in practice:

$$N_{l_1r_1u_1d_1m_1,l_2r_2u_2d_2m_2} = \tilde{N}_{l_1r_1u_1d_1,l_2r_2u_2d_2} \otimes \delta_{m_1,m_2}$$

the actual equation becomes: $\tilde{N}X = M$

Non-truncated

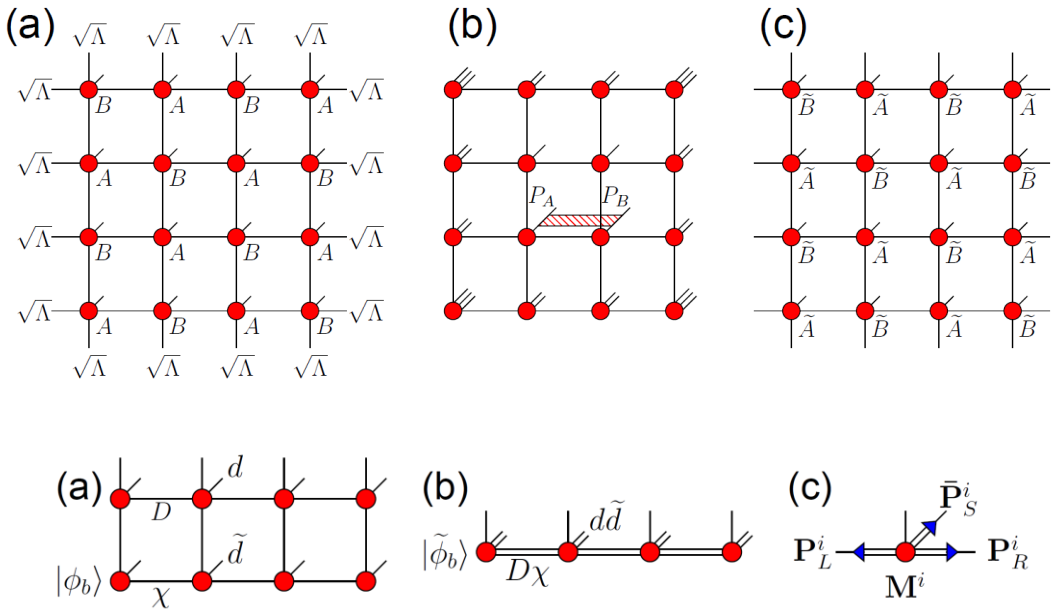


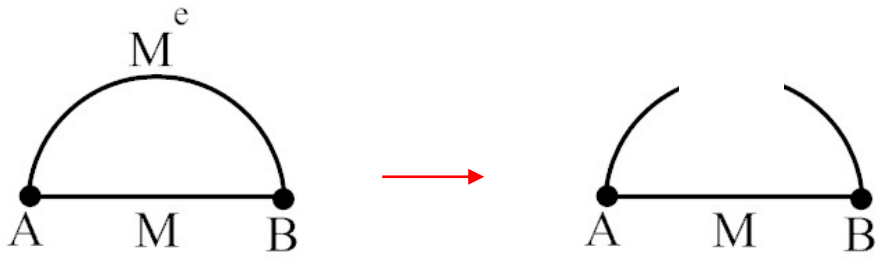
(3). Cluster update

Ling Wang and FV, arXiv. 1110.4362

Single-Layer update: I. Pizorn, Phys. Rev. A 83, 052321 (2011)

- ✓ Choose a small cluster containing the targeted system
- ✓ Use the local entanglement spectra (bond vector/field) as the environment of the cluster
- ✓ Then update can be reduced to a local optimization



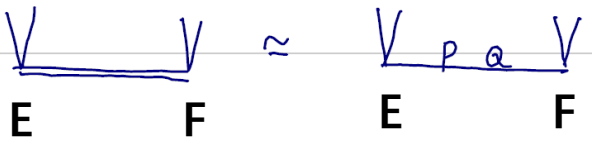


$$EF = EF\left[(EF)^{-1}EF\right] = E\left[F(EF)^{-1}E\right]F$$

$$EF = u\Lambda v^{+} \Rightarrow (EF)^{-1} = v\Lambda^{-1}u^{+}$$

$$\Rightarrow F(EF)^{-1}E = Fv\Lambda^{-1}u^{+}E = (Fv\Lambda^{-1/2})\cdot(\Lambda^{-1/2}u^{+}E) = PQ$$

$$\Rightarrow \quad \simeq$$



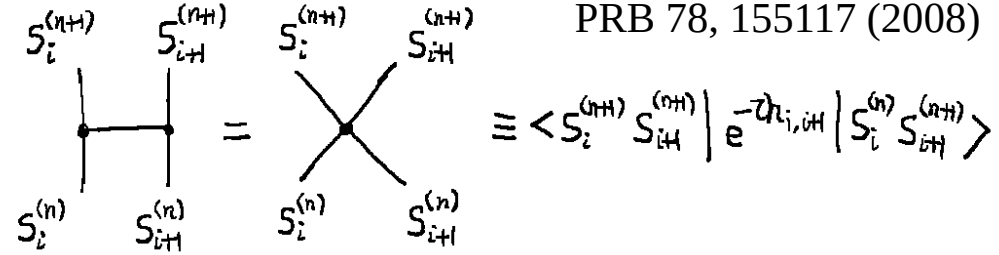
Essence: for convenience, use projector to realize SVD

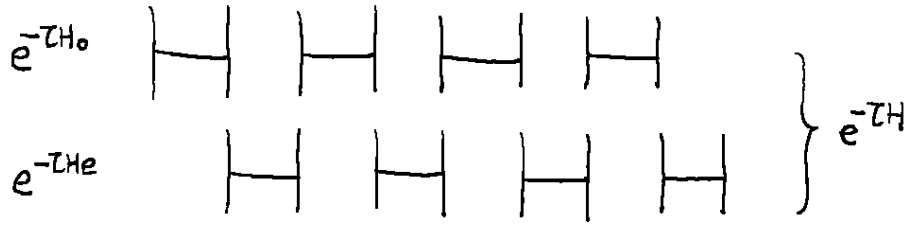
Time-evolving block decimation (TEBD)

PRL 91, 147902 (2003)
PRL 93, 040502 (2004)
PRL 98, 070201 (2007)
PRB 78, 155117 (2008)

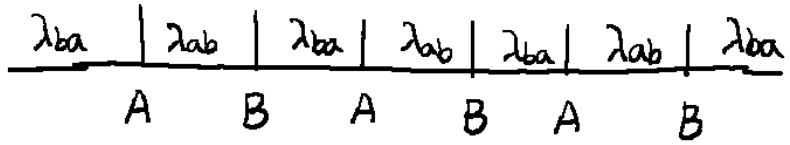
$H = H^e + H^o$, $H_e = \sum_{i\in e} h_{i,i+1}$, $H_o = \sum_{i\in o} h_{i,i+1}$

$e^{-\beta H} = (e^{-\tau H})^M \simeq (e^{-\tau H_o} e^{-\tau H_e})^M$

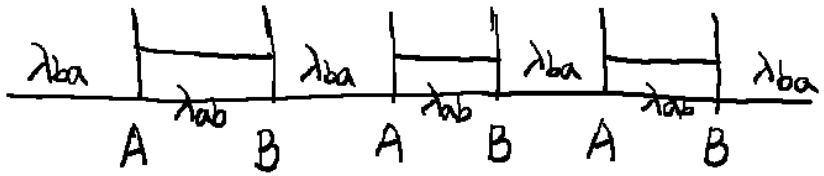




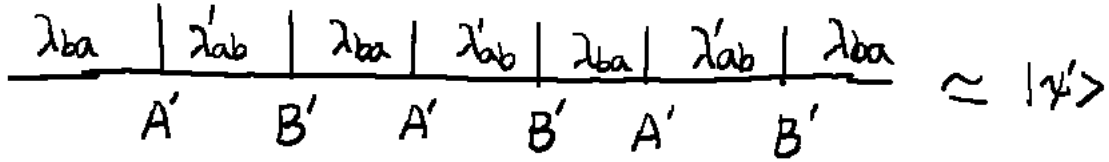
$|\psi_o\rangle$ as an MPS: (with entanglement spectra λ_{ab}, λ_{ba}; OBC)



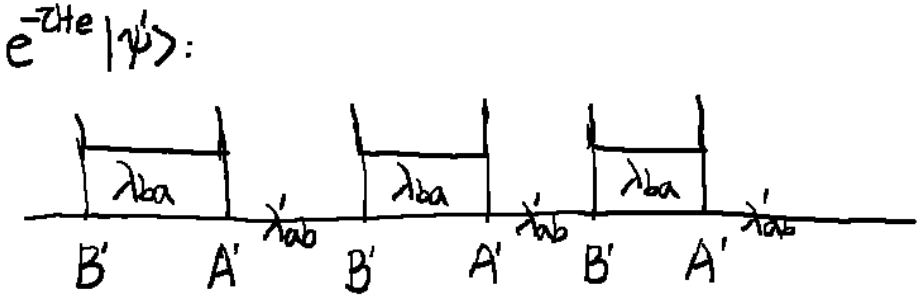
$e^{-\tau H_e}|\psi_o\rangle$:



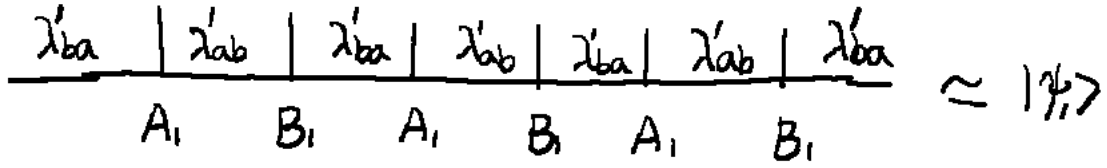
truncation:



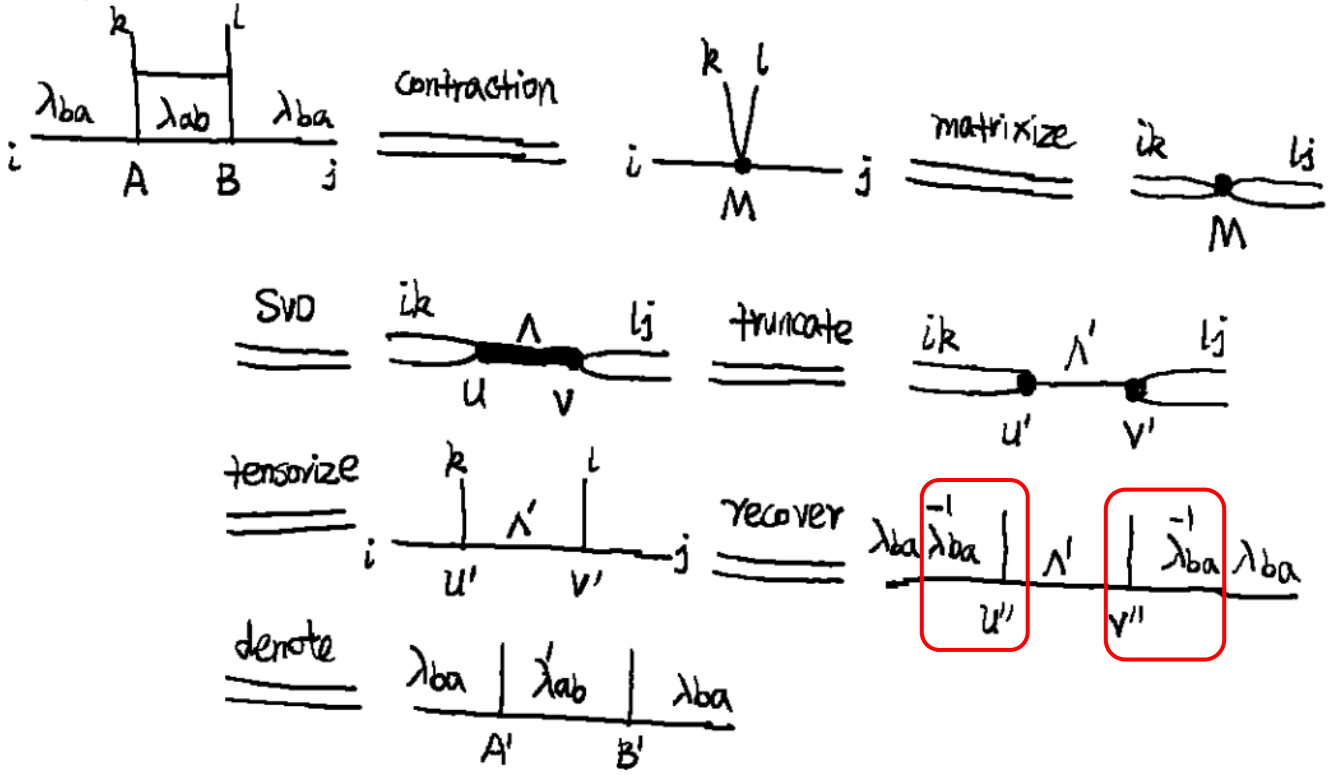
Time-evolving block decimation (TEBD)



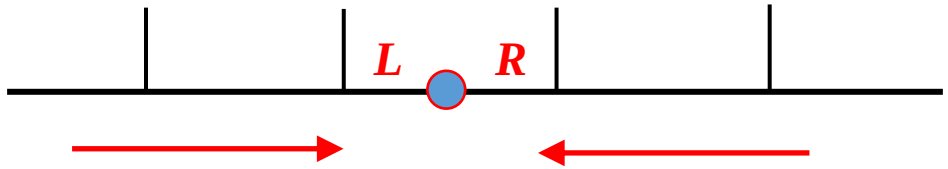
Truncate



Simple update:



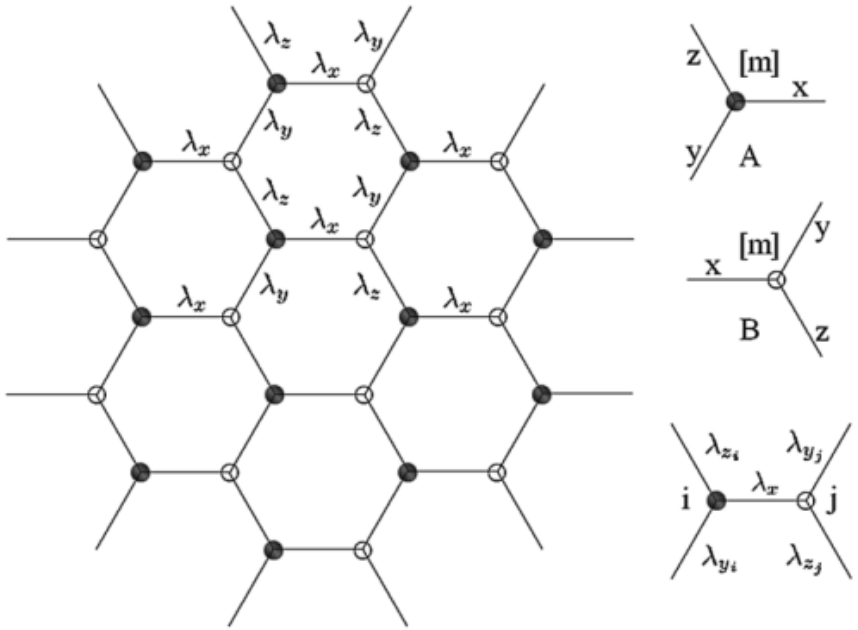
1. $e^{-\tau h} \sim 1$ when τ is small
2. Generally: canonicalization



Simple update of PEPS: honeycomb lattice

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

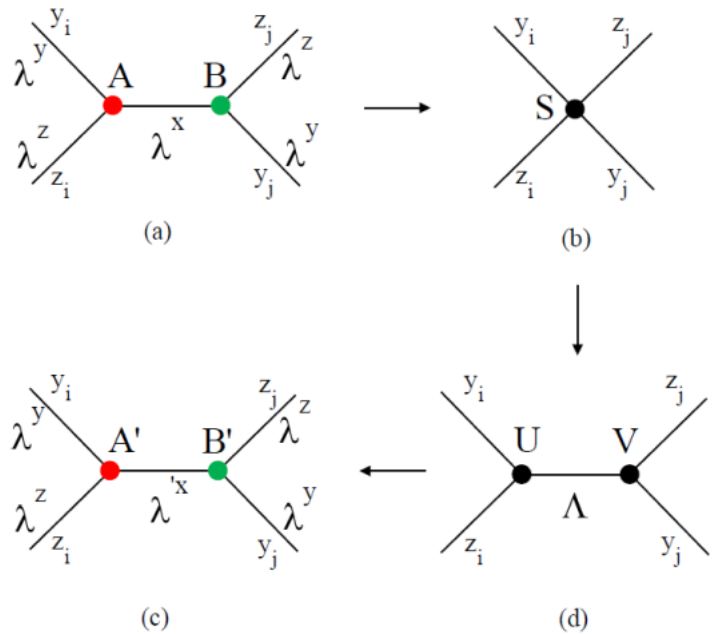
$$H = H_x + H_y + H_z, \qquad H_\alpha = \sum_{i \in \text{black}} H_{i,i+\alpha} \qquad (\alpha = x, y, z).$$



$$|\Psi\rangle = Tr \prod_{i \in b, j \in w, \langle ij \rangle} \lambda_i^x \lambda_i^y \lambda_i^z A_{x_i y_i z_i}[m_i] B_{x_j y_j z_j}[m_j] |m_i m_j\rangle$$

将投影算符分为三个方向，交替投影

$$e^{-\tau H} \approx e^{-\tau H_z} e^{-\tau H_y} e^{-\tau H_x} + o(\tau^2).$$

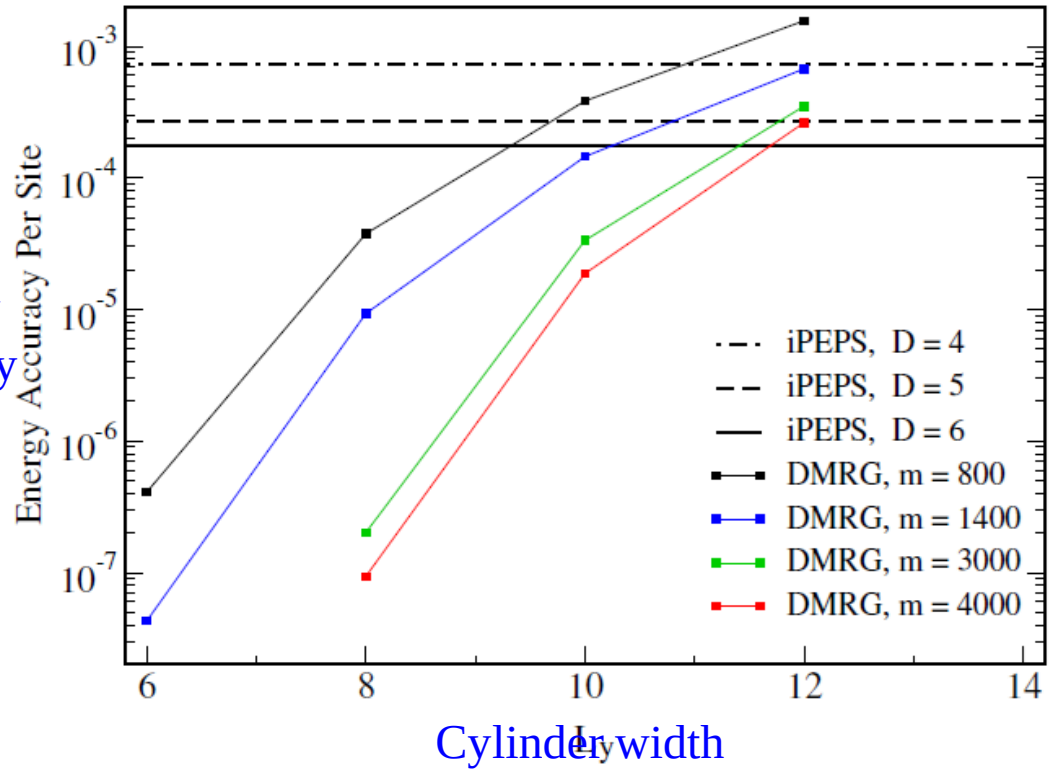


tensor network state has achieved great success

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

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

Energy accuracy



DMRG:
jumps fast as width(Ly) grows

PEPS:
improves as D grows

6 > 4000

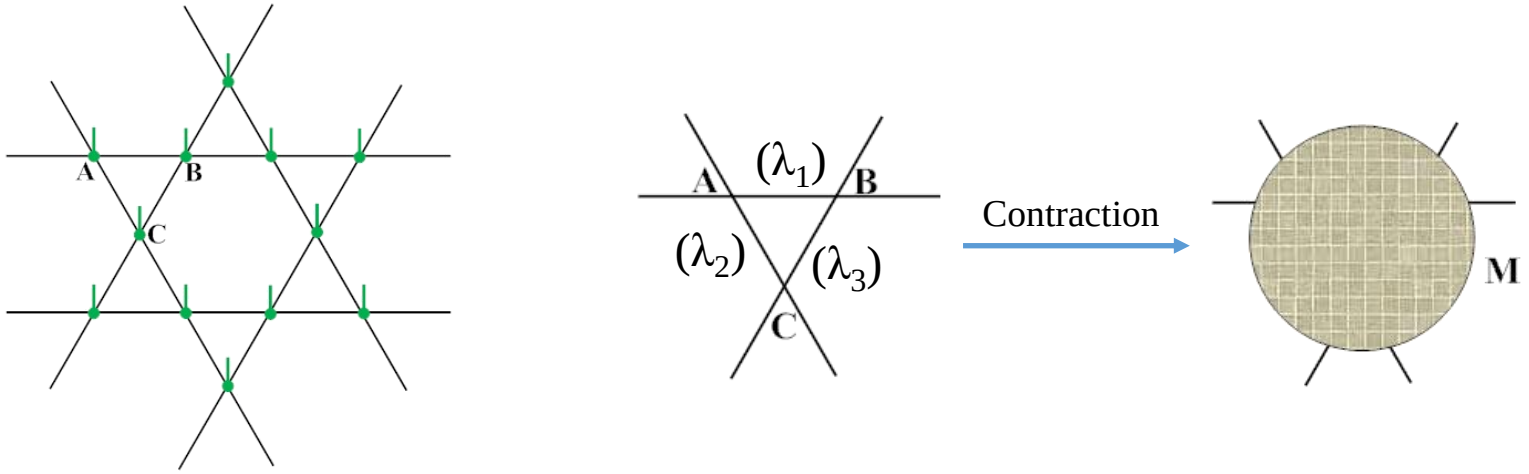
Augmented DMRG with disentanglers

CPL (EL) 40, 057102 (2023) by M.P.Qin's Group

Note:
iPEPS reference: VMC extrapolation in Sandvik PRB 56, 11678(1997)
DMRG reference: DMRG extrapolation in truncation error at given size.

Frustrated situation

- Conventional Ansatz: Only emphasized local pair entanglement, but can not effectively describe the many-body entanglement, e.g., among spins in a small triangle/simplex
- For the Kagome Heisenberg model: when local update is employed, ***hidden frustration*** occurs:
  - ✓ Each local bond spectra λ has nearly full two-fold degeneracy.

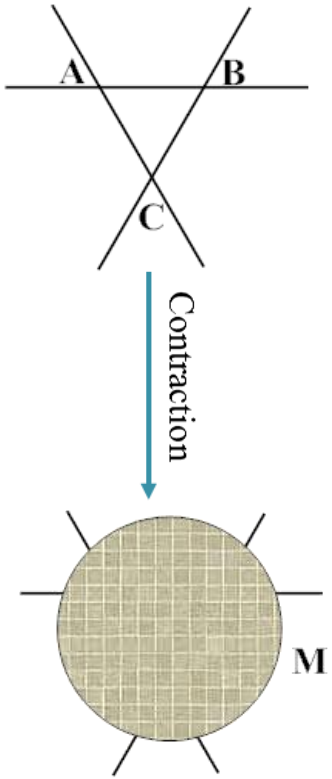


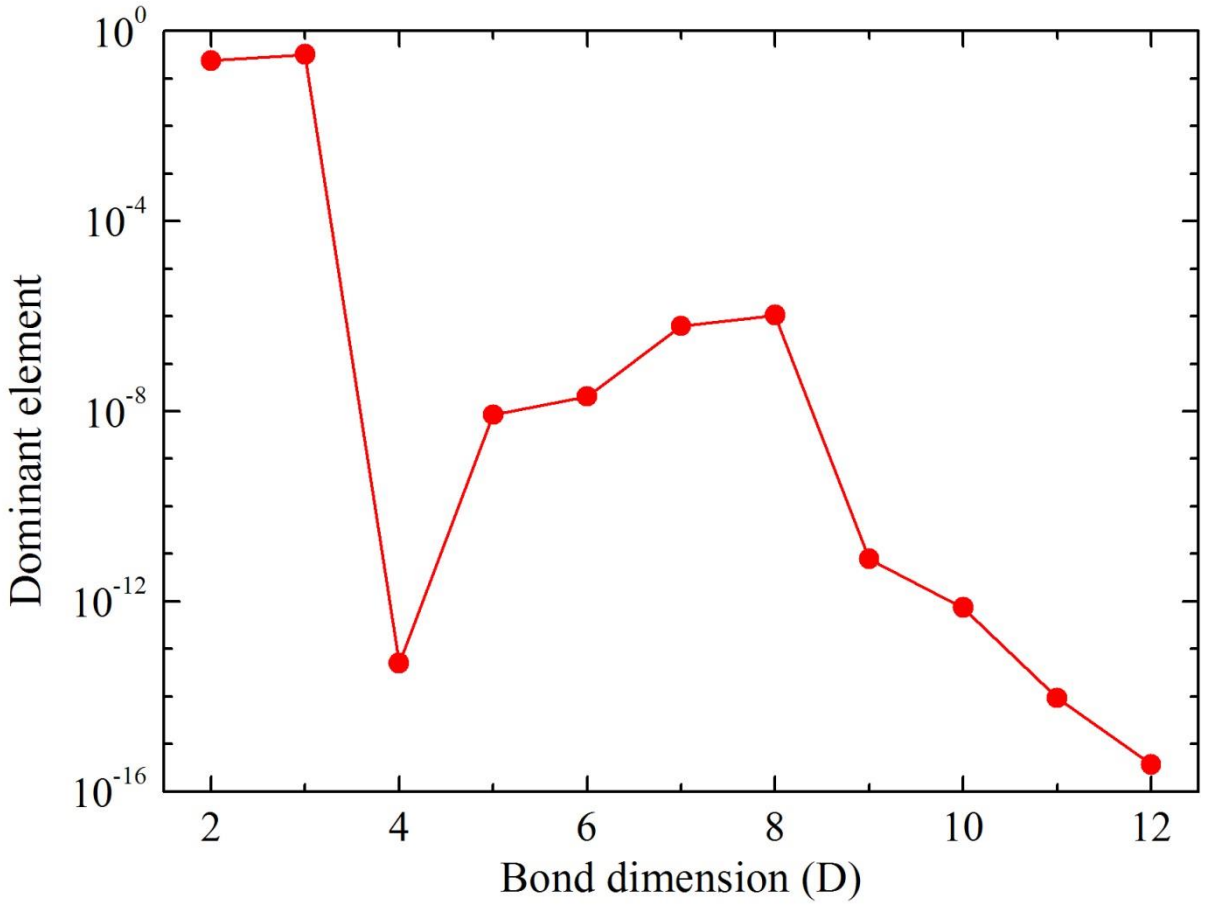
  - ✓ information cancelation:

A, B, C has dominant element 1 → M has dominant element << 1

Information cancelation

The fact is:





- ✓ pair entanglement is not so important in this system

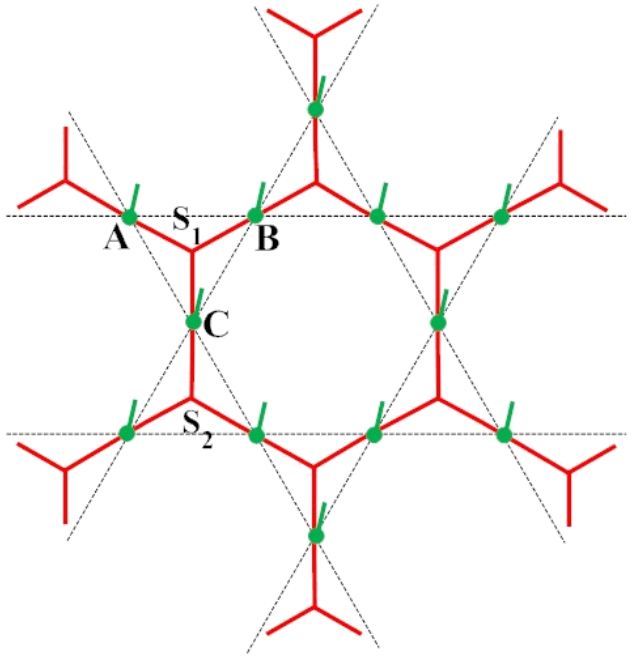
  the basis relevant for different pairs almost orthogonal/cancel with each other: hidden frustration

- ✓ Indication: not an effective representation for frustrated system.

Solution: generalization pair entanglement to simplex entanglement
Projected entangled ***simplex*** states(PESS) ansatz

ZYXie, etal., PRX 4, 011025(2014).

Simplex ~ possible building block, such as triangle for Kagome



- Introduce a simplex tensor S: the triangle/simplex entanglement, instead of pair
- defined on unfrustrated lattice:

  honeycomb, no hidden frustration here!
- Only tree approximation is needed when

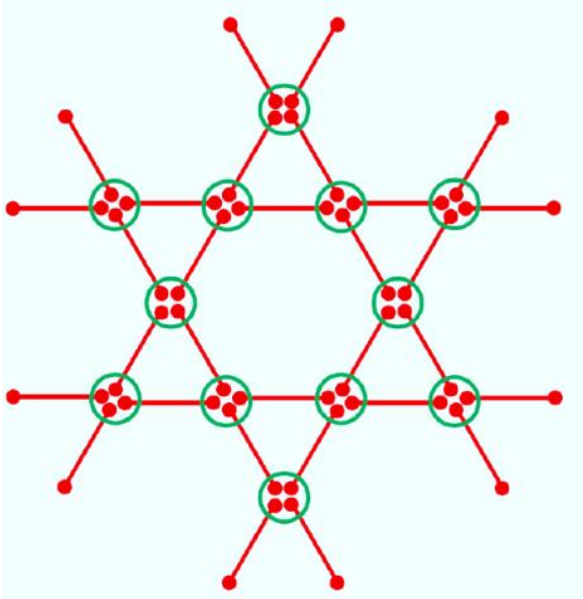
  local update is performed: low cost!

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

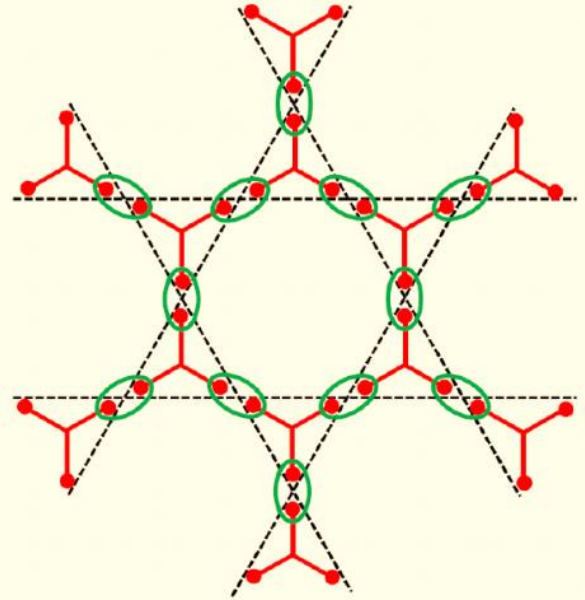
Exact examples: to show explicitly the difference

- **Spin-2** AKLT state: 2: 4*1/2, 1/2+1/2: pair singlet
- **Spin-2** Simplex Solid (SS): 2: 2*1, 1+1+1: simplex singlet

D. P. Arovas, PRB **77**, 104404 (2008)
They two are the same in this case



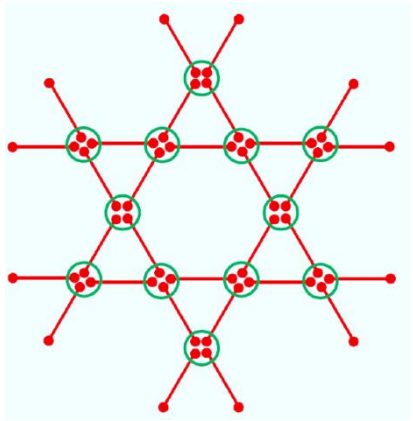
PEPS for AKLT



PESS for SSS

A: Projection tensor, C-G matrix, map virtual to physical
S: Simplex tensor, a fully anti-symmetric tensor, singlet entanglement

- PEPS representation: spin-2 AKLT state on Kagome lattice



(1). Represent a spin-2 in terms of 4 vspin-1/2 (D=2).

(2). Vspins satisfy Bond singlet configuration.

$$|\alpha_0\beta_1\rangle - |\alpha_1\beta_0\rangle = \sum_{\alpha\beta} |\alpha\rangle\epsilon_{\alpha\beta}|\beta\rangle, \epsilon_{01} = -\epsilon_{10} = 1$$

(3). Project virtual product space to the physical **spin-2** space:

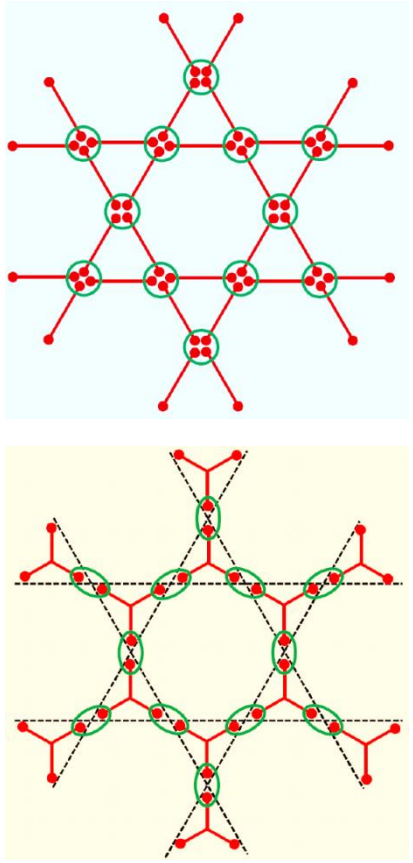
$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = 0_2 \oplus 1_3 \oplus 2 \to 2$$

$$P_2 = |S_2\rangle\langle S_2| = \sum_{\sigma=-2}^{2} |\sigma\rangle\langle\sigma|$$

$$= \sum_{\sigma=-2}^{2} \sum_{\alpha\beta\gamma\delta} |\sigma\rangle\langle\sigma|\alpha\beta\gamma\delta\rangle\langle\alpha\beta\gamma\delta|$$

$$= \sum_{\sigma=-2}^{2} A_{\alpha\beta\gamma\delta}[\sigma]|\sigma\rangle\langle\alpha\beta\gamma\delta|$$

➢ PESS: spin-2 simplex solid state on Kagome lattice



(1). Represent a spin-2 in terms of 2 vspin-1 (D=3).

(2). Vspins satisfy simplex singlet configuration.

$$|S_0\rangle = \sum_{\alpha\beta\gamma} \epsilon_{\alpha\beta\gamma} |\alpha\rangle|\beta\rangle|\gamma\rangle$$

(3). Project virtual space to the physical **spin-2** space:

$$1 \otimes 1 = 0 \oplus 1 \oplus 2 \to 2$$

$$P_2 = |S_2\rangle\langle S_2| = \sum_{\sigma=-2}^{2} |\sigma\rangle\langle\sigma|$$

$$= \sum_{\sigma=-2}^{2} \sum_{\alpha\beta} |\sigma\rangle\langle\sigma|\alpha\beta\rangle\langle\alpha\beta|$$

$$= \sum_{\sigma=-2}^{2} A_{\alpha\beta}[\sigma]|\sigma\rangle\langle\alpha\beta|$$

Bond spin cannot be 2+2=4

$$P_4 = \sum_{n=0}^{4} c_n T^n \qquad P_4|i\rangle = \sum_{n=0}^{4} c_n T^n |i\rangle = \sum_{n=0}^{4} c_n [i(i+1)]^n |i\rangle$$

$$P_4|0\rangle = 0, P_4|1\rangle = 0, P_4|2\rangle = 0, P_4|3\rangle = 0, \langle 4|P_4|4\rangle = 1$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 4 & 8 & 16 \\ 1 & 6 & 36 & 6^3 & 6^4 \\ 1 & 12 & 12^2 & 12^3 & 12^4 \\ 1 & 20 & 20^2 & 20^3 & 20^4 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$P_4(ij) = -\frac{1}{280} T_{ij} + \frac{3}{1120} T_{ij}^2 - \frac{1}{2016} T_{ij}^3 + \frac{1}{40320} T_{ij}^4$$

$$T_{ij} \equiv (S_i + S_j)^2 = S_i^2 + S_j^2 + 2S_i S_j = 12 + 2S_i S_j$$

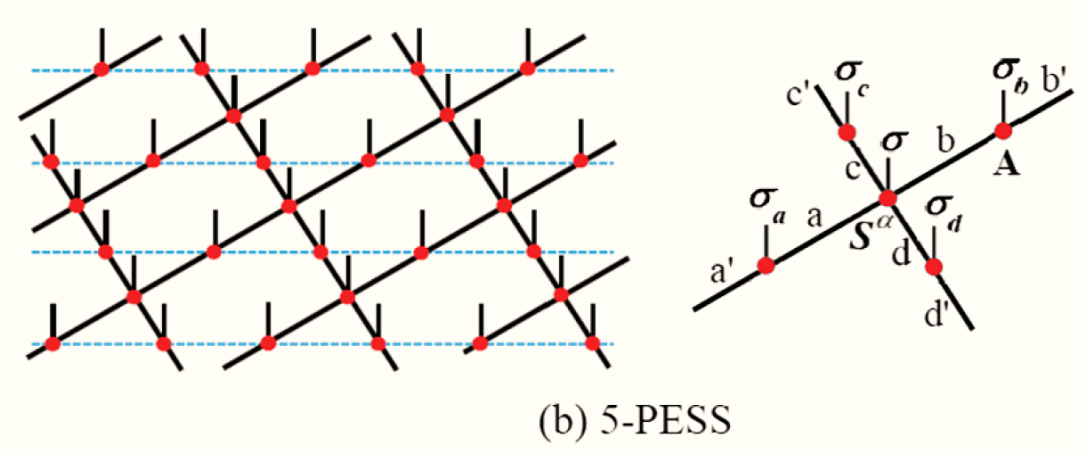
- If three-body interaction are allowed, then physics is much more richer:

- arbitrary non-negative linear combination of {P4, P5, P6}, since simplex spin cannot be larger than 1+1+1=3

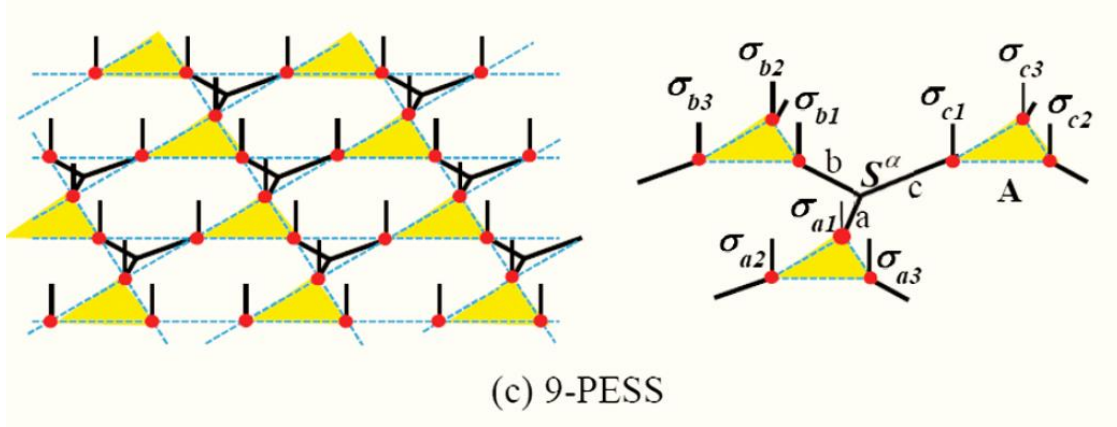
$$H = \sum_{\alpha} (J_4 P_{\alpha,4} + J_5 P_{\alpha,5} + J_6 P_{\alpha,6})$$

$$P_{ijk} = \sum_{n=0}^{6} c_n T_{ijk}^n \quad \text{with} \quad T_{ijk} \equiv (S_i + S_j + S_k)^2$$

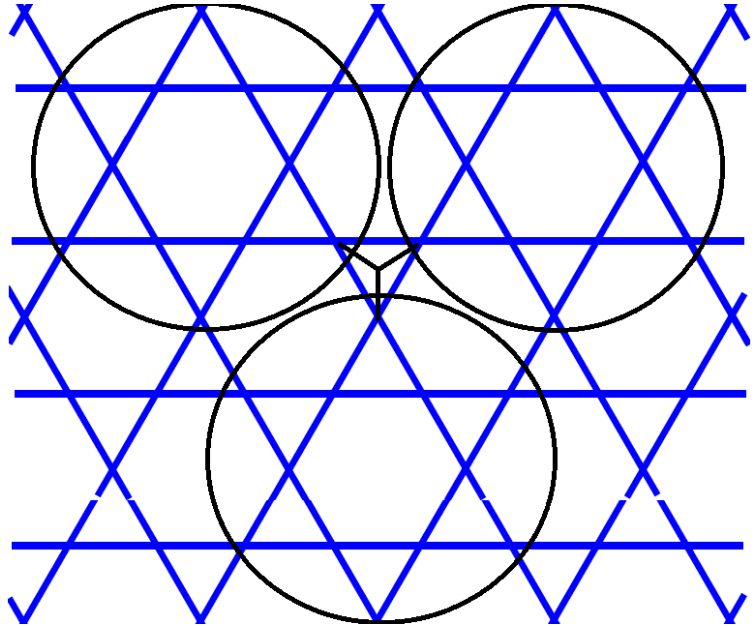
***n*-PESS**: *n*-body entanglement is described by a sinlge simplex tensor $\boldsymbol{S}$



(b) 5-PESS

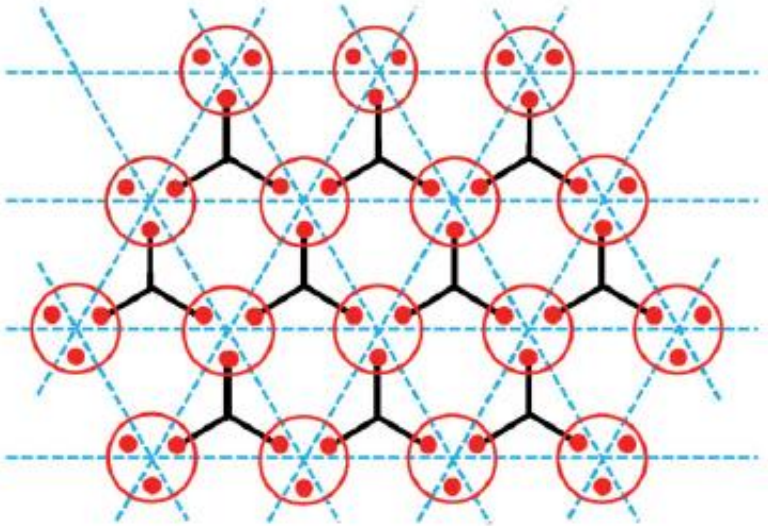


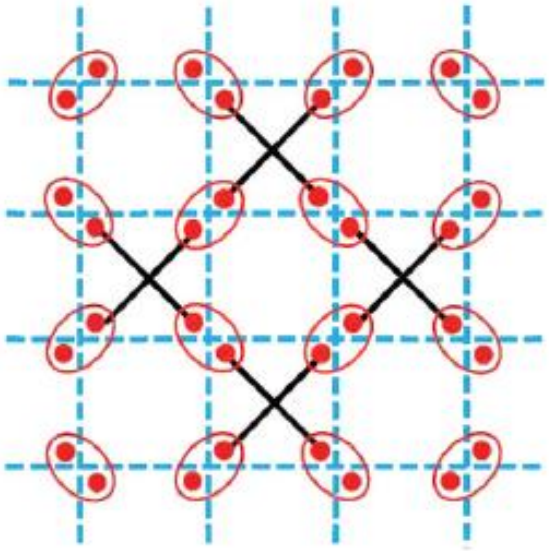
(c) 9-PESS

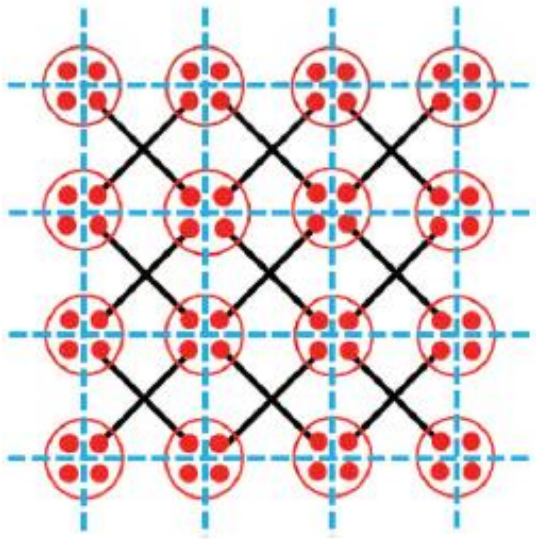


36-PESS

PESS on Other lattice

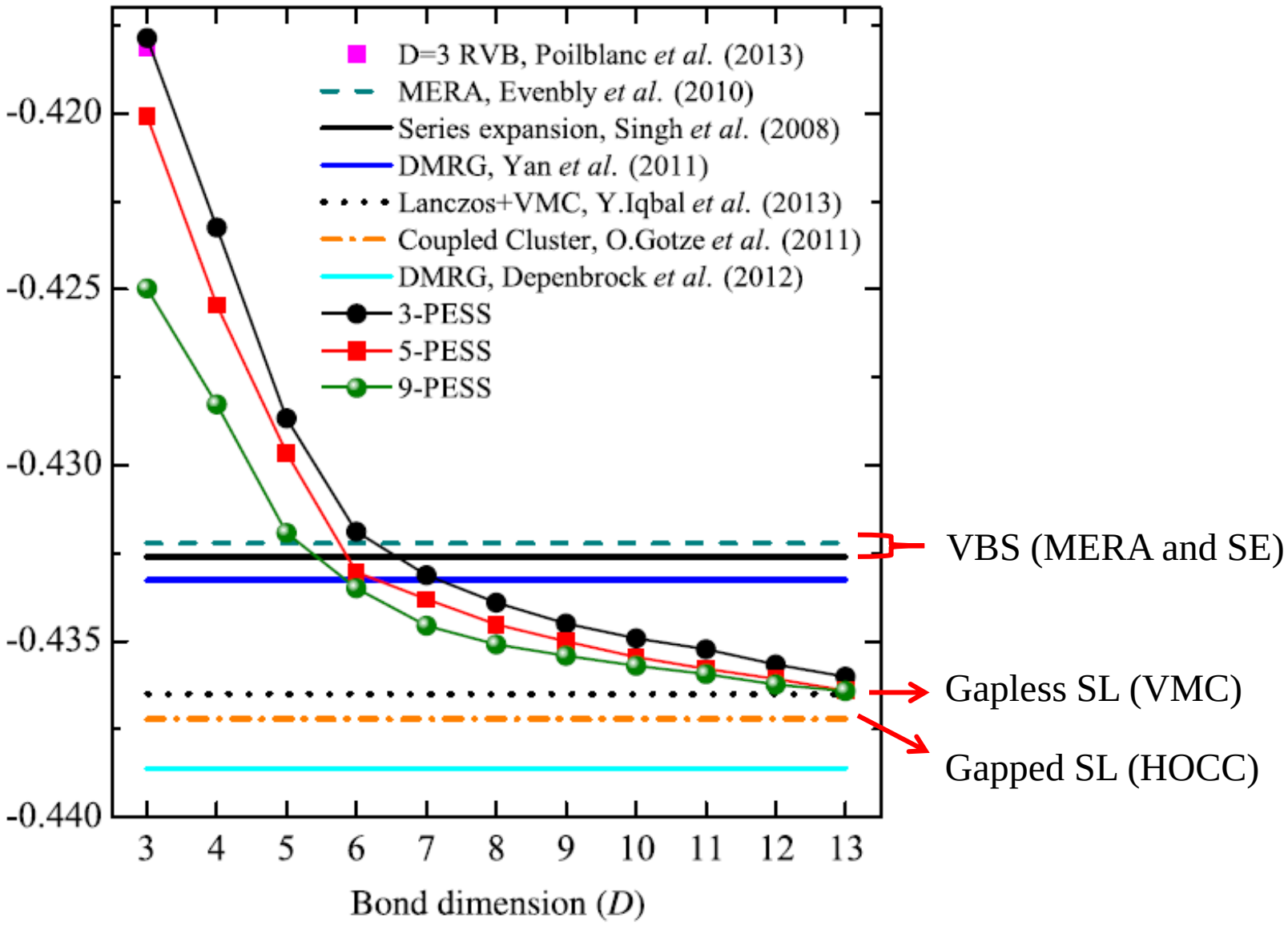






With D up to 13

Our group, PRX 4, 011025(2014).



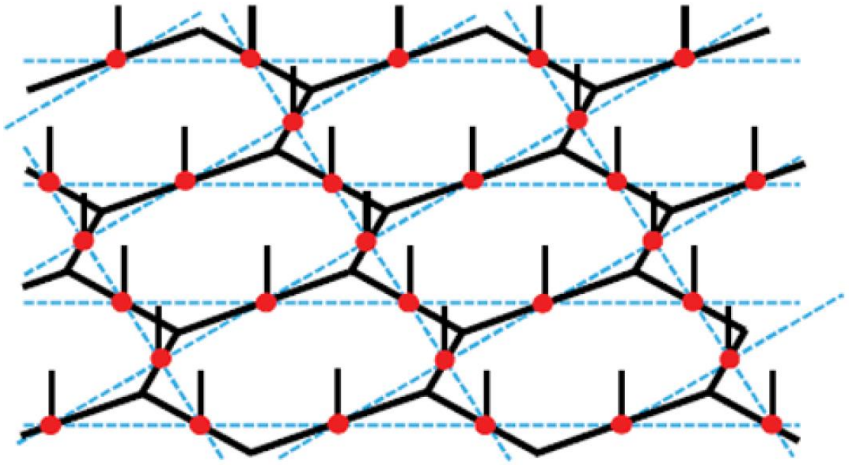
Simple update in PESS as an example

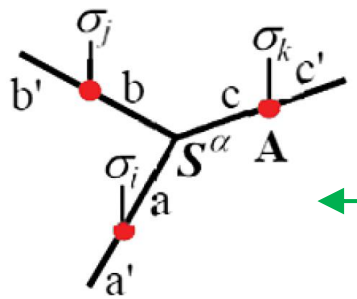
Replace the lambda into simplex tensor (as effective lambda)

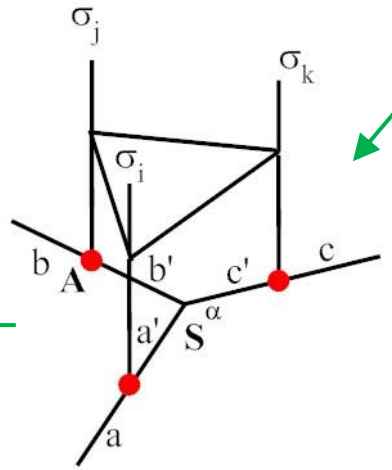
$$e^{-\beta H} = (e^{-\tau H})^M \approx (e^{-\tau H_\nabla} e^{-\tau H_\Delta} + O(\tau^2))^M, \quad (M = \beta/\tau)$$

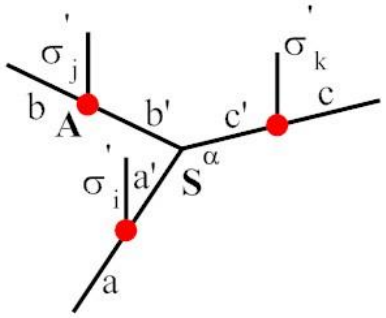
$$e^{-\tau H_\nabla} |\Psi_0\rangle = \mathrm{Tr}(\ldots T^{\alpha_\nabla}_{a\sigma_i, b\sigma_j, c\sigma_k} S^{\beta_\Delta}_{ade} \ldots) |\ldots \sigma_i \sigma_j \sigma_k \ldots\rangle$$

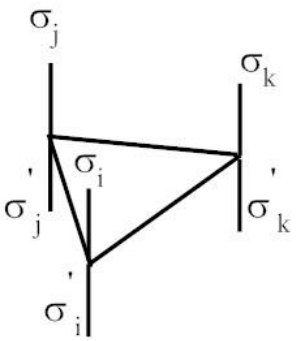
$$T^{\alpha_\nabla}_{a\sigma_i, b\sigma_j, c\sigma_k} = \sum_{\sigma_i' \sigma_j' \sigma_k' a' b' c'} \langle \sigma_i \sigma_j \sigma_k | e^{-\tau H_{\nabla\alpha}} | \sigma_i' \sigma_j' \sigma_k' \rangle \; S^{\alpha_\nabla}_{a' b' c'} A_{a' a}[\sigma_i'] A_{b' b}[\sigma_j'] A_{c' c}[\sigma_k']$$





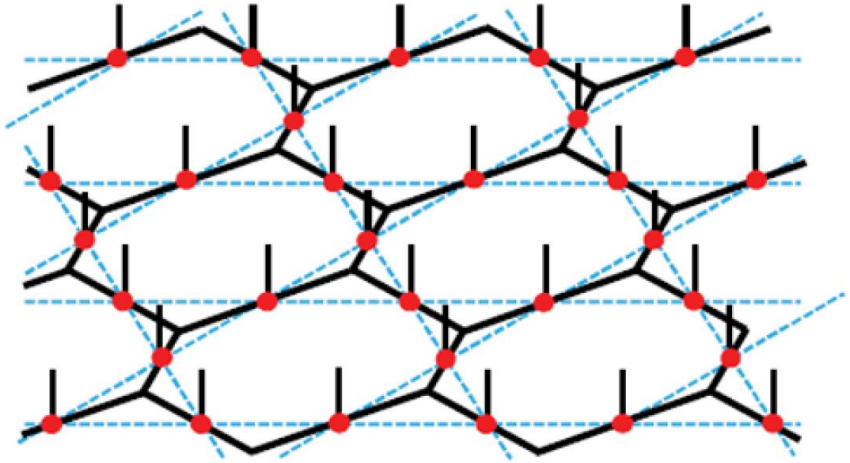


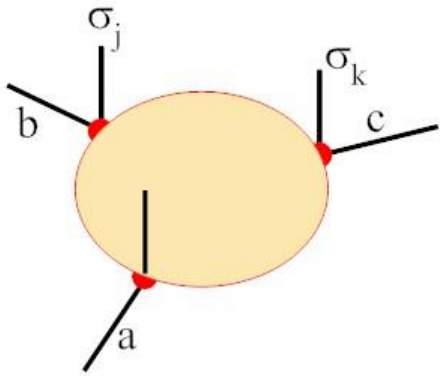


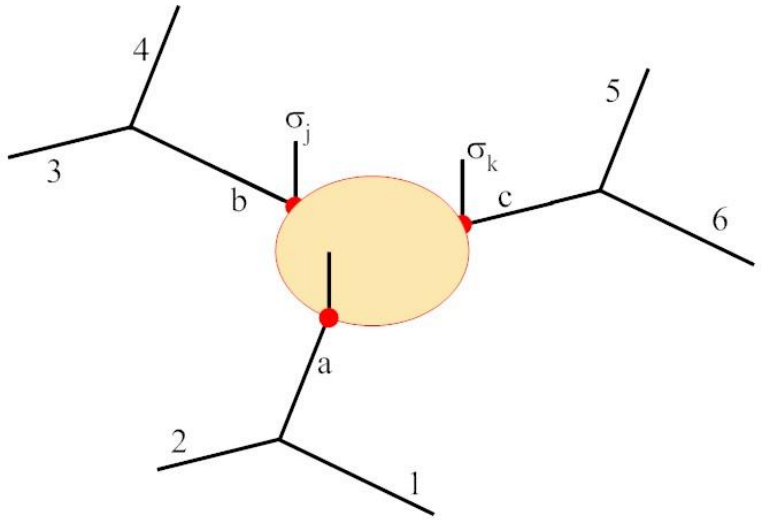


To construct the local environment, i.e., simplex tensor

$$\tilde{T}^{\alpha}_{12\sigma_i,34\sigma_j,56\sigma_k} = \sum_{abc} T^{\alpha}_{a\sigma_i,b\sigma_j,c\sigma_k} S^{\beta}_{a12} S^{\beta}_{b34} S^{\beta}_{c56}$$







Rank is too high to deal with ….

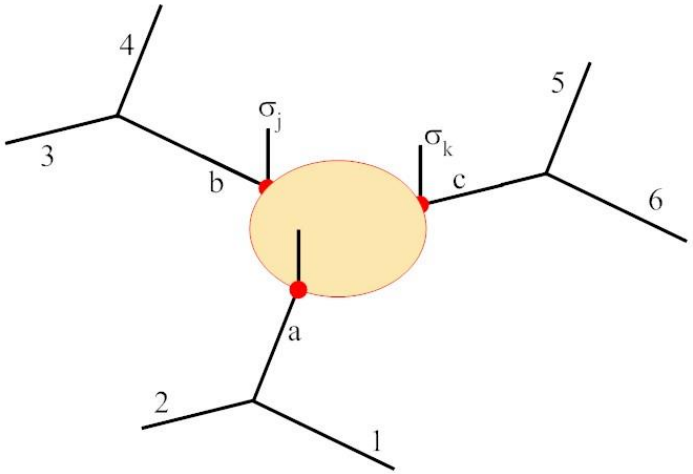
Fortunately, the HOSVD of the high-rank tensor, can be obtained by two steps equivalently!

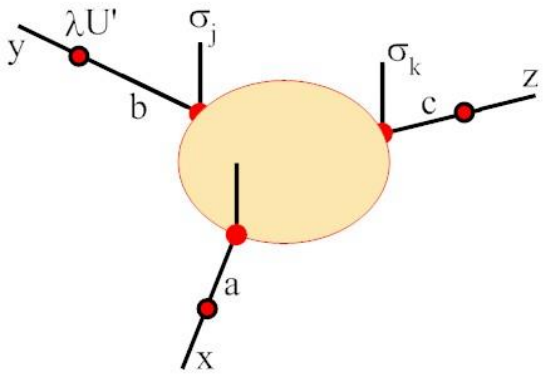
- Do SVD of environment simplex $S^{\beta}_{a'12} = \sum_{x=1}^{D} U^{\beta}_{a,x} \lambda_x V^{\beta}_{12,x}$
- Construct another low-rank tensor, and HOSVD, finally determine everything from this.

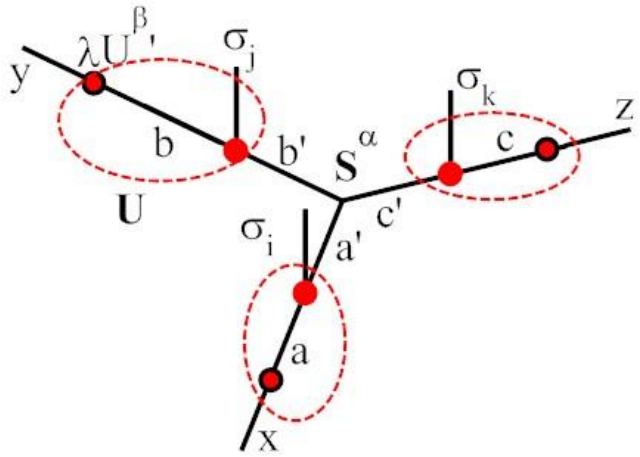
$$\bar{T}^{\alpha}_{x\sigma_i,y\sigma_j,z\sigma_k} = \sum_{abc} T^{\alpha}_{a\sigma_i,b\sigma_j,c\sigma_k} \lambda_x \lambda_y \lambda_z U^{\beta}_{a,x} U^{\beta}_{b,y} U^{\beta}_{c,z} = \sum_{a'b'c'} C^{\alpha}_{a'b'c'} U_{x\sigma_i,a'} U_{y\sigma_j,b'} U_{z\sigma_k,c'}$$

$$\sum_{a} (U^{\beta}\lambda)_{a,x} A_{aa'}[\sigma_i] = U_{x\sigma_i,a'}$$

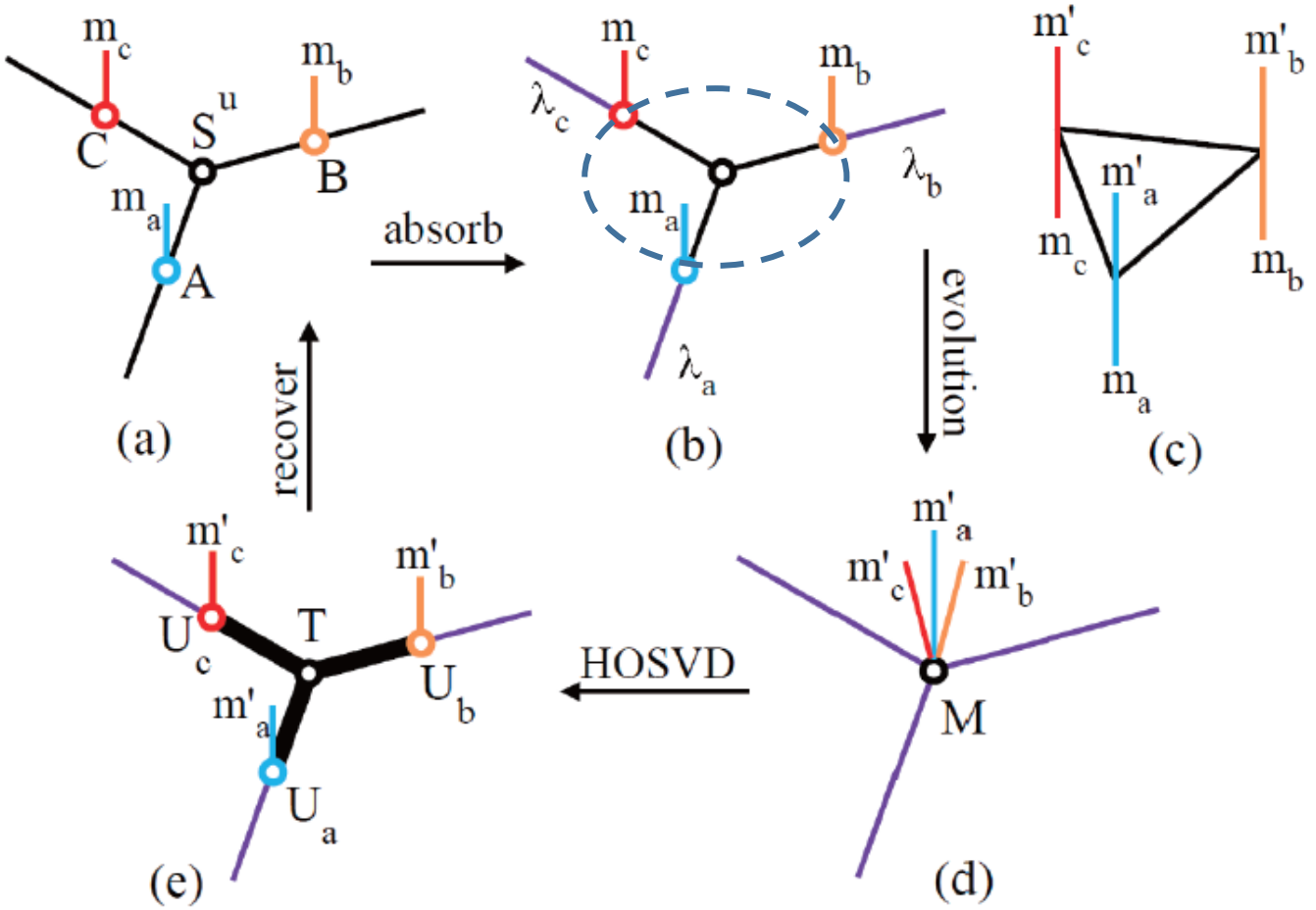
Important: unitary transformation does not change the core tensor, i.e., entanglement structure remains







Sketch of simple update



A small trick: for two-component trotter-Suzuki decomposition

$$e^{-\tau H} = e^{-\tau H_\nabla} e^{-\tau H_\Delta} + O(\tau^2)$$

$$e^{-\tau H} = e^{-\frac{\tau}{2} H_\nabla} e^{-\tau H_\Delta} e^{-\frac{\tau}{2} H_\nabla} + O(\tau^3)$$

Can we reduce the trotter error while avoiding the complexity of high order?

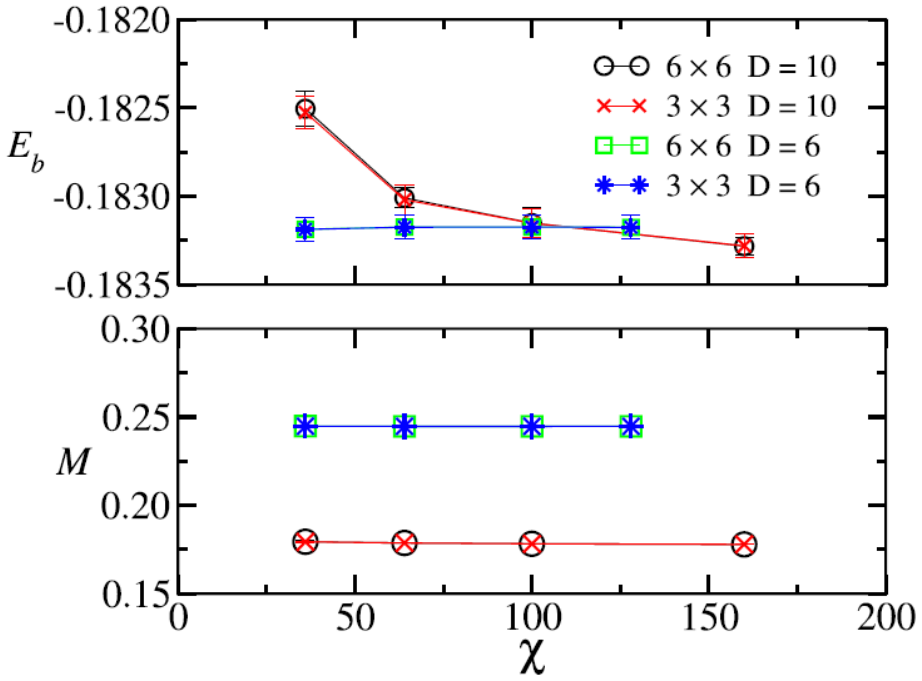
$$\left[e^{-\frac{\tau}{2} H_\nabla} e^{-\tau H_\Delta} e^{-\frac{\tau}{2} H_\nabla}\right]^n$$

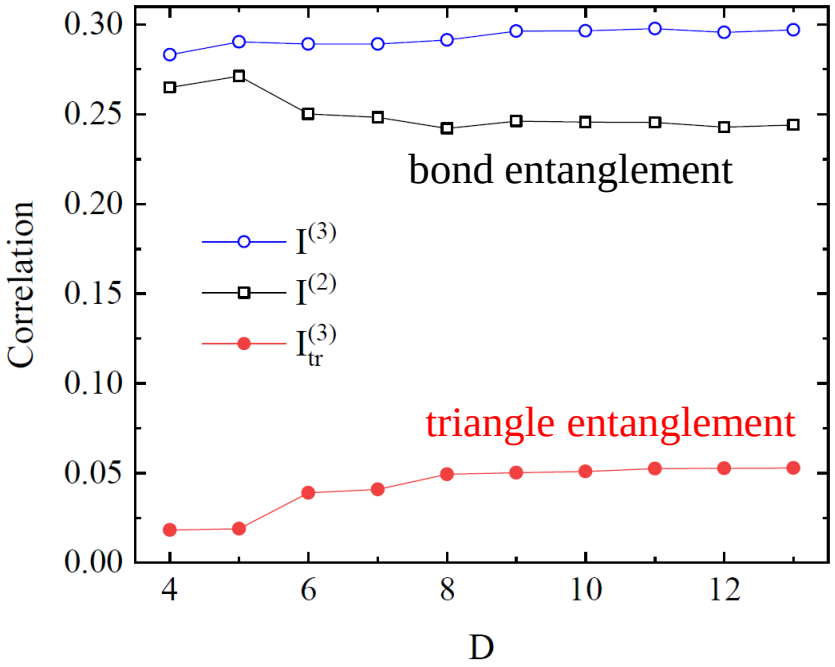
$$= e^{-\frac{\tau}{2} H_\nabla} \cdot \left[e^{-\tau H_\Delta} e^{-\frac{\tau}{2} H_\nabla} e^{-\frac{\tau}{2} H_\nabla}\right]^n \cdot e^{\frac{\tau}{2} H_\nabla}$$

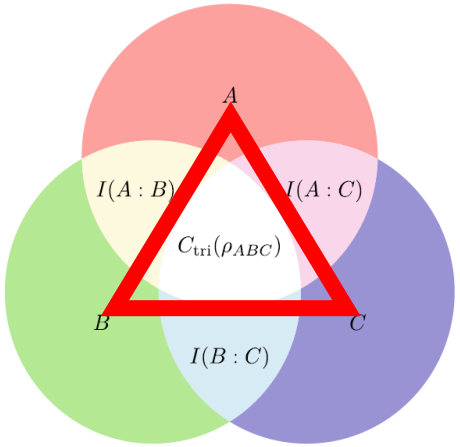
$$= e^{-\frac{\tau}{2} H\nabla} \cdot \left[e^{-\tau H_\Delta} e^{-\tau H_\nabla}\right]^n \cdot e^{\frac{\tau}{2} H_\nabla}$$

Indifferent, can be regard as different starting wf.

- Just do 1st Trotter decomposition as usual, but in the end add a half step evolution with half trotter!







$$\rho^{(3)}_{II'} = \sum_J |\Psi_{IJ}\rangle\langle\Psi_{I'J}|$$

$$S = -\mathrm{Tr}\rho\ln\rho$$

B. Zeng, *et al*, QI meets QM (2019): mutual information
R. Orus, *et al*, PRL 113, 257202 (2014): geometric entanglement

Independent of parameters: $D(\chi)$, unitcell-size

- 1st evidence: PESS can grasp many-body entanglement
- Three-body entanglement are indeed become stronger

$$\begin{aligned} I_{ab} &= S_a + S_b - S_{ab} \\ I^{(3)} &= S_a + S_b + S_c - S_{abc} \\ I^{(3)}_{tr} &= I^{(3)} - I_{ab} - I_{bc} - I_{ca} \end{aligned}$$

PRB 105, 184418 (2022)

3. Expectation value calculation

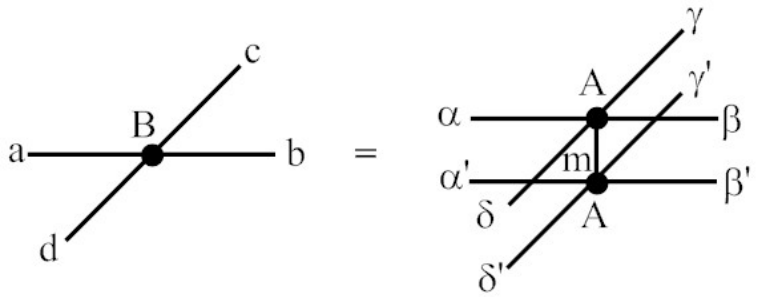
Expectation value calculation

- Calculate the expectation value via the formula:

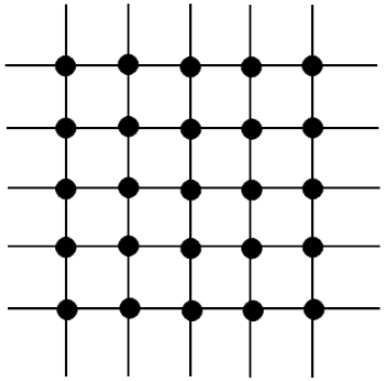
$$\langle O \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$|\Psi\rangle = \mathbf{Tr} \prod_i A^{(i)}_{\alpha\beta\gamma\delta}[m_i]|m_i\rangle$$

$$\langle \Psi | \Psi \rangle = \mathbf{Tr} \prod_i A^{(i)}_{\alpha\beta\gamma\delta}[m_i] A^{(i)}_{\alpha'\beta'\gamma'\delta'}[m_i] = \mathbf{Tr} \prod_i B^{(i)}_{abcd}$$



$$B_{abcd} \equiv \sum_m A_{\alpha\beta\gamma\delta}[m] A_{\alpha'\beta'\gamma'\delta'}[m]$$

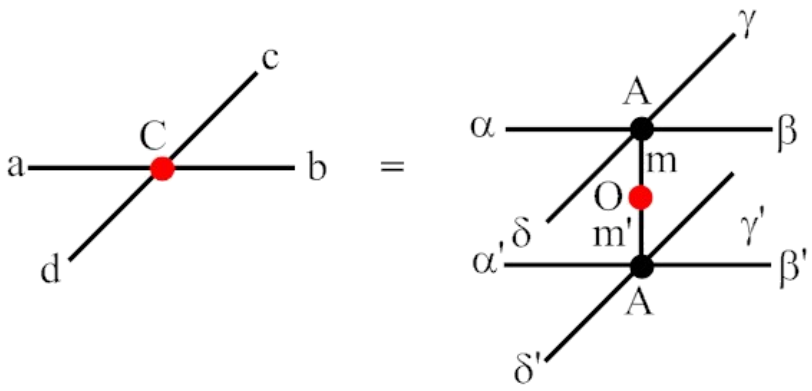


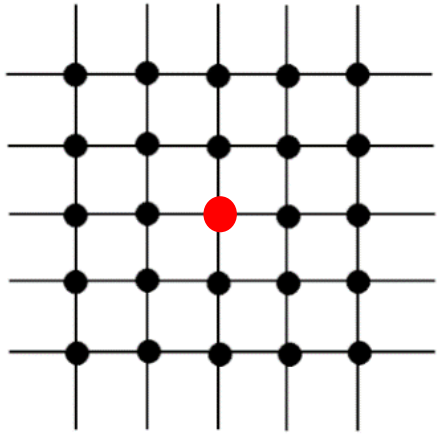
2D network scalar: identical to classical partition function!

About the numerator:

$$\langle\Psi|\hat{O}_j|\Psi\rangle = \mathbf{Tr}\sum_{m_j,m_j'} A^{(j)}_{\alpha\beta\gamma\delta}[m_j]A^{(j)}_{\alpha'\beta'\gamma'\delta'}[m_j]\langle m_j|\hat{O}_j|m_j'\rangle\prod_{i\neq j}B^{(i)}_{abcd}$$

$$= \mathbf{Tr}[C^j_{a'b'c'd'}\prod_{i\neq j}B^i_{abcd}]$$

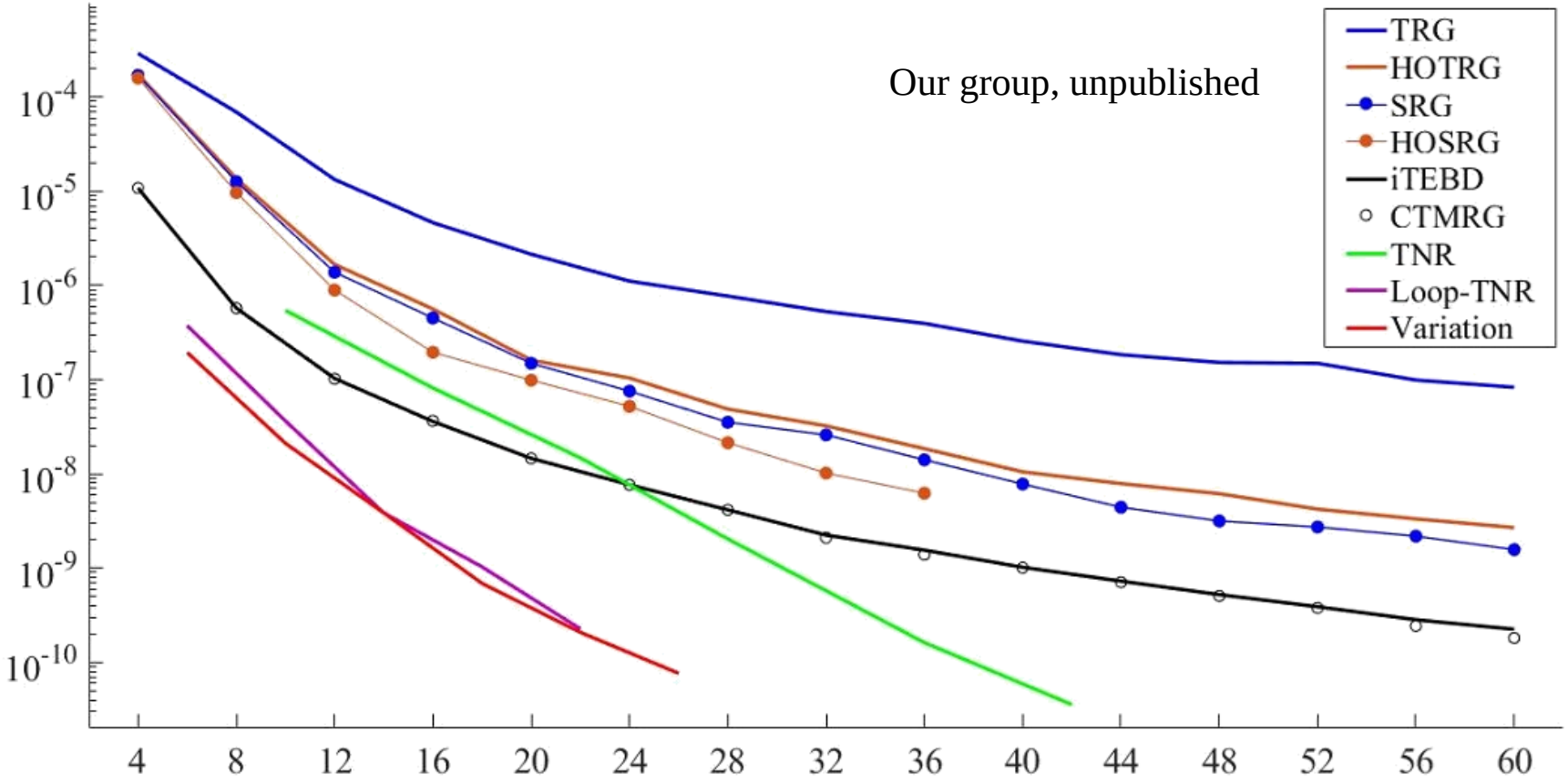




$$C_{abcd} \equiv \sum_{m,m'} A_{\alpha\beta\gamma\delta}[m]A_{\alpha'\beta'\gamma'\delta'}[m']\langle m|\hat{O}|m'\rangle$$

2D network scalar too!

Comparison at critical point of 2D Ising model



* Variation is intentionally avoided: nonlinear optimization
* Variation is very important in entanglement-related algorithms.

VUMPS: V. Z. Stauber, et al,
PRB 97, 045145 (2017)

Fixed-point CTMRG:
M. T. Fishman, et al.,
PRB 98, 235148 (2018)

Variational CTMRG
X. F. Liu, Y. F. Fu, et al.,
CPL (Express Letter)
39, 067502 (2022)

Honeycomb CTMRG
L. V. Lukin, and G. Sotnikov,
PRB 107, 054424 (2023)

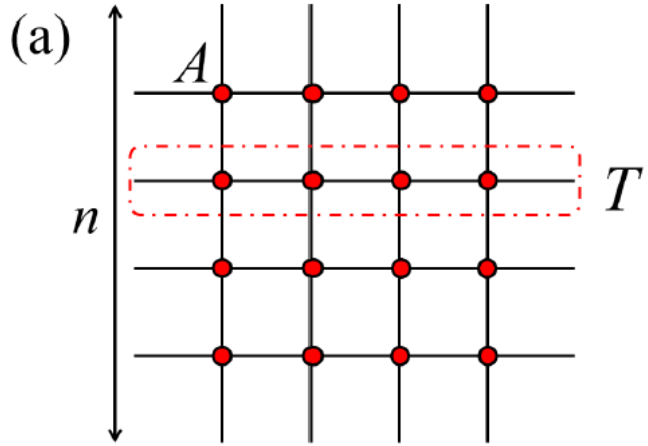
Apart from coarse-graining RG method …

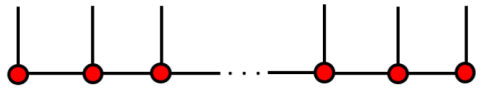
✓ Time Evolving Block Decimation(TEBD) / Boundary MPS： (equivalent to DMRG)

Target: effective MPS representation of the dominant eigenvector

PRL **91**, 147902 (2003)
PRB 78, 155117 (2008)

$$Z = \mathrm{Tr}T^n \simeq \lambda_{dom}^n$$



$\phi \approx$ 

Power method to get the fixed point: $T^n|\Psi\rangle \rightarrow |\Psi_{dom}\rangle$

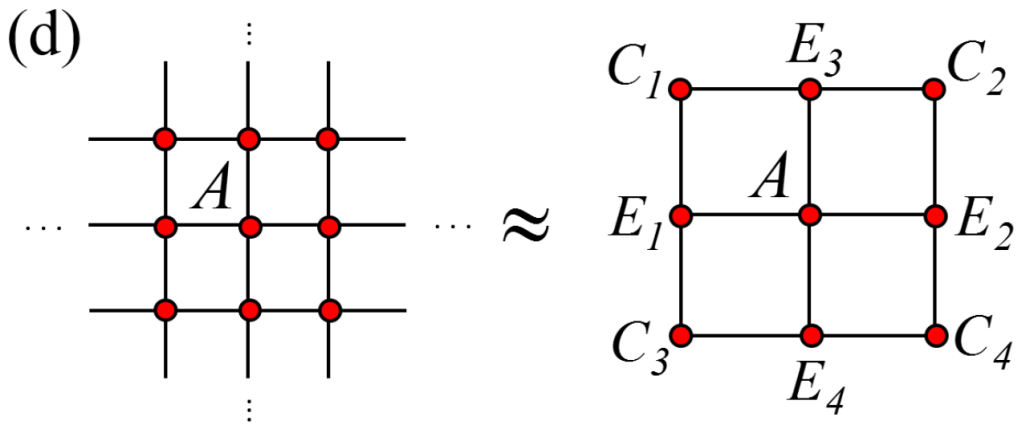
✓ Corner Transfer Matrix Renormalization Group(CTMRG)

Target: effective representation of the surrounding environment

JPSJ 65, 891 (1996)
PRB 80, 094403 (2009)
PRL 113, 046402 (2014)

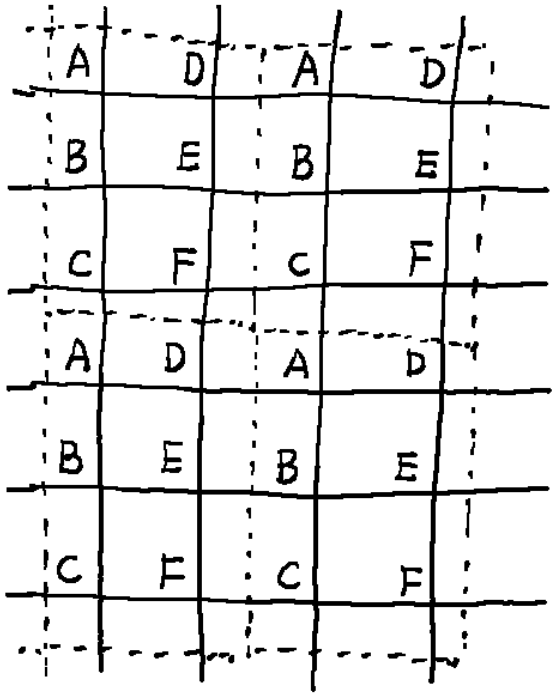
$$Z = \mathrm{Tr}(TT^e)$$

$$T^e = \{C_1, C_2, C_3, C_4, E_1, E_2, E_3, E_4\}$$

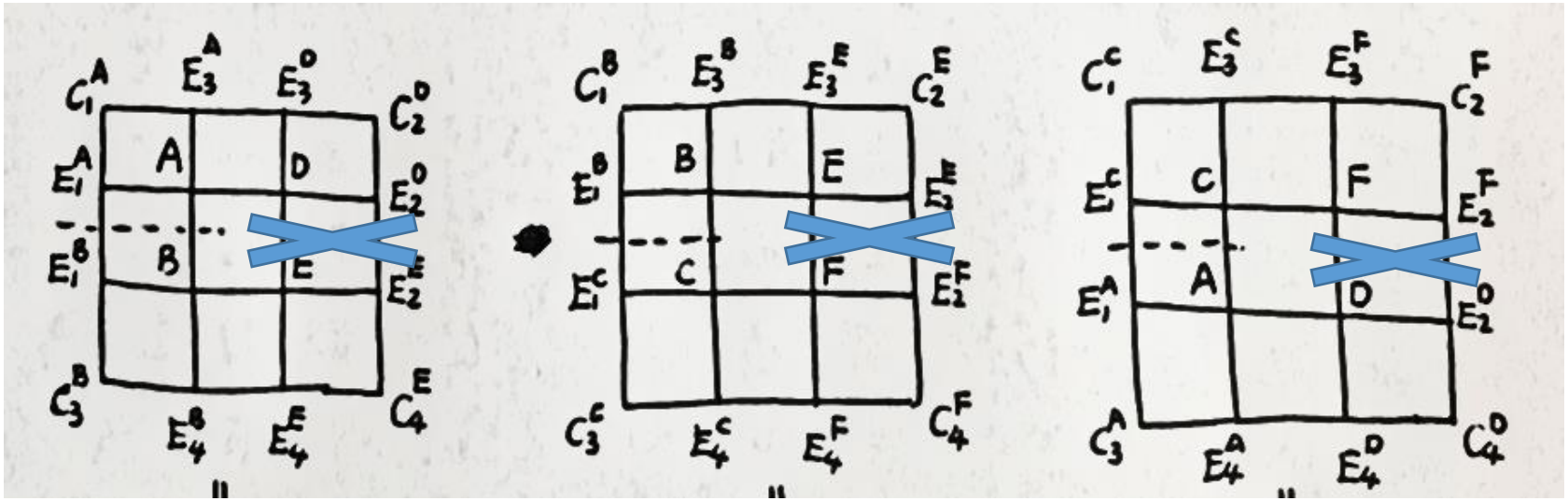


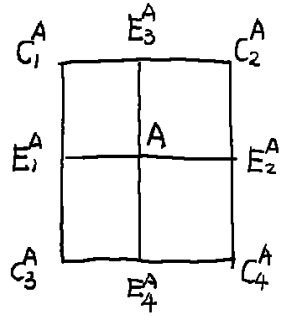
Enlarge the corner by absorbing A and then basis transformation, to get the fixed point

Practical CTMRG for 3 × 2 as an example

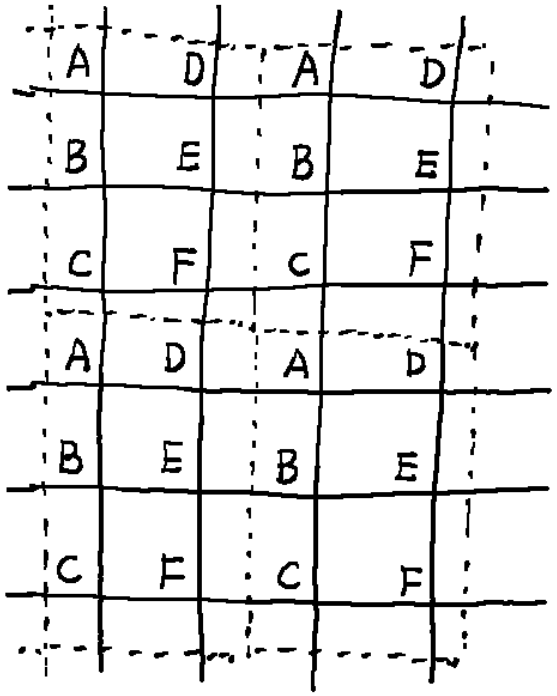


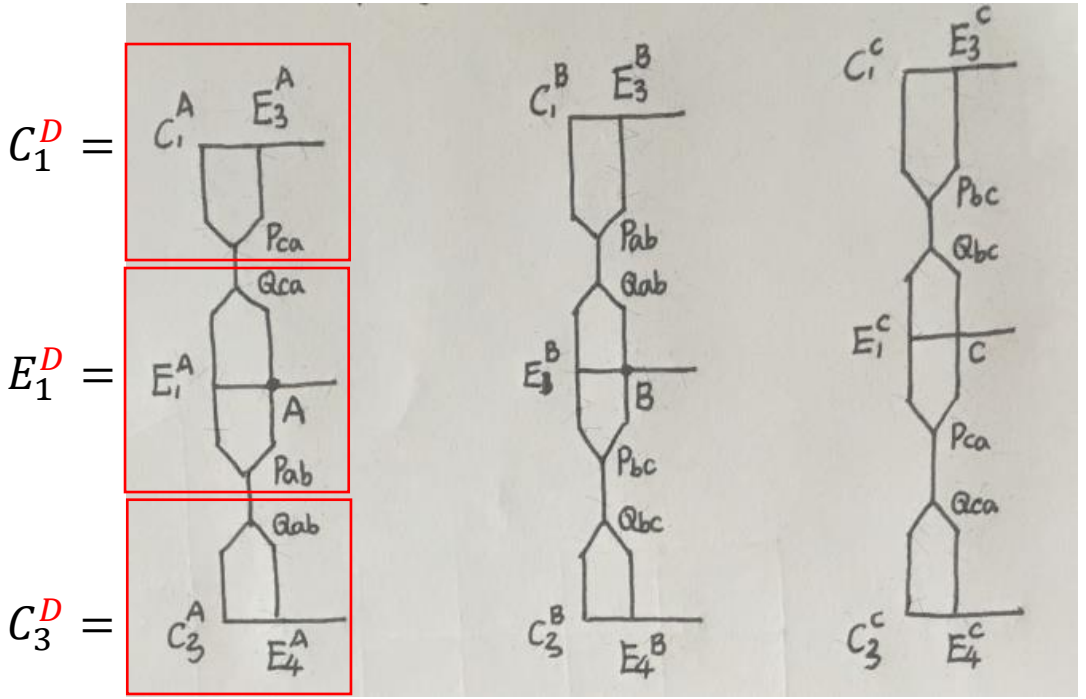
- A single step of left move

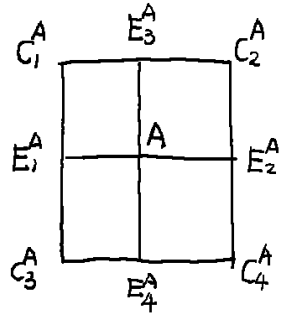




Practical CTMRG for 3 × 2 as an example



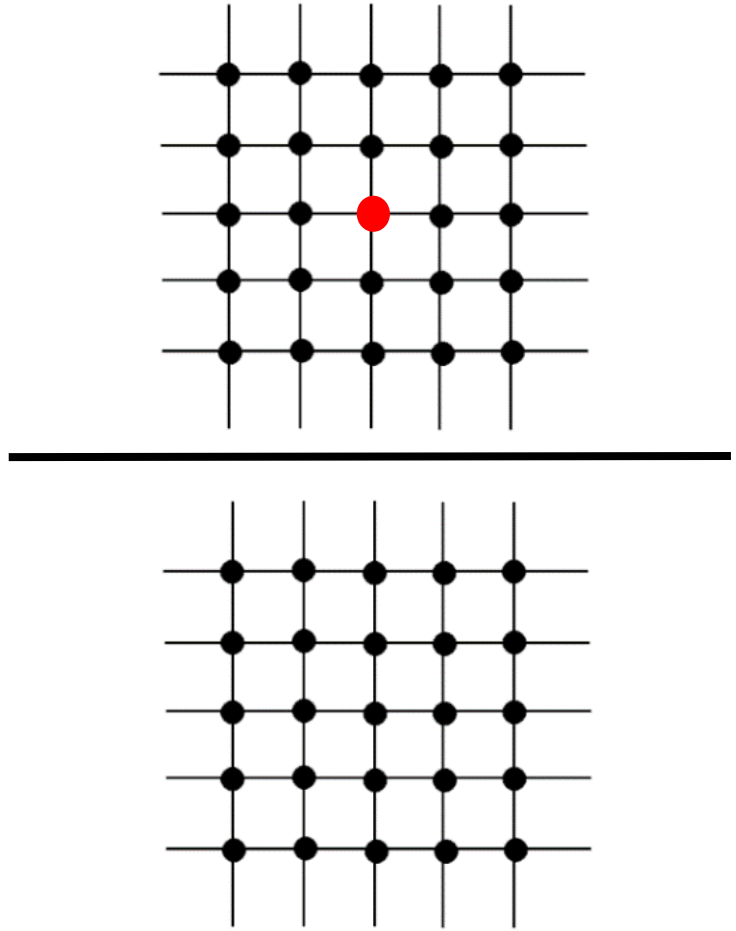




- next single step of left move: D, E, F
- next move: right * 2, up * 3, down * 3
- **next iteration**

The main bottleneck of TNS probably: D^2 dimension

$$\langle \hat{O}_i \rangle = \frac{\langle \Psi | \hat{O}_i | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\mathbf{Tr}[C^j_{a'b'c'd'} \prod_{i \neq j} B^i_{abcd}]}{\mathbf{Tr} \prod_i B^{(i)}_{abcd}}$$

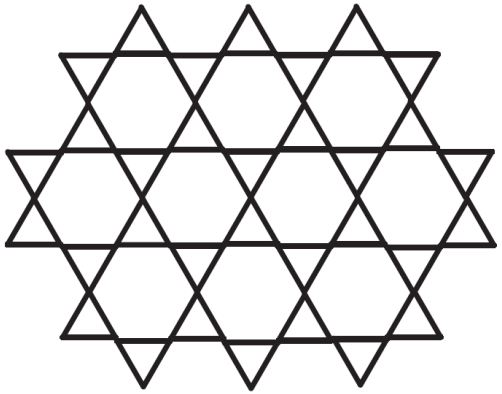


Note:

- The bond dimension is squared in both two terms, i.e., D^2
- If no arnoldi or partial SVD is used, then cost scales $M \sim D^8$, $C \sim D^{12}$
- Full update need this calculation in every evolution step
- D is usually no more than 13
- Even the wf can have very large D (~270), but exp. Cal. D is limited
- Other method without square: MERA even higher, D^{16} in 2D

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

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



Kaomge lattice

Valence bond crystal

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

Gapped spin liquid (Topological)

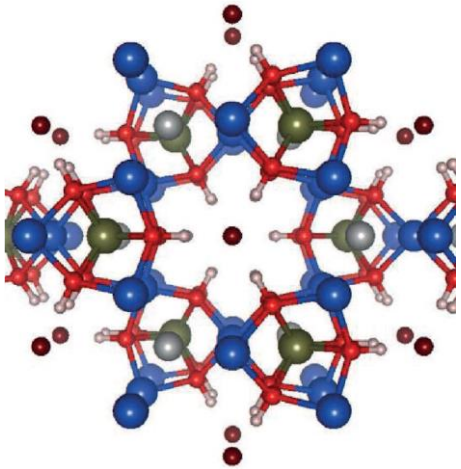
Jiang, Weng & Sheng, PRL 2008 DMRG
Yan, Huse & White, Science 2011 DMRG
Depenbrock, McCulloch & Schollwock, PRL 2012 DMRG
Jiang, Wang & Balents, Nature Physics 2012 DMRG
Gong, Zhu & Sheng, Scientific Reports 2014 DMRG
Li, arXiv:1601.02165 VMC
Mei, Chen, He & Wen, arXiv:1606.09639 SU(2)-TNS

Gapless spin liquid (Algebra)

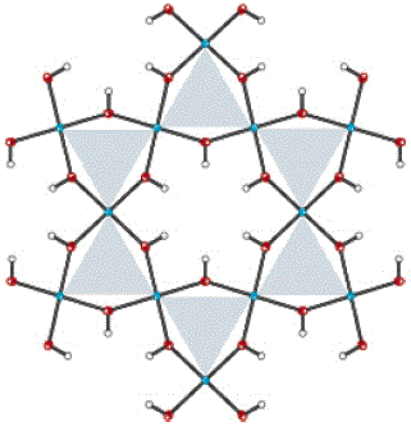
Hastings, PRB 2000
Ran, Hermele, Lee & Wen, PRL 2007 VMC
Iqbal, Becca, Sorella & Poilblanc, PRB 2013 VMC+Lanczos
Hu, Gong, Becca & Sheng, PRB 2015 VMC
Jiang, Kim, Han & Ran, arXiv:1610.02024 SU(2)-TNS
He, Zaletel, Oshikawa & Pollmann, arXiv:1611.06238 DMRG

Experiment:

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



$Cu_3Zn(OH)_6FBr$



Herbertsmithite
$ZnCu_3(OH)_6Cl_2$

For Monte Carlo: Larger Size is important!

Finite size vs Thermodynamic limit

qualitatively different: Kagome AFH

T. Li, arXiv: 1601.02165
Y. Iqbal, et al, arXiv: 1606.02255
T. Li, arXiv: 1807.09463

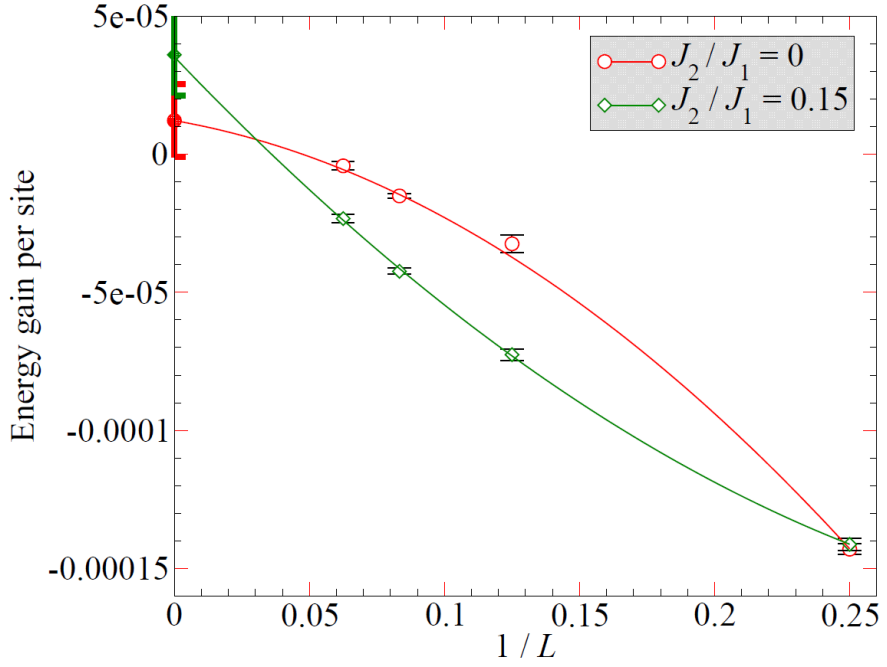
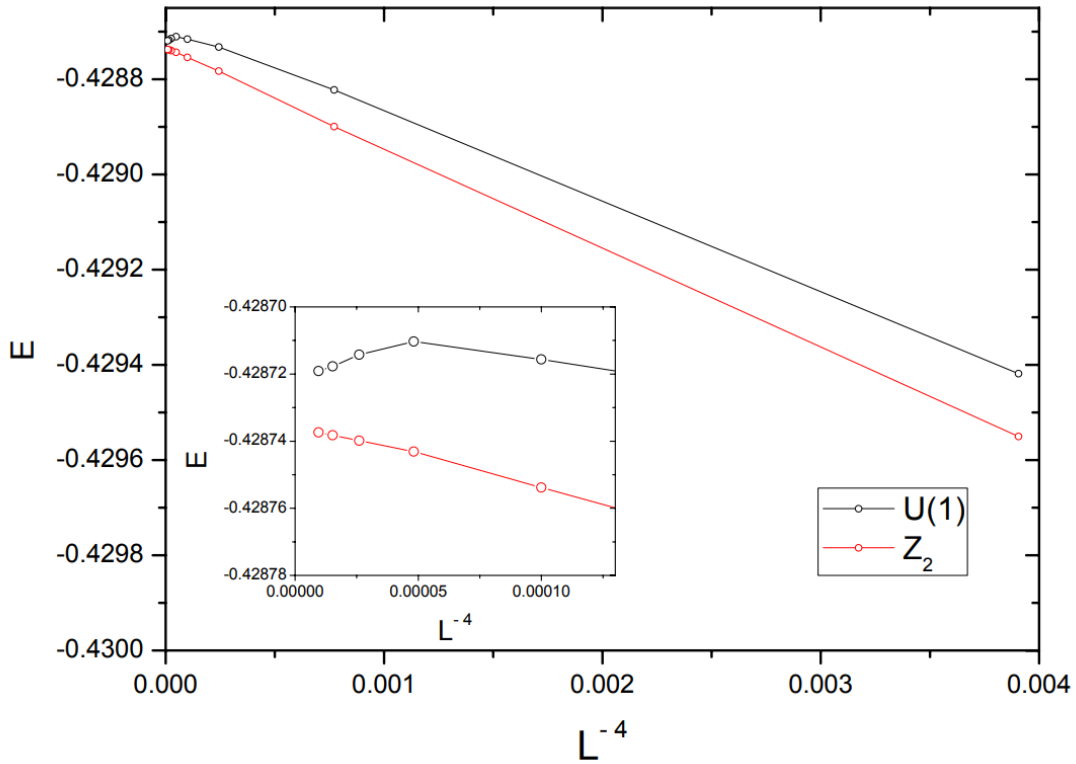
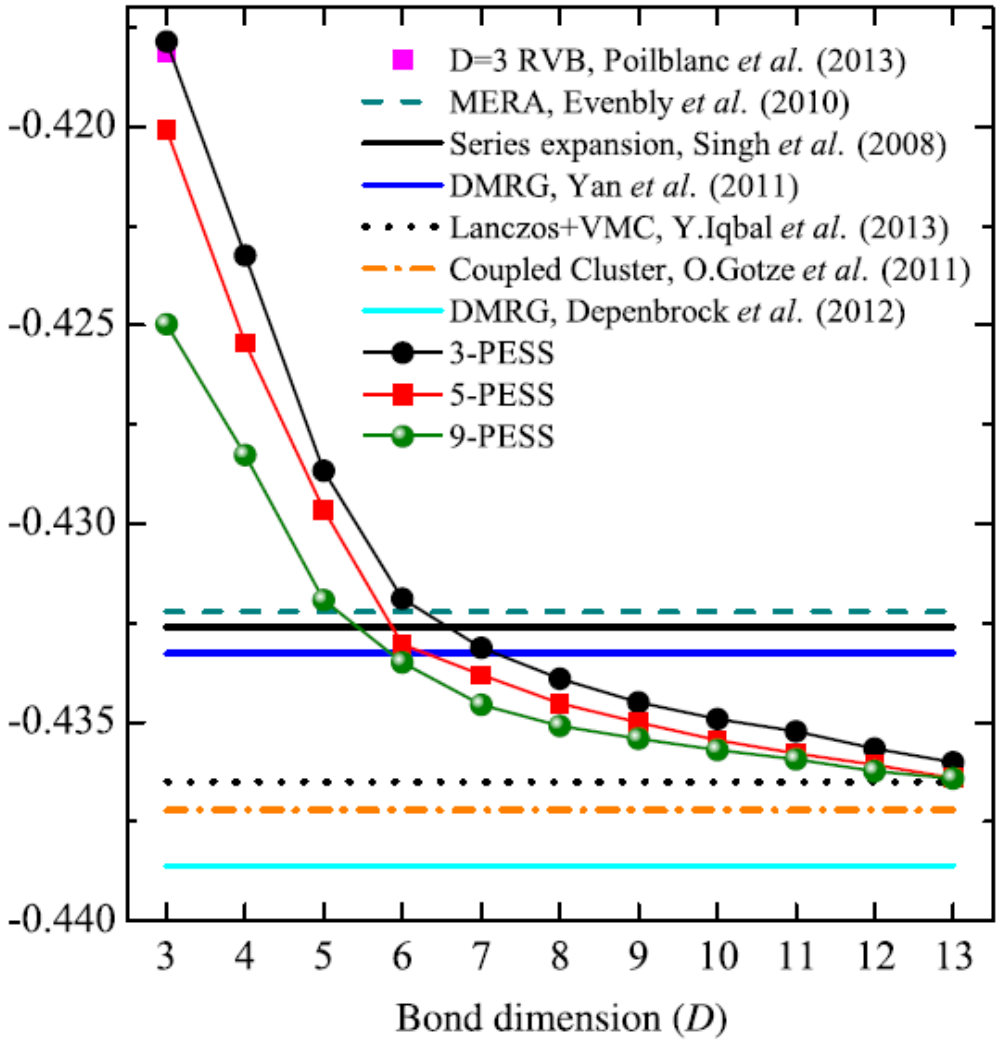
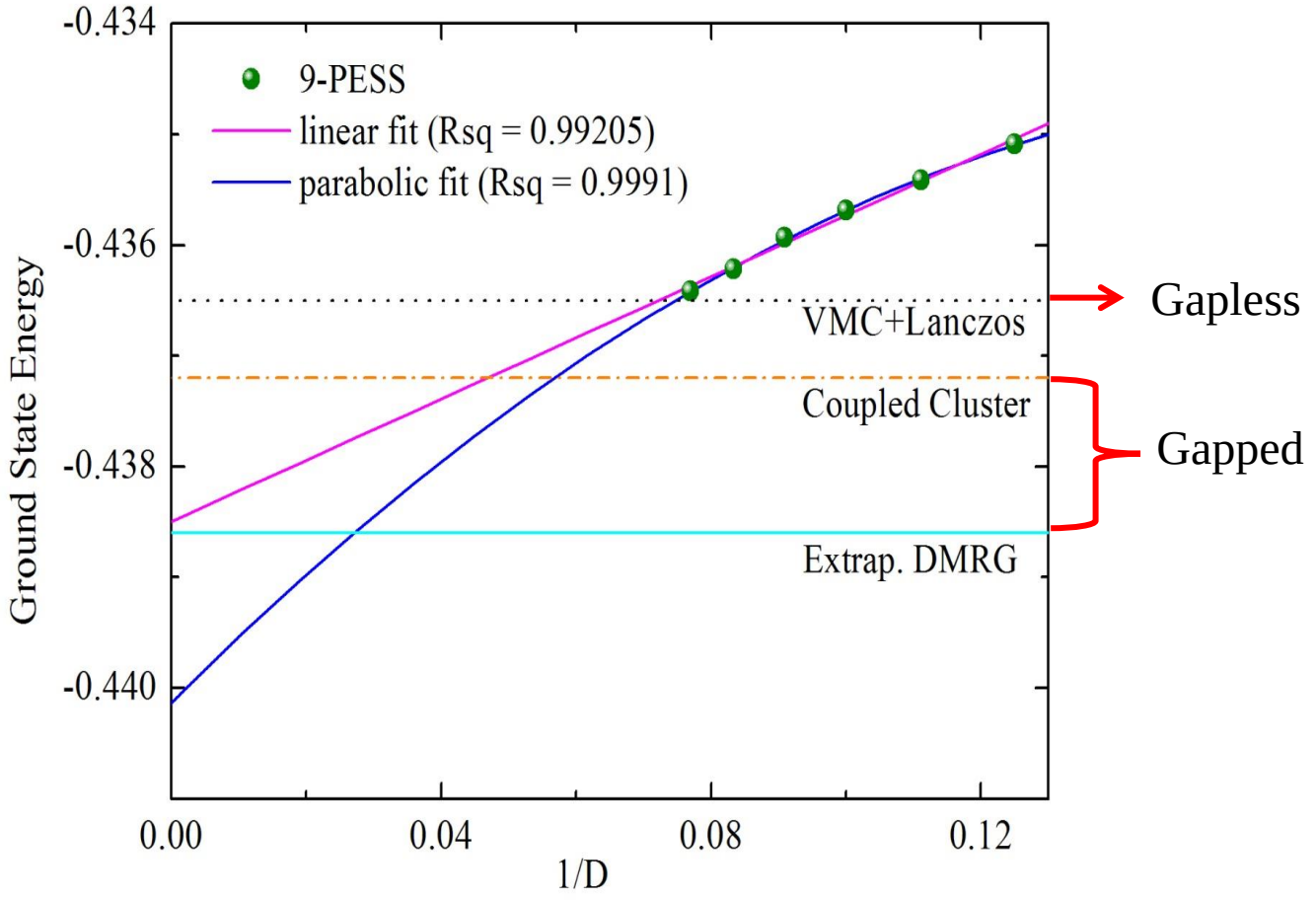


FIG. 1. The size scaling of the energy gain per site $\Delta E = E_{\mathbb{Z}_2} - E_{U(1)}$ is shown for $J_2 = 0$ and $J_2/J_1 = 0.15$, for $L = 4$, 8, 12 and 16 clusters. The results for $L = 4$ and 8 are from Ref. [4].



For TNS: Larger D is important!





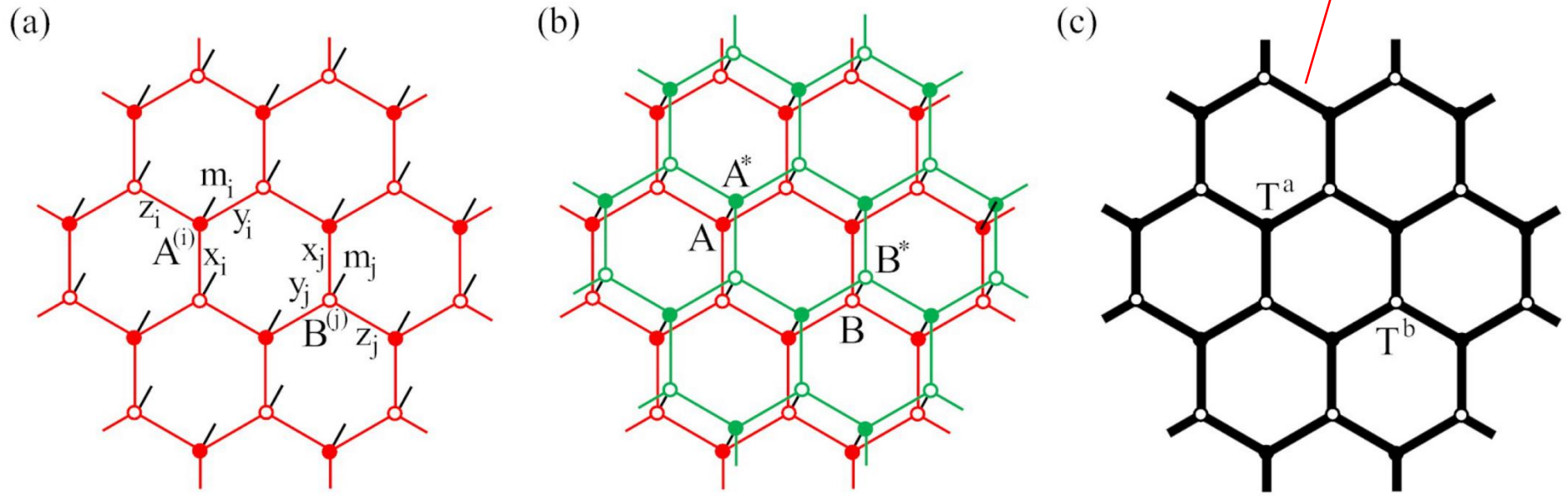
Which extrapolation is the correct one!
Gapped or gapless?

Reduced Tensor Network: physical index are summed over firstly

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

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

Bond dimension: D^2



$$T^a_{xx',yy',zz'} = \sum_m A_{xyz}[m]A^*_{x'y'z'}[m],$$

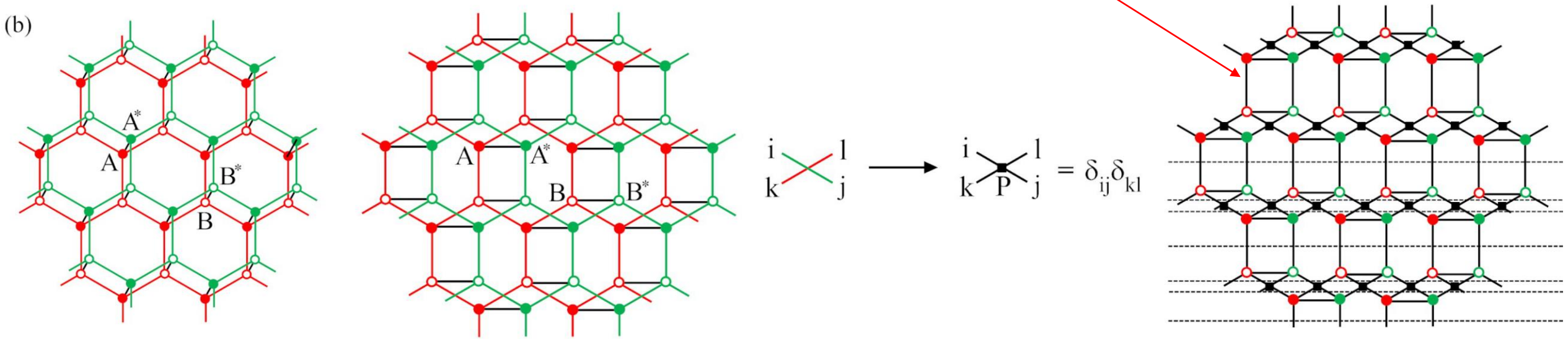
$$T^b_{xx',yy',zz'} = \sum_m B_{xyz}[m]B^*_{x'y'z'}[m].$$

Nested Tensor Network: Dimension Reduction Technique

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

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

Bond dimension: D

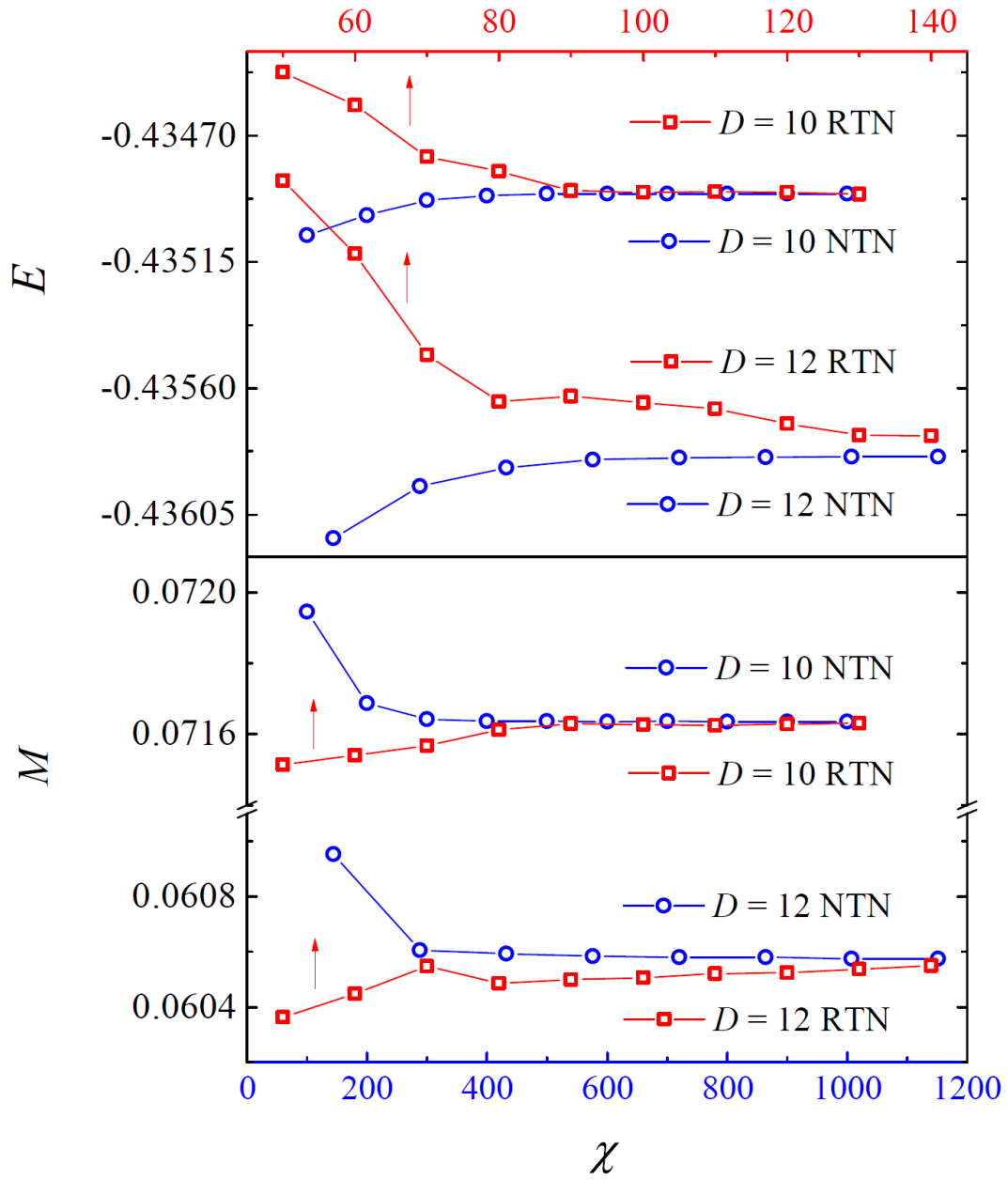


Seems trivial, but the consequence is non-trivial:

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

Our group, PRB 96, 045128 (2017)

Convergence Test: Kagome Heisenberg model

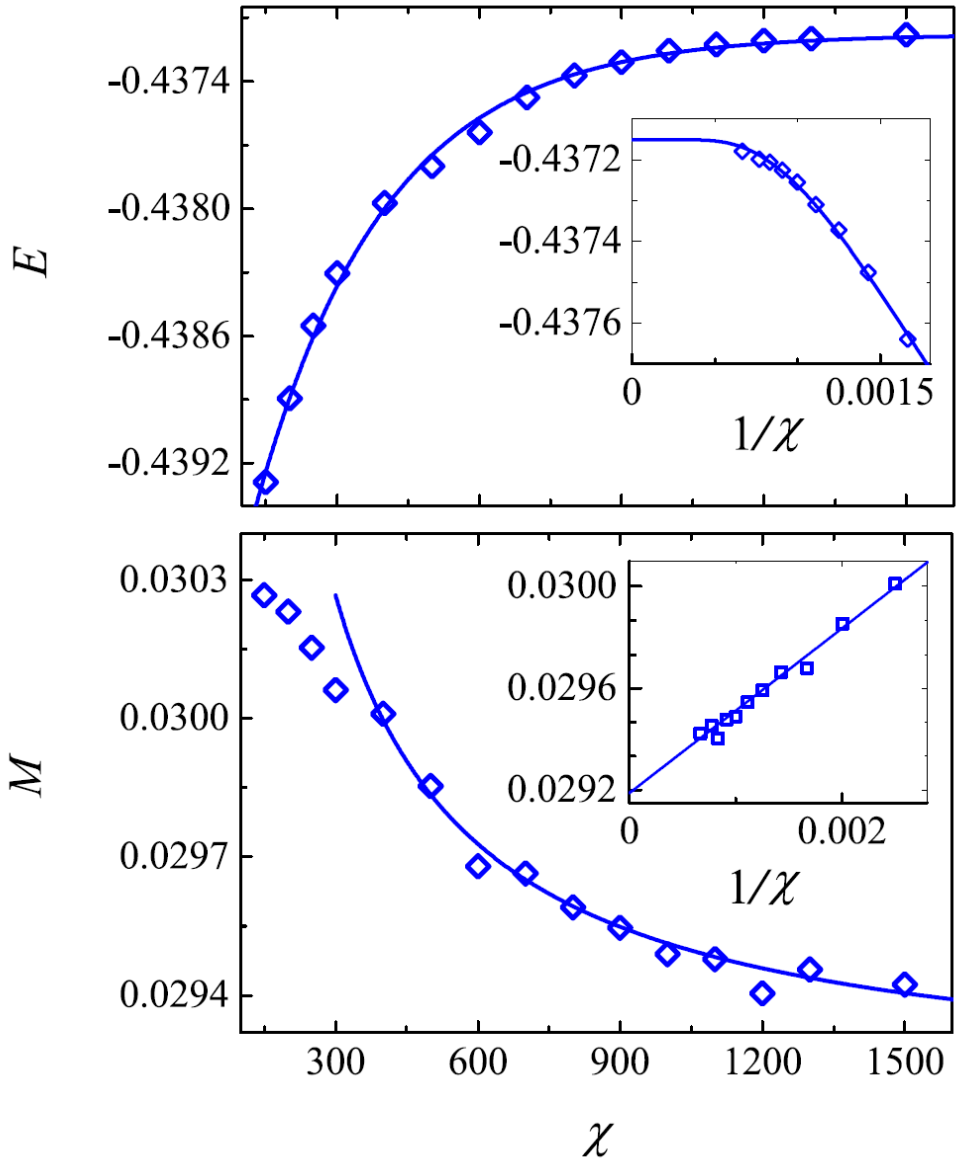


This is important to ensure the convergence: $X \sim D^2$

RTN: X~100

NTN: X~1000

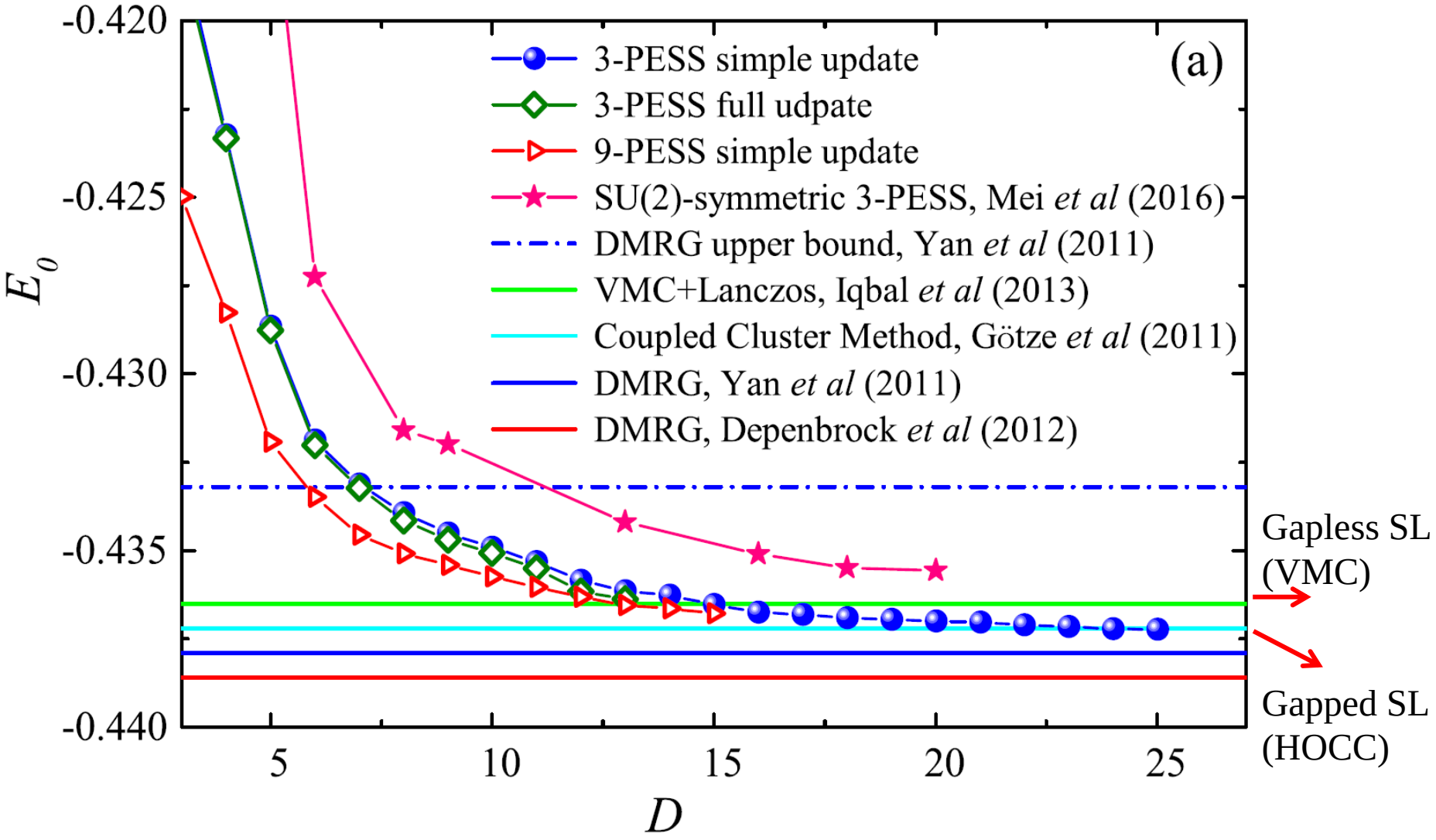
When RTN can not work: D = 24 e.g.



Energy: already exp. converged
Mag: only pow. converged, need to increase X

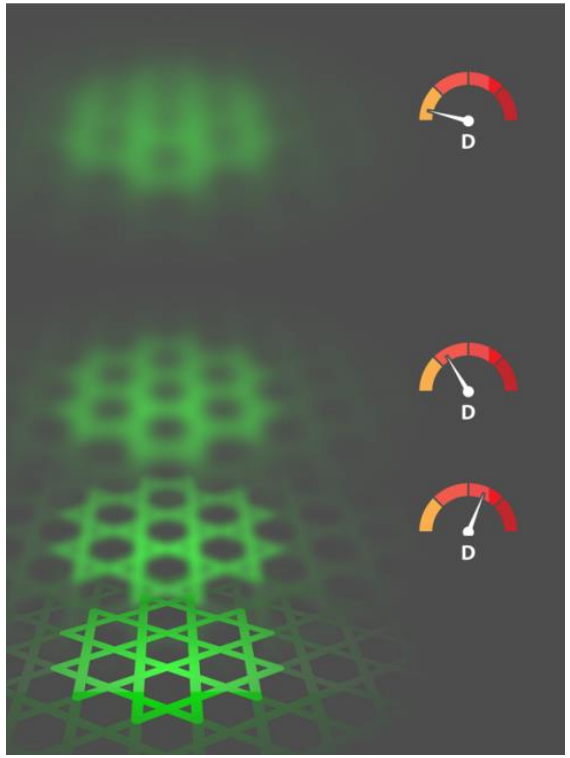
Latest Result: Ground State Energy, SL region

Our group, PRL 118, 137202 (2017)

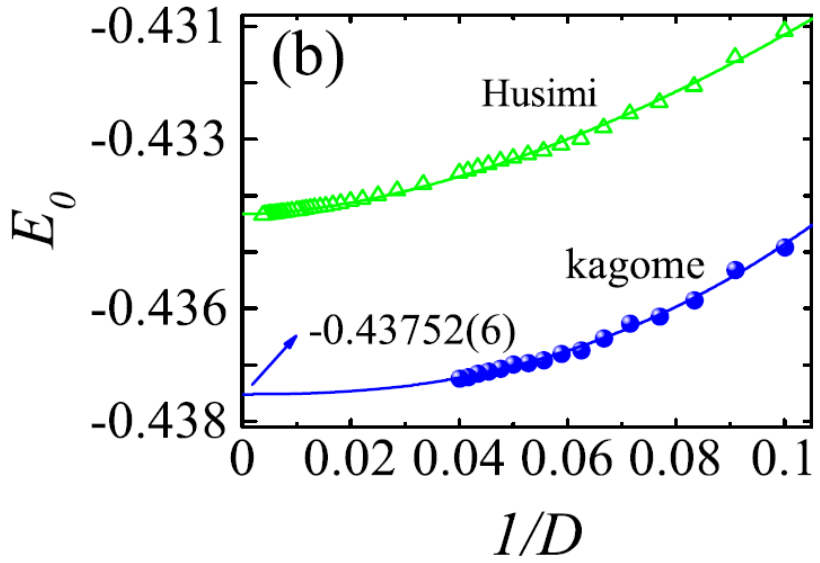


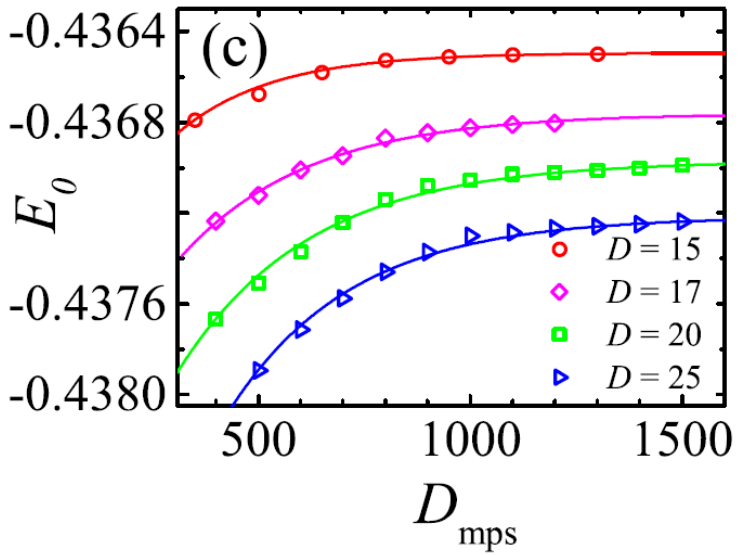
Gapless SL (VMC)

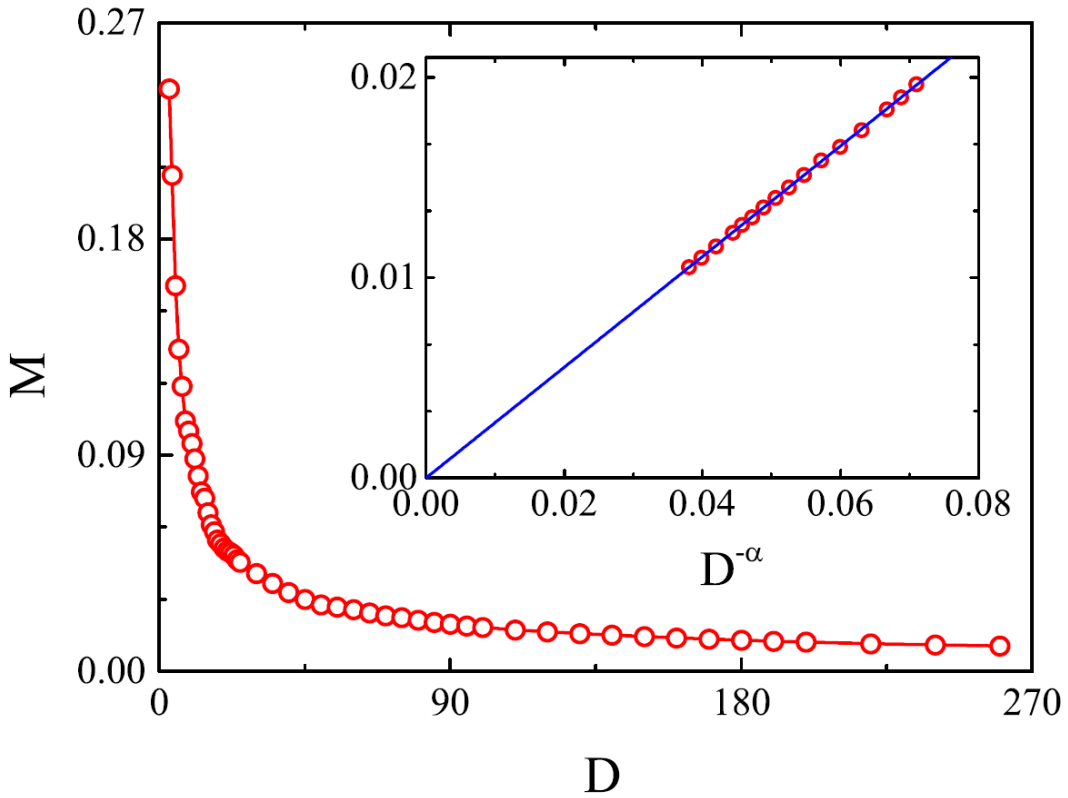
Gapped SL (HOCC)

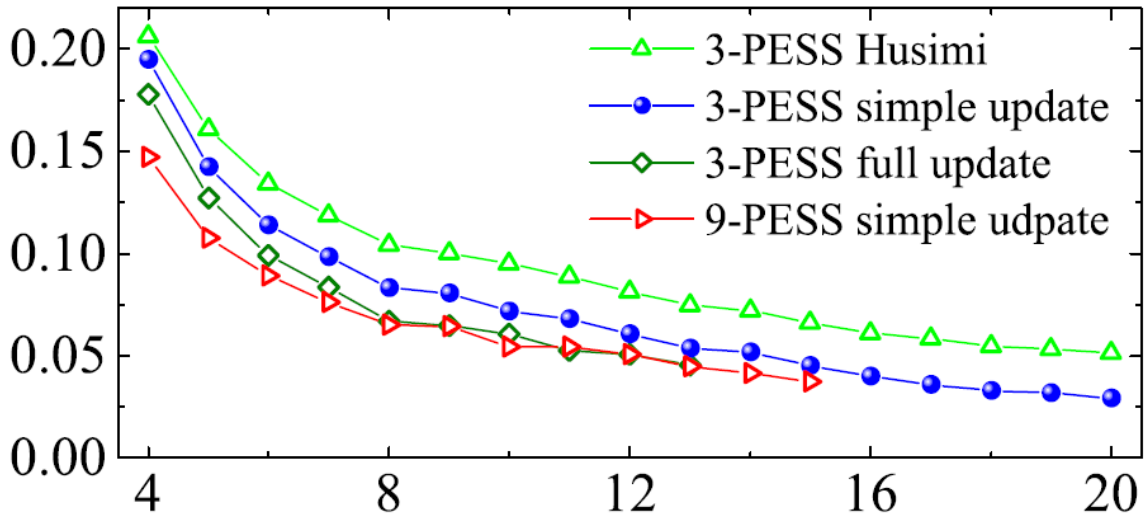


B. Clark, Physics **10**, 33 (2017)







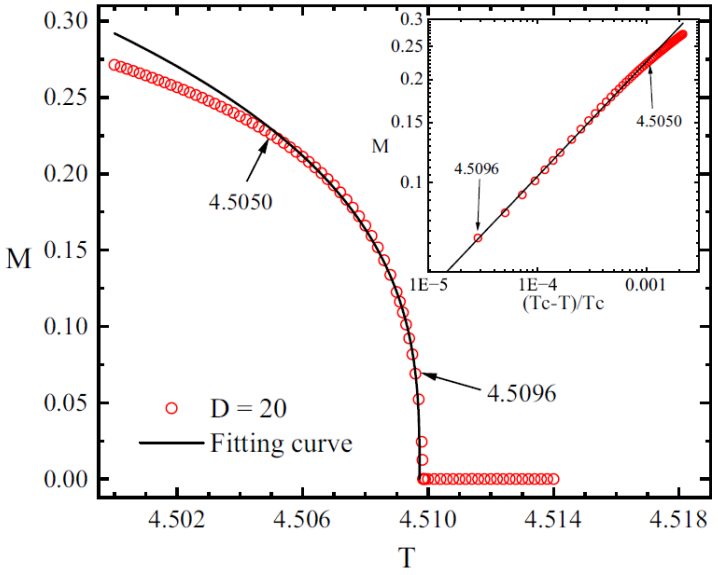


PRL 118, 137202 (2017)

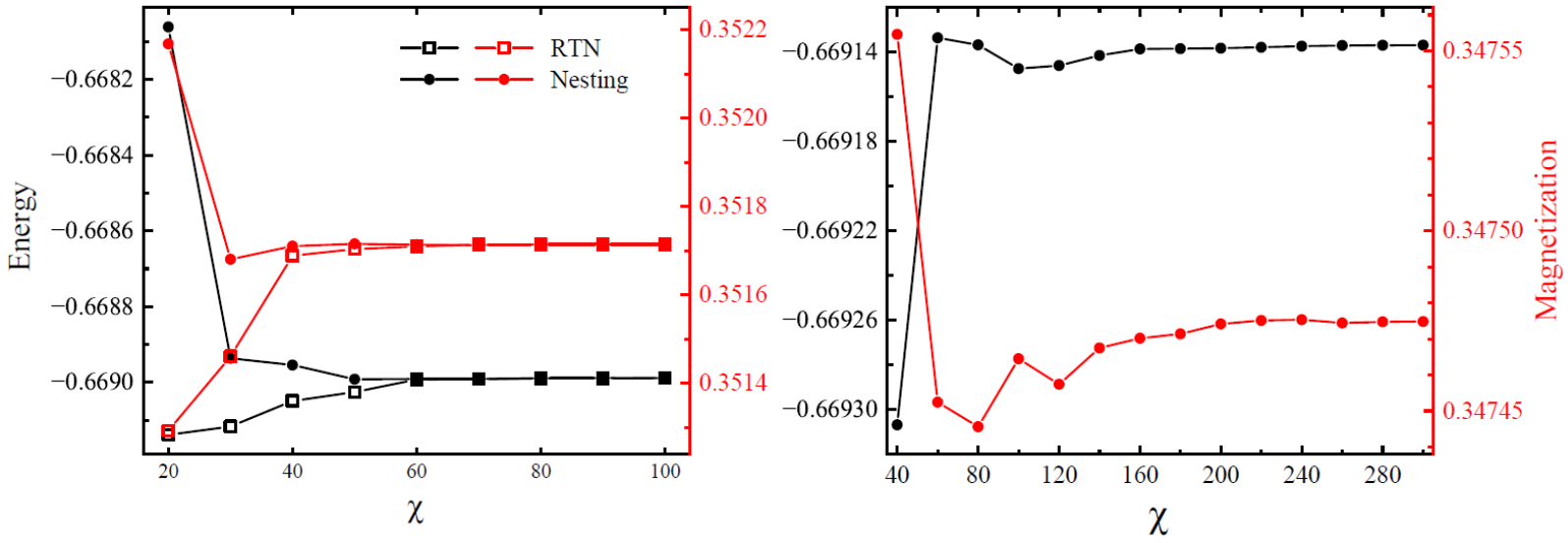
Natural nested technique based on PESS ansatz

L. P. Yang, Y. F. Fu, et al., PRB **107**, 165127 (2023)

3D Ising model



AF Heisenberg model on square lattice: local update



D=10 D=20

Not mentioned: variation assisted by AD: PRX 9, 031041 (2019), PRB 101, 220409 (2020), PRB 101, 195109 (2020).

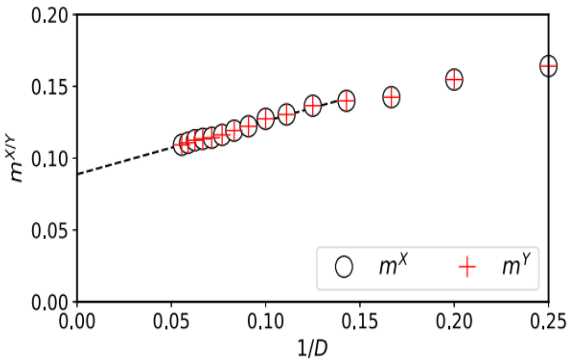
这套方法在典型阻挫系统的应用

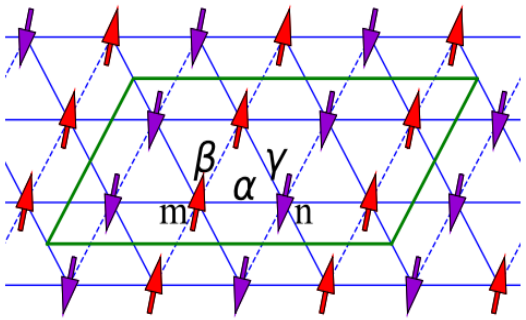
① 三角晶格反铁磁海森堡模型：磁矩上限

Method	E_b	M_0	Year	Max. size
This work	−0.18334(10)	0.161(5)	2020	∞
SB+1/N [30]		0.224	2018	432
DMRG [29]	−0.1837 (7)		2016	
CC [28]	−0.1838	0.21535	2016	10*
SB [26]		0.2739	2015	∞
SWT [26]		0.2386	2015	∞
SE [26]		0.198(34)	2015	∞
CC [27]	−0.18403(7)	0.198(5)	2015	10*
CC [24]	−0.1843	0.1865	2014	10*
VMC [25]	−0.18163(7)	0.2715(30)	2014	324
SWT [26]	−0.18228	0.24974	2009	∞

Q. Li, et al, PRB 105, 184418 (2022)

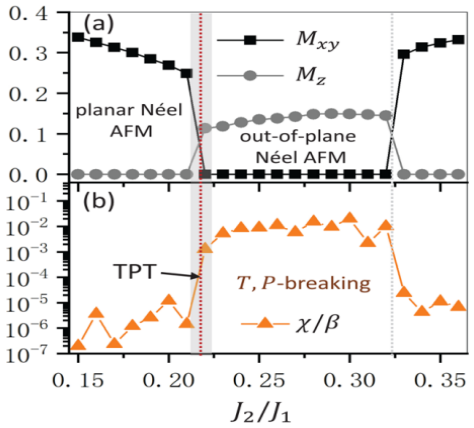
② 三角晶格反铁磁海森堡系统: 量子自旋轨道液体

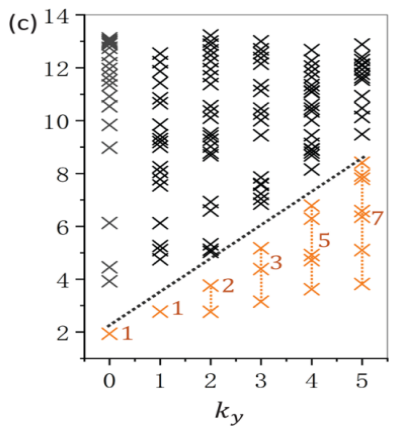




Y. Liu, et al, PRB 107, L041106 (2023) **Letter**

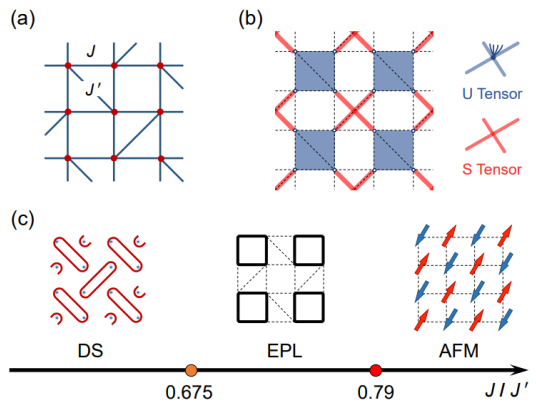
③ 六角晶格阻挫XY模型：非均匀手征自旋液体

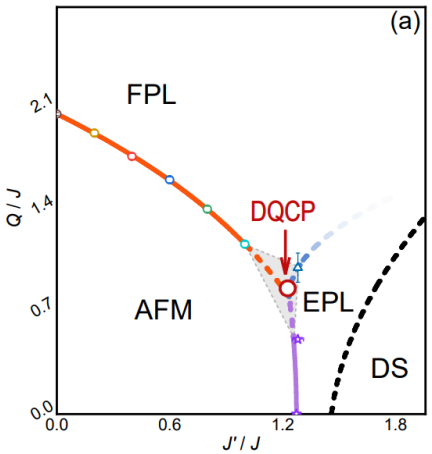




R. Wang, et al, PRB 106, L121117 (2022) **Letter**

④ Shastry-Sutherland模型：解禁闭量子临界点

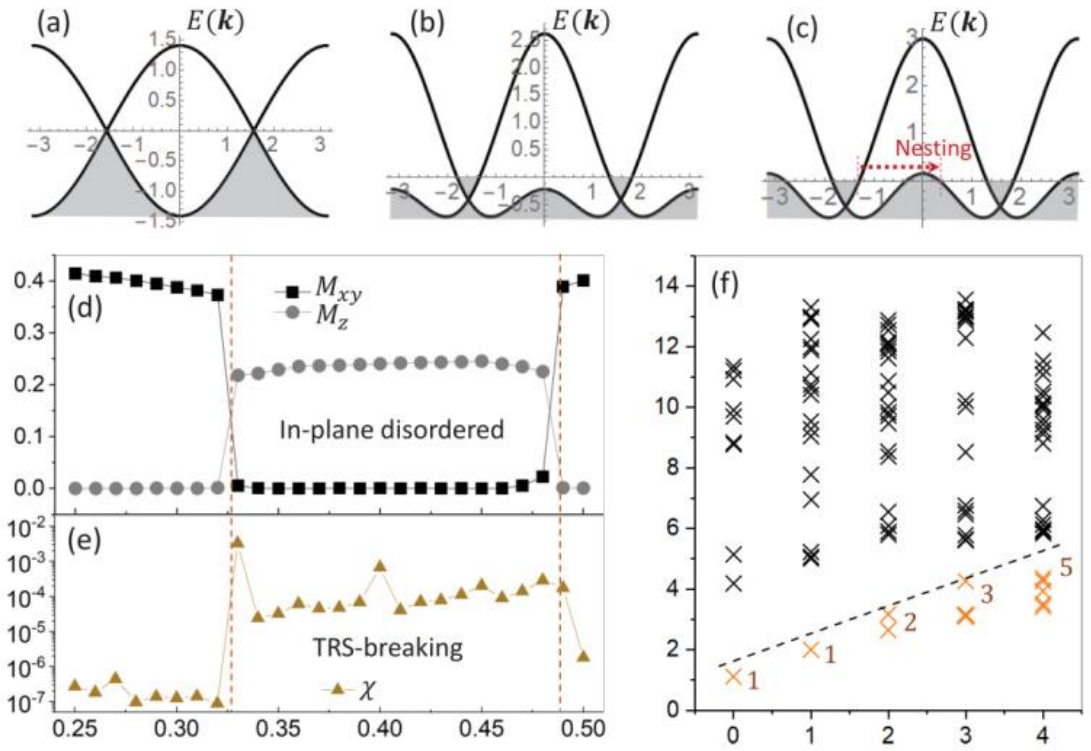




N. Xi, et al, PRB 107, 220408 (2023) **Letter**

这套方法在典型阻挫系统的应用

⑤ 正方晶格阻挫XY系统：非均匀手征自旋液体



R. Wang, et al, PRB Accepted (2024) **Letter**

⑥ 正方晶格阻挫磁海森堡系统: QSL vs DQCP

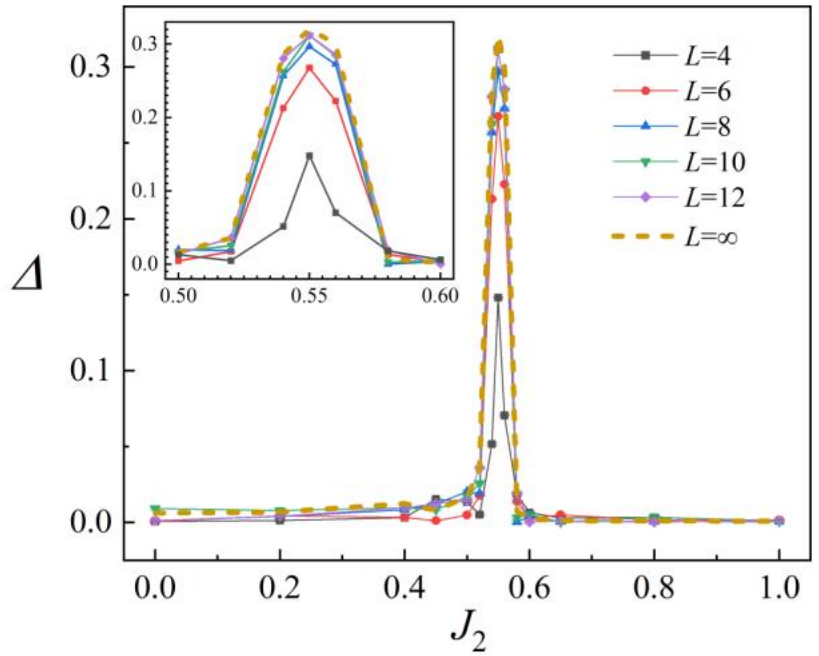


FIG. 6. The relevant order parameter to the columnar VBS phase for $D = 4$ and a series of lattice sizes. The orange dashed line shows a direct extrapolation to the thermodynamic limit.

H. Y. Lin, et al, PRB Accepted (2024)

量子纠缠与量子多体系统专题 《物理》第46 卷，2017 年第7期

张量重正化群方法及其应用*

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（中国人民大学物理系　北京　100872）

2017－06－08收到
† email：qingtaoxie@ruc.edu.cn
DOI：10.7693/wl20170703

机器学习与量子物理专题 《物理》第50 卷，2021年第2期

张量网络与神经网络在物理学中的应用和交融*

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（中国人民大学物理系　北京　100872）

2020－12－25收到
† email：qingtaoxie@ruc.edu.cn
DOI：10.7693/wl20210203

Thanks!

Excellent References:

R. Orus, Annals of Physics 349, 117 (2014)
R. Orus, Eur. Phys. J. B 87, 280 (2014)
R. Orus, Nature Reviews Physics 1, 538 (2019)
J. Cirac, D. P. Garcia, N. Schuch, F. Verstraete, RMP 93, 045003 (2021)
T. Xiang, *Density Matrix and Tensor Network Renormalization*, CUP (2023)

TEBD 算法示例：自旋1/2反铁磁海森堡链

```
function TEBD
% AF spin-1/2 Heisenberg chain
% Energy = 0.25 - log2 ~ -0.4431, from Bethe Ansatz

warning off
rmpath( 'C:\Users\401b\Desktop\HOTRG\ToolBox' );
rmpath( 'D:\Software\matlab2017a\toolbox\RUCTool' );
addpath( 'C:\Users\401b\Desktop\Typical\TEBD\ToolBox' );

[ Inface ] = UserInterface;

[ Wa, Wb, Imp, tau, TrunError ] = GetMPS( Inface );
[ Energy ] = GetExpVal( Wa, Wb, Imp );

fprintf( 'tau-E1-E2-E3-Er: %g, %g, %g, %g, %g \n', tau, Energy(1), Energy(2), Energy(3), TrunError );
save( 'wf.mat', 'Wa', 'Wb' );

end
```

```
function [ Wa, Wb, Te, tau, TrunError ] = GetMPS( Inface )

tau = Inface.FinalTau;
[ Ga, Gb, Te, Wa, Wb ] = ConstructTensor( tau, Inface.Dbond, Inface.MarshallSign );

if( Inface.CanoFlag == 1 )
   disp( '==========use canonicalization of MPS==========' );
   [ Wa, Wb, TrunError ] = CanoTEBD( Ga, Gb, Te, Wa, Wb, Inface );
else
   disp( '==========use mean field entanglement approximation==========' );
   [ Wa, Wb, TrunError ] = BondSVD( Ga, Gb, Te, Wa, Wb, Inface );
end
```

```
function [ A, B, TrunError, BondDiff, CoefDiff ] = CanoTEBD( Ga, Gb, Te, A, B, Inface )


[ tcab, tcba, tlba, tlab ] = copyvalue( 10, 10, 10, 10 );
[ Dbond, Maxiter, CtrlError ] = GetFields( Inface, 'Dbond', 'Maxiter', 'CtrlError' );

for iterNo = 1 : Maxiter

   % Gate act on Wa-Wb bond
   A = TensorContract3( Ga, A, 3, 2, 3, 3, [ 3, 2, 4, 1 ], [ 1, 2, 1 ] );
   B = TensorContract3( Gb, B, 3, 2, 3, 3, [ 2, 3, 4, 1 ], [ 2, 1, 1 ] );
   [ A, B, Coefab, ~, ~, TRab ] = BlackBoxTEBD( A, B, Dbond );

   % Gate act on Wb-Wa bond
   B = TensorContract3( Ga, B, 3, 2, 3, 3, [ 3, 2, 4, 1 ], [ 1, 2, 1 ] );
   A = TensorContract3( Gb, A, 3, 2, 3, 3, [ 2, 3, 4, 1 ], [ 2, 1, 1 ] );
   [ B, A, Coefba, Lba, Lab, TRba ] = BlackBoxTEBD( B, A, Dbond );

   CoefError = max( abs( Coefab - tcab ), abs( Coefba - tcba ) );
   LamError = max( Maxdiff( Lab, tlab ), Maxdiff( Lba, tlba ) );
   ConError = max( CoefError, LamError );

   if( ConError <= CtrlError )&&( iterNo > 100 )
      break
   else
      [ tlba, tlab, tcab, tcba ] = copyvalue( Lba, Lab, Coefab, Coefba );
      if( ~mod( iterNo, 100 ) )
         [ Energy ] = GetExpVal( A, B, Te );
         fprintf( 'iter-Cab-Cba-ABer-Baer-Energy-Conv: %d, %g, %g, %g, %g, %g, %g \n', ...
            iterNo, Coefab, Coefba, TRab, TRba, Energy(3), ConError );
      end
   end
end
TrunError = max( TRab, TRba );
d = min( numel( Lab ), numel( Lba ) );
BondDiff = Maxdiff( Lab( 1:d ), Lba( 1:d ) );
CoefDiff = abs( Coefab - Coefba );

end
```

```
function [ A, B, TrunError, BondDiff, CoefDiff ] = BondSVD( Ga, Gb, Te, A, B, Inface )

Lab = sort( rand( size( A, 1 ), 1 ), 'descend' );
[ Lba, tcab, tcba, tlba, tlab ] = copyvalue( Lab, 10, 10, 10, 10 );
[ Dbond, Maxiter, CtrlError ] = GetFields( Inface, 'Dbond', 'Maxiter', 'CtrlError' );

for iterNo = 1 : Maxiter

   % Gate act on A-B bond
   A = TensorPosAct2( A, diag(Lab), 2 );
   A = TensorContract3( Ga, A, 3, 2, 3, 3, [ 3, 2, 4, 1 ], [ 1, 2, 1 ] );
   B = TensorContract3( Gb, B, 3, 2, 3, 3, [ 2, 3, 4, 1 ], [ 2, 1, 1 ] );
   [ A, B, Coefab, Lab, TRab ] = BlackBoxSVD( A, B, Lba, Dbond );

   % Gate act on B-A bond
   B = TensorPosAct2( B, diag(Lba), 2 );
   B = TensorContract3( Ga, B, 3, 2, 3, 3, [ 3, 2, 4, 1 ], [ 1, 2, 1 ] );
   A = TensorContract3( Gb, A, 3, 2, 3, 3, [ 2, 3, 4, 1 ], [ 2, 1, 1 ] );
   [ B, A, Coefba, Lba, TRba ] = BlackBoxSVD( B, A, Lab, Dbond );

   CoefError = max( abs( Coefab - tcab ), abs( Coefba - tcba ) );
   LamError = max( Maxdiff( Lab, tlab ), Maxdiff( Lba, tlba ) );
   ConError = max( CoefError, LamError );

   if( ConError <= CtrlError )&&( iterNo > 100 )
      break
   else
      [ tlba, tlab, tcab, tcba ] = copyvalue( Lba, Lab, Coefab, Coefba );
      if( ~mod( iterNo, 100 ) )
         Wa = TensorPosAct2( A, diag(Lab), 2 );
         Wb = TensorPosAct2( B, diag(Lba), 2 );
         [ Energy ] = GetExpVal( Wa, Wb, Te );
         fprintf( 'iter-Cab-Cba-ABer-Baer-Energy-Conv: %d, %g, %g, %g, %g, %g, %g \n', ...
            iterNo, Coefab, Coefba, TRab, TRba, Energy(3), ConError );
      end
   end
end

TrunError = max( TRab, TRba );
d = min( numel( Lab ), numel( Lba ) );
BondDiff = Maxdiff( Lab( 1:d ), Lba( 1:d ) );
CoefDiff = abs( Coefab - Coefba );

A = TensorPosAct2( A, diag(Lab), 2 );
B = TensorPosAct2( B, diag(Lba), 2 );
end
```

```
function [ Energy ] = GetExpVal( Wa, Wb, Te )

Wab = TensorContract3( Wa, Wb, 3, 2, 3, 1, [ 1, 3, 2, 4 ], [ 1, 1, 2 ] );
Wba = TensorContract3( Wb, Wa, 3, 2, 3, 1, [ 1, 3, 2, 4 ], [ 1, 1, 2 ] );

[ Energy1 ] = GetEnergy( Wab, Te );
[ Energy2 ] = GetEnergy( Wba, Te );
Energy = [ Energy1, Energy2, ( Energy2 + Energy1 ) / 2 ];
end

function [ Energy ] = GetEnergy( Wab, Te )

T1 = MergeTPS( Wab, Wab );
T2 = TensorPosAct2( Wab, Te, 3 );
T2 = MergeTPS( T2, Wab );

[ Rvec, Coef ] = eigs( T1, 1 );
[ Lvec, Coef ] = eigs( T1', 1 );
Energy = Lvec' * T2 * Rvec / ( Lvec' * T1 * Rvec );
end
```