

Tensor network approach to two-dimensional frustrated spin systems

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Computational
Science
Alliance

The University of Tokyo

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- Introduction
 - Motivations and difficulties in quantum many-body problems
 - Outline of tensor network quantum states
- Area law of entanglement and tensor network state
 - Quantum entanglement
 - Tensor network states and breakdown of MPS
- Tensor product states (TPS) / Projected entangled pair states (PEPS)
 - Contraction
 - Expressive power of iTPS
 - Optimizations
- Finite temperature simulation
- Summary

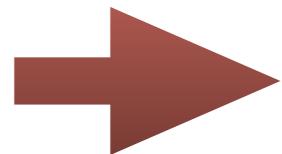
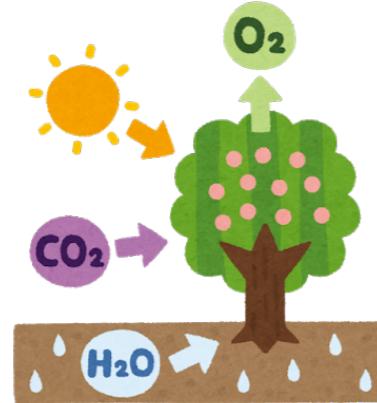
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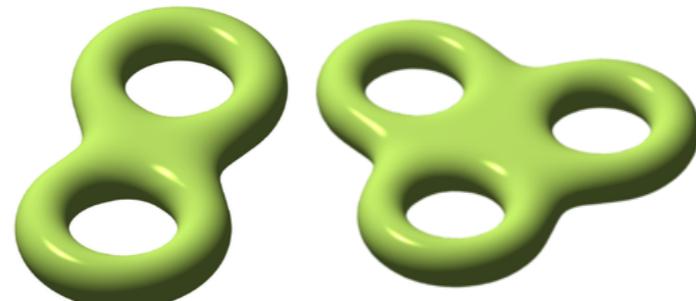
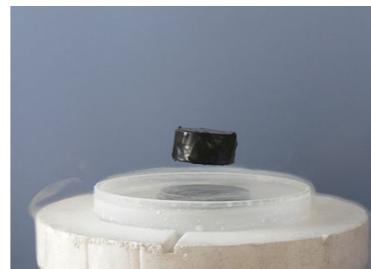
Quantum many-body problems

A variety of phenomena in condensed matter physics

- Chemical reaction
- Superconductivity
- Topological states
- ...



Quantum many-body problems

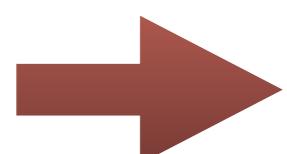


Cited from wikipedia: "Meissner effect", "Torus"

(Time independent) Schrödinger equation = Eigen value problem

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

- Dimension of the vector space increases **exponentially** as # of particles increases
- Quantum many-body problem ~ Eigenvalue problem of **huge** matrices



To solve the problem numerically by (classical) computer,
we need **huge memory** and **huge computation time**.

Phase transition in magnets and spin models

(Quantum) Spin model:

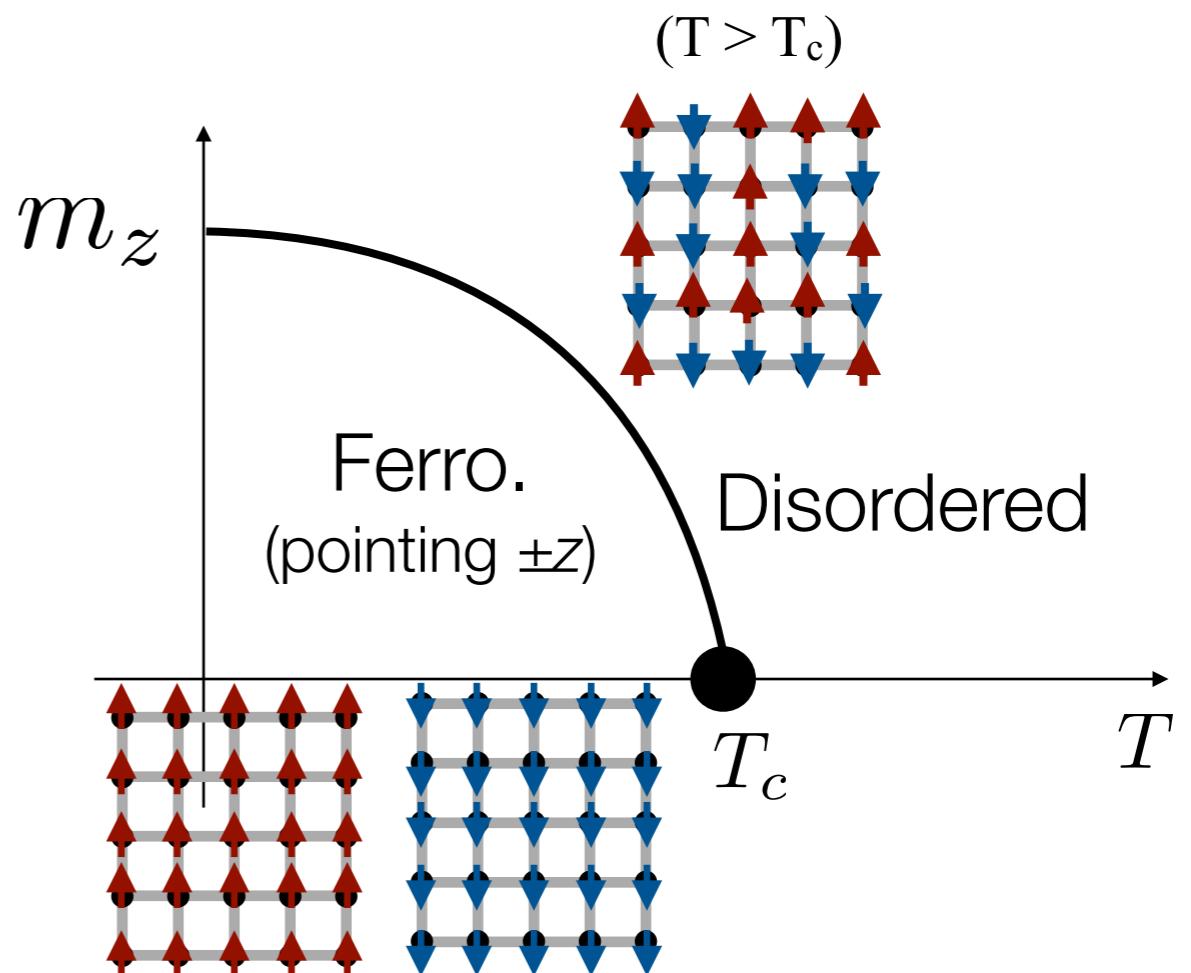
Spin degree of freedoms defined on a **lattice** and **interact** each other

Ex.1: (classical) Ising model

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_{i,z} S_{j,z}$$

$S_{i,z} = \pm 1$

Phase transition **by varying temperature**



Phase transition in magnets and spin models

(Quantum) Spin model:

Spin degree of freedoms defined on a **lattice** and **interact** each other

Ex.1: (classical) Ising model

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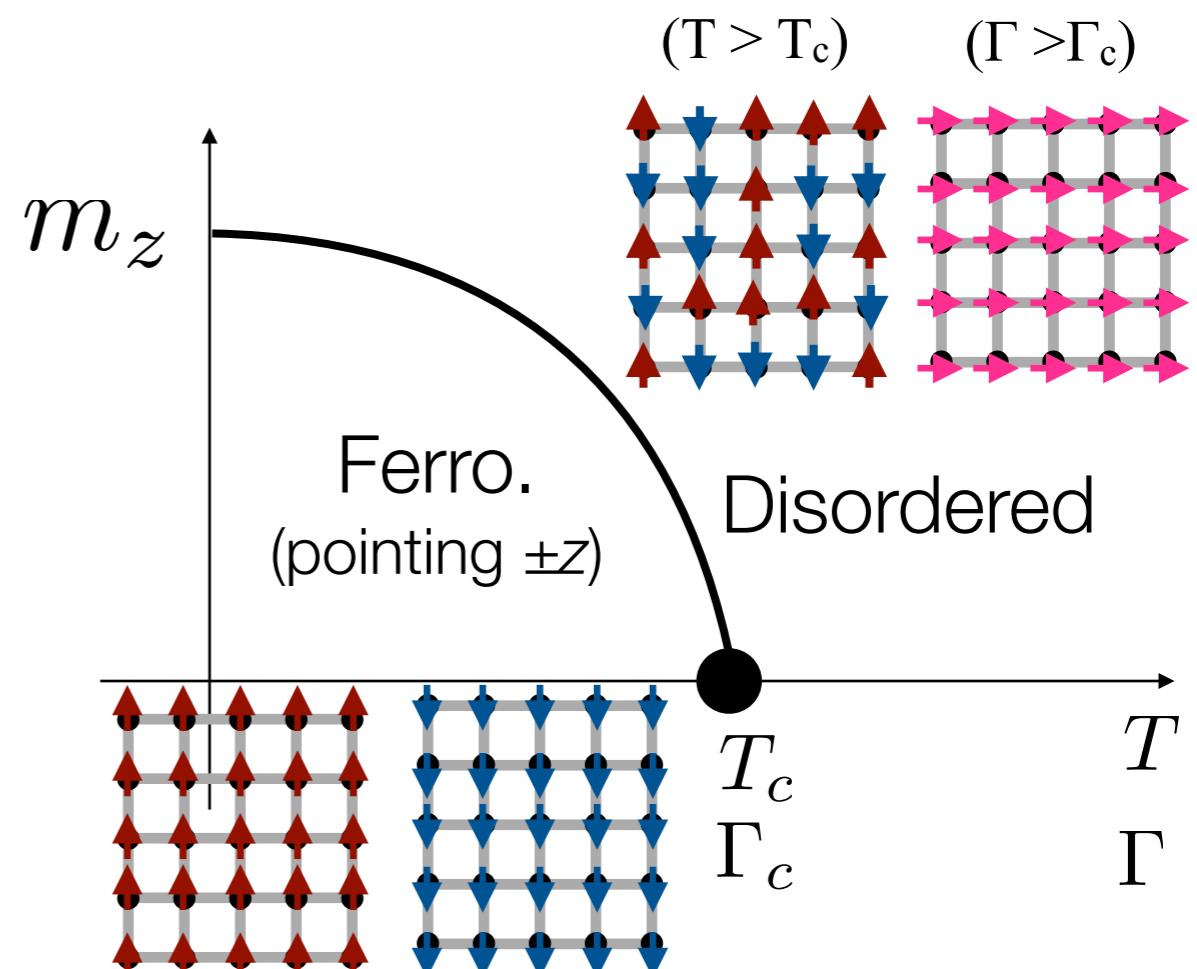
Phase transition **by varying temperature**

Ex.2: Transverse field Ising model

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_{i,z} S_{j,z} - \Gamma \sum_i S_{i,x}$$

$S_{i,z}, S_{i,x}$: spin **operator**

Phase transition by **varying Γ at $T=0$** .



Origin of a variety of physics in magnets: Frustration



Competition among several optimization conditions

Frustration in magnets:

Optimization : minimization of the total energy

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \quad J > 0$$

Antiferromagnetic

local energy minimization : anti-parallel spin pair

Origin of a variety of physics in magnets: Frustration



Competition among several optimization conditions

Frustration in magnets:

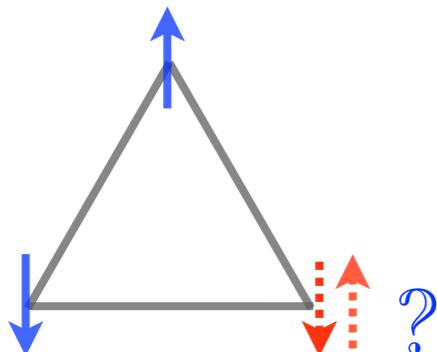
Optimization : minimization of the total energy

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \quad J > 0$$

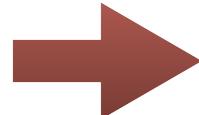
Antiferromagnetic

local energy minimization : anti-parallel spin pair

Ising spin



One of three pairs is necessarily parallel



Increase of degeneracy

Origin of a variety of physics in magnets: Frustration



Competition among several optimization conditions

Frustration in magnets:

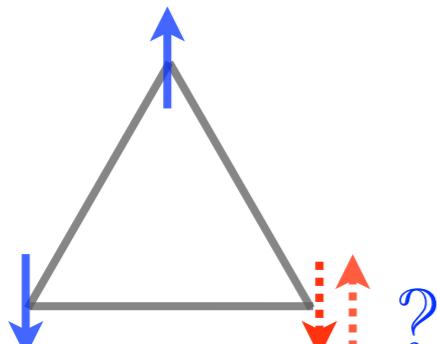
Optimization : minimization of the total energy

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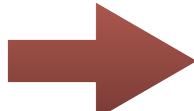
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local energy minimization : anti-parallel spin pair

Ising spin

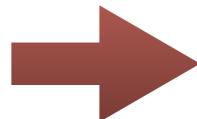


One of three pairs is necessarily parallel



Increase of degeneracy

Typical example: Kagome lattice, pyrochlore lattice,...



- Classical spin models:
 - No magnetic long-range order due to the huge degeneracy
 - Novel orders induced from weak perturbations
- Quantum spin models:
 - Spin liquids stabilized by quantum fluctuations
 - Hidden orders, topologies

Numerical methods for quantum spin systems

- **Numerical diagonalization**

Exact and applicable for any systems, but **system size is limited**.

$S=1/2$ spin models ~ 50 sites  We need careful extrapolation.

- **Quantum Monte Carlo (QMC)**

Within statistical error, solving problem “exactly”!

Easy calculation for **very large system**.

But, **frustrated interactions** are usually
suffered from the **sign problem**!

- **Variational method**

Assuming a wave-function ansatz

- Variational Monte Carlo: **larger systems than ED**
- **Tensor network method:** **Very large system size (infinite)**

Data compression in quantum many-body systems

Quantum state vector: Exponentially large dimension

$$S = \frac{1}{2} \rightarrow 2^N \text{ dim.}$$

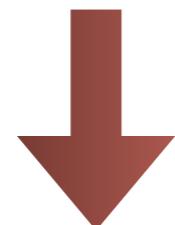
It is impossible to treat it in (classical) computers.



Efficient data compression by reducing effective dimension of the Hilbert space!

Low-energy states:

- Smaller quantum correlation than general (random) states
 - c.f. Area law of the entanglement entropy: $S \propto L^{d-1}$
- We can represent a quantum state efficiently **within** a proper subspace.



Quantum information Theory

Tensor network representation

Hilbert space



Important
subspace

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When we efficiently compress a vector?

$$\vec{v} = \sum_{i=1}^M C_i \vec{e}_i \quad \vec{v} \in \mathbb{C}^M$$

If we can find a basis where the coefficients have a structure (correlation).

All of C_i are not necessarily independent.

→ We store "**structure**" and "**independent elements**".

$$\{(i, C_i)\}$$

E.g. Product state ("generalized" classical state)

A vector is decomposed into product of small vectors.

$$|\Psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots$$

structure: "**product state**"

independent elements: **small vectors**

e.g. $|\phi_1\rangle = \alpha|0\rangle + \beta|1\rangle$
 $|\phi_1\rangle = |01\rangle - |10\rangle$

Tensor network decomposition of a wave function

Target:

Exponentially large Hilbert space

$$\vec{v} \in \mathbb{C}^M \text{ with } M \sim a^N$$

+

Total Hilbert space is decomposed as
a product of "local" Hilbert space.

$$\mathbb{C}^M = \mathbb{C}^a \otimes \mathbb{C}^a \otimes \cdots \otimes \mathbb{C}^a$$

eg. array of quantum bits

→ **Tensor network decomposition**

$$v_i = v_{i_1, i_2, \dots, i_N} = \sum_{\{x\}} T^{(1)}[i_1]_{x_1, x_2, \dots} T^{(2)}[i_2]_{x_1, x_3, \dots} \cdots T^{(N)}[i_N]_{x_3, x_{100}, \dots}$$

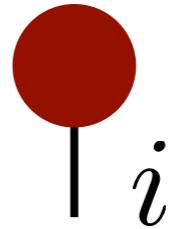
$i_n = 0, 1, \dots, a - 1$: index of local Hilbert space

$T[i]_{x_1, x_2, \dots}$: local tensor for "state" i

Graphical representations for tensor network

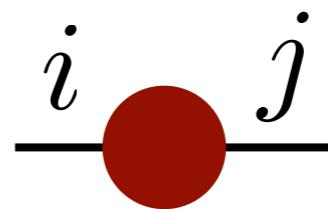
- Vector

$$\vec{v} : v_i$$



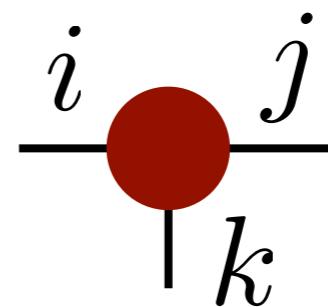
- Matrix

$$M : M_{i,j}$$



- Tensor

$$T : T_{i,j,k}$$



* **n-rank tensor = n-leg object**

When indices are not presented in a graph, it represent a tensor itself.

$$\vec{v} = \text{---} \bullet$$

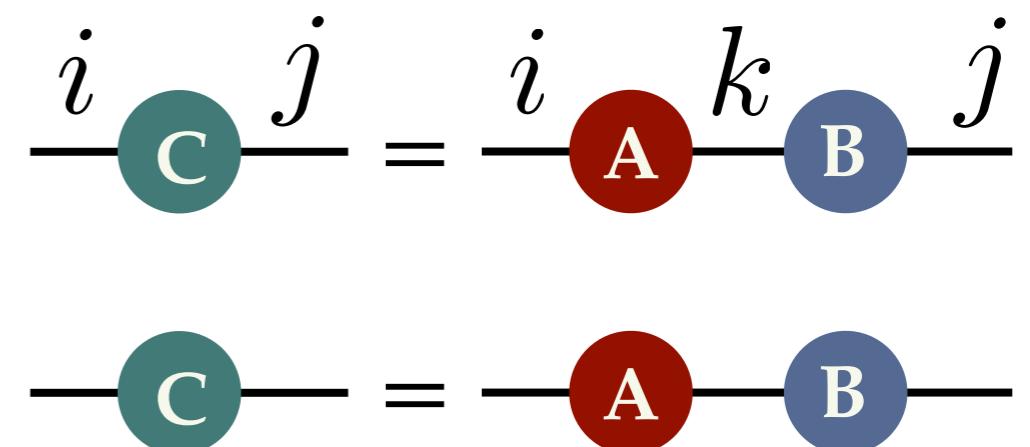
$$T = \text{---} \bullet \text{---}$$

Graphical representations for tensor network

Matrix product

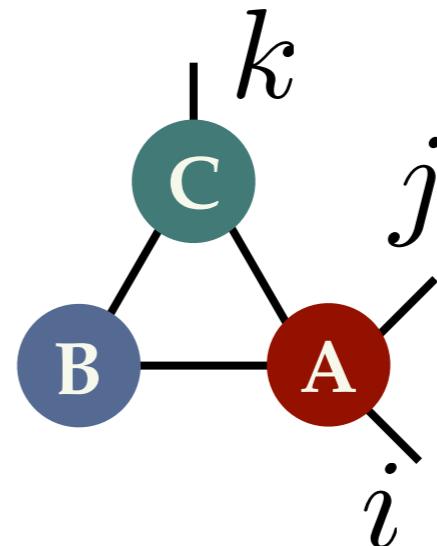
$$C_{i,j} = (AB)_{i,j} = \sum_k A_{i,k} B_{k,j}$$

$$C = AB$$



Generalization to tensors

$$\sum_{\alpha, \beta, \gamma} A_{i,j,\alpha,\beta} B_{\beta,\gamma} C_{\gamma,k,\alpha}$$

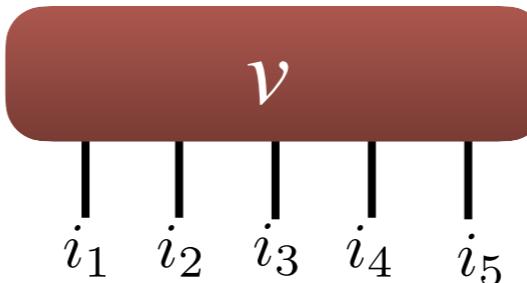


Contraction of a network = Calculation of a lot of multiplications

Graph for a tensor network decomposition

- Vector

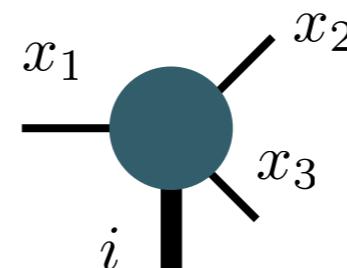
$$v_{i_1, i_2, i_3, i_4, i_5}$$



*Vector looks like a tensor

- Tensor

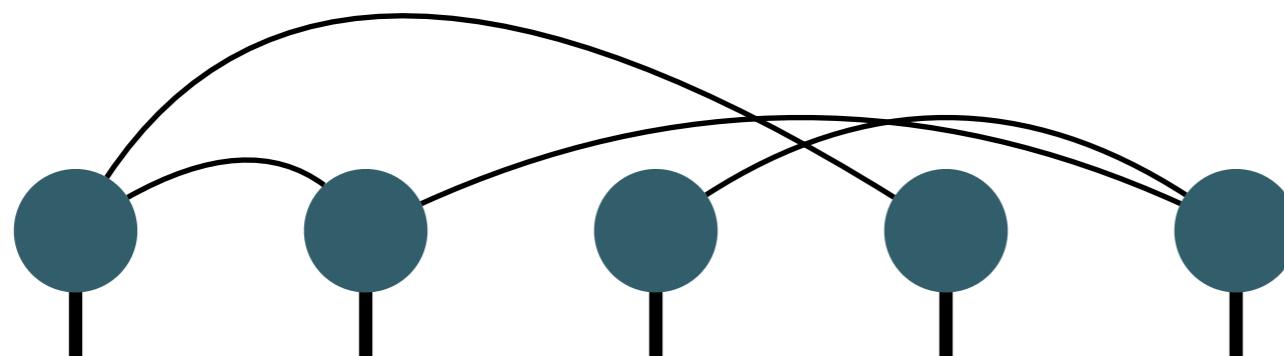
$$T[i]_{x_1, x_2, x_3}$$



*We treat i as an index
of the tensor.

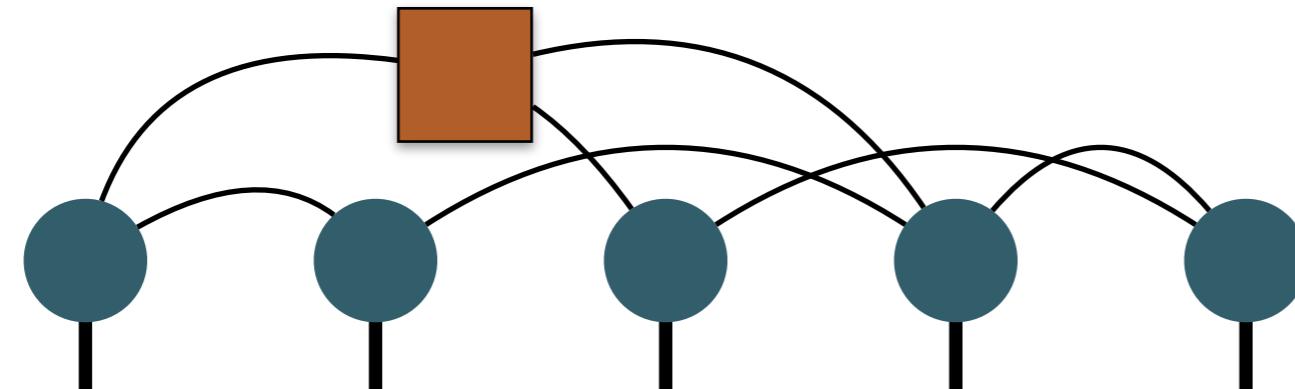
Tensor network decomposition

$$\vec{v} =$$



*We can consider tensors
independent of i .

$$\vec{w} =$$



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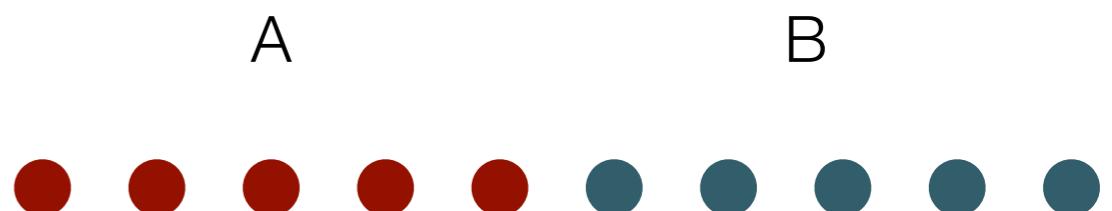
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Schmidt decomposition of a quantum physics

Quantum state $|\Psi\rangle = \sum_{\{i_1, i_2, \dots, i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$

Schmidt decomposition

Divide a system into two parts, A and B:



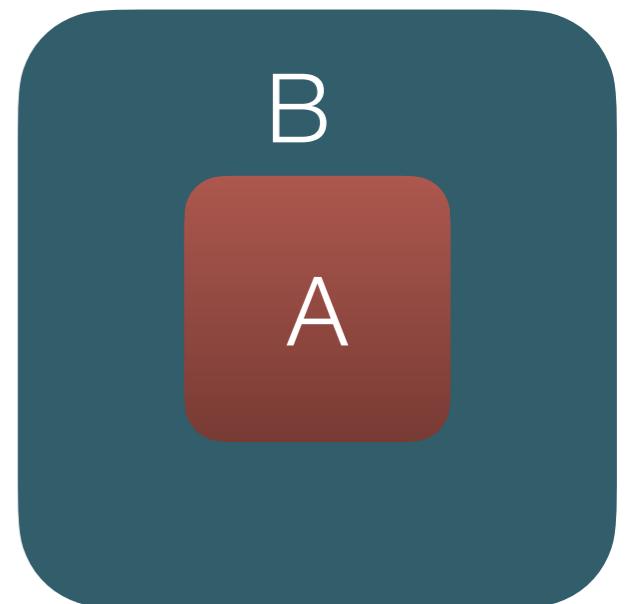
→ General wave function can be represented by a superposition of orthonormal basis set.

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle = \sum_i \lambda_i |\alpha_i\rangle \otimes |\beta_i\rangle$$

$$M_{i,j} \equiv \underbrace{\Psi_{(i_1, \dots), (\dots, i_N)}}_{\text{A} \quad \text{B}} \quad |A_i\rangle = |i_1, i_2, \dots\rangle$$
$$|B_j\rangle = |\dots, i_{N-1}, i_N\rangle$$

Orthonormal basis: $\langle A_i | A_j \rangle = \langle B_i | B_j \rangle = \delta_{i,j}$,
 $\langle \alpha_i | \alpha_j \rangle = \langle \beta_i | \beta_j \rangle = \delta_{i,j}$

Schmidt coefficient: $\lambda_i \geq 0$



Relation between SVD and Schmidt decomposition

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle$$

Singular values: $\lambda_m \geq 0$

SVD

$$M_{i,j} = \sum_m U_{i,m} \lambda_m V_{m,j}^\dagger$$

Singular vectors:

$$\sum_i U_{m,i}^\dagger U_{i,m'} = \delta_{m,m'}$$
$$\sum_j V_{m,j}^\dagger V_{i,m'} = \delta_{m,m'}$$

Relation to the Schmidt decomposition:

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle = \sum_m \lambda_m |\alpha_m\rangle \otimes |\beta_m\rangle$$

$$|\alpha_m\rangle = \sum_i U_{i,m} |A_i\rangle$$

$$|\beta_m\rangle = \sum_j V_{m,j}^\dagger |B_j\rangle$$



$$\langle \alpha_m | \alpha_{m'} \rangle = \langle \beta_m | \beta_{m'} \rangle = \delta_{m,m'}$$

SVD of the quantum state is directly related to the Schmidt decomposition.



of non-zero Schmidt coefficients is the rank of the matrix M

Schmidt rank of a quantum state

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle = \sum_m \lambda_m |\alpha_m\rangle \otimes |\beta_m\rangle$$

Schmidt rank:

of non-zero Schmidt coefficients (= rank of the matrix M)

Schmidt rank characterizes the quantum correlation between A and B .

- Schmidt rank = 1 $|\Psi\rangle = |\alpha\rangle \otimes |\beta\rangle$



The quantum state is represented as **a single product of two states.**

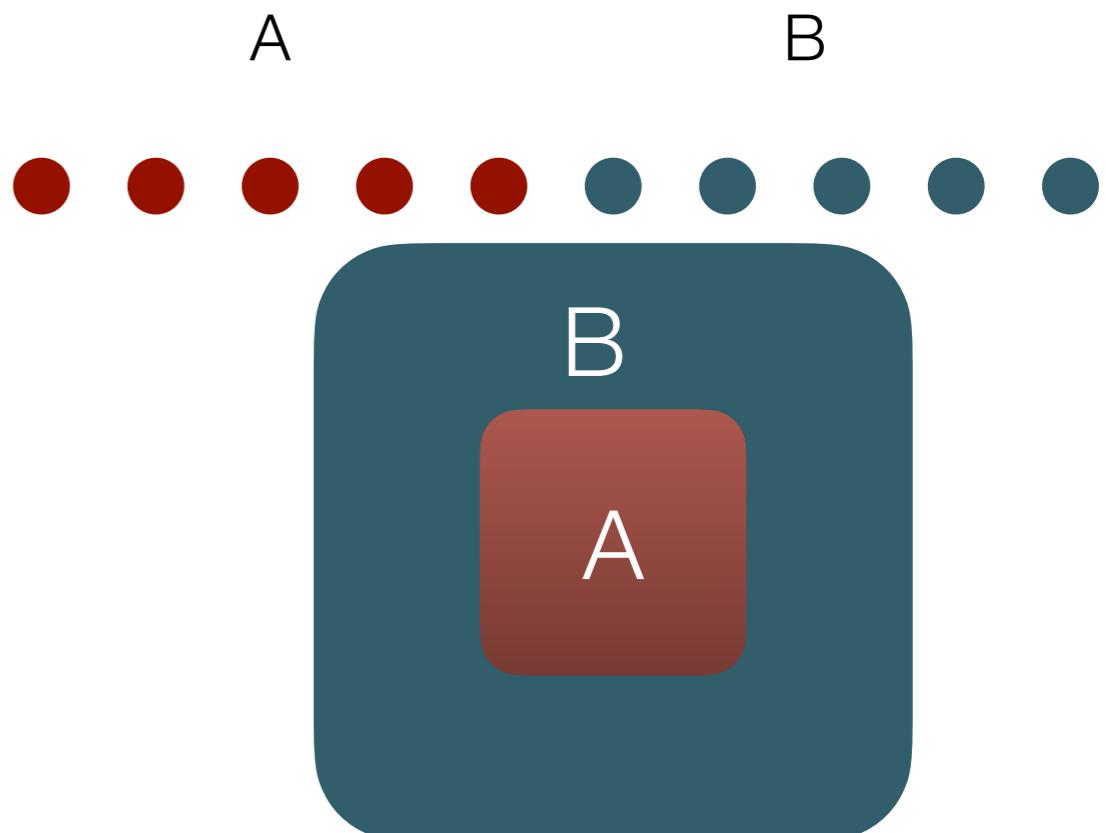
Product state

- Schmidt rank > 1 $|\Psi\rangle = \sum_m \lambda_m |\alpha_m\rangle \otimes |\beta_m\rangle$



The quantum state is represented as **a sum of product states.**

(The Origin of the **nonlocal correlation**)

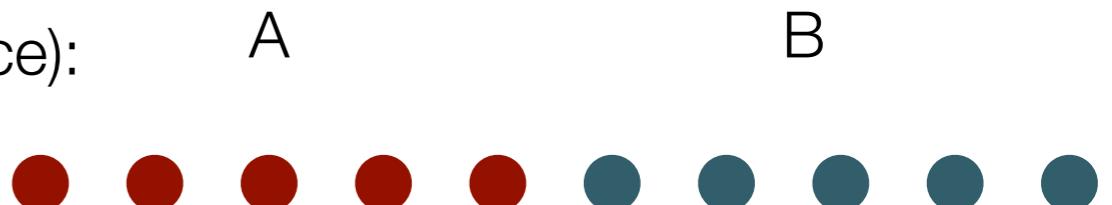


Entanglement entropy

Entanglement entropy:

Reduced density matrix of a sub system (sub space):

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi|$$



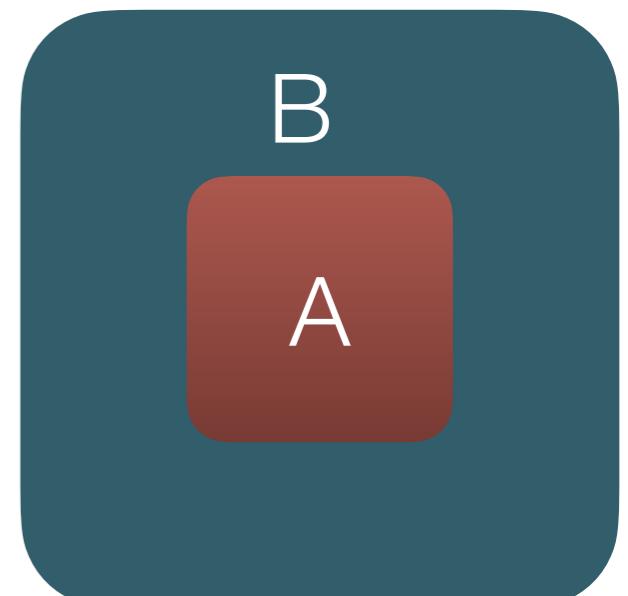
Entanglement entropy = von Neumann entropy of ρ_A

$$S = -\text{Tr}(\rho_A \log \rho_A)$$

Schmidt decomposition $|\Psi\rangle = \sum_i \lambda_i |\alpha_i\rangle \otimes |\beta_i\rangle$

→ $\rho_A = \sum_i \lambda_i^2 |\alpha_i\rangle\langle\alpha_i|$ (*Exercise)

→ $S = -\sum_i \lambda_i^2 \log \lambda_i^2$ $(\sum_i \lambda_i^2 = 1)$



Entanglement entropy is calculated through
the spectrum of Schmidt coefficients.
(It also indicates $S = -\text{Tr}(\rho_B \log \rho_B)$)

Area law of the entanglement entropy **in physics**

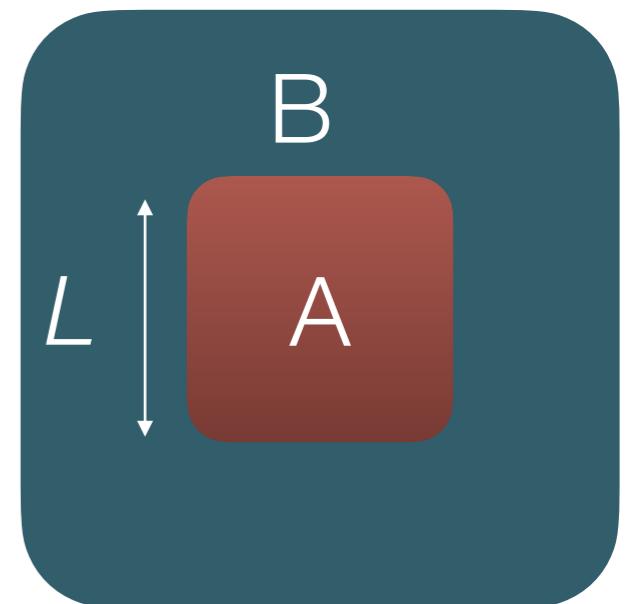
General wave functions (vector):

EE is proportional to its **volume (# of qubits)**.

$$S = -\text{Tr}(\rho_A \log \rho_A) \propto L^d \quad (\text{c.f. random vector})$$

Ground state wave functions:

For a lot of ground states, EE is proportional to its area.



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

$$S = -\text{Tr}(\rho_A \log \rho_A) \propto L^{d-1}$$

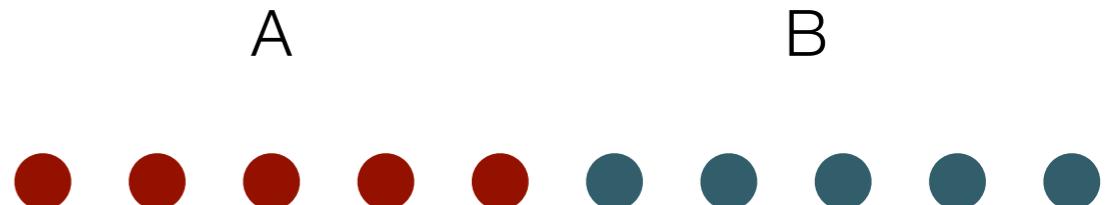
In the case of **one-dimensional system**:

Gapped ground state for **local Hamiltonian**

M.B. Hastings, J. Stat. Mech.: Theory Exp. P08024 (2007)

$$S = O(1)$$

**Ground state are in a small part
of the huge Hilbert space**



Expected entanglement scaling for spin systems

Table 1

Entanglement entropy scaling for various examples of states of matter, either disordered, ordered, or critical, with smooth boundaries (no corners).

Physical state	Entropy	Example
Gapped (brok. disc. sym.)	$aL^{d-1} + \ln(\deg)$	Gapped XXZ [143]
$d = 1$ CFT	$\frac{c}{3} \ln L$	$s = \frac{1}{2}$ Heisenberg chain [21]
$d \geq 2$ QCP	$aL^{d-1} + \gamma_{\text{QCP}}$	Wilson–Fisher O(N) [136]
Ordered (brok. cont. sym.)	$aL^{d-1} + \frac{n_G}{2} \ln L$	Superfluid, Néel order [147]
Topological order	$aL^{d-1} - \gamma_{\text{top}}$	\mathbb{Z}_2 spin liquid [159]

(Nicolas Laflorencie, Physics Reports **646**, 1 (2016))

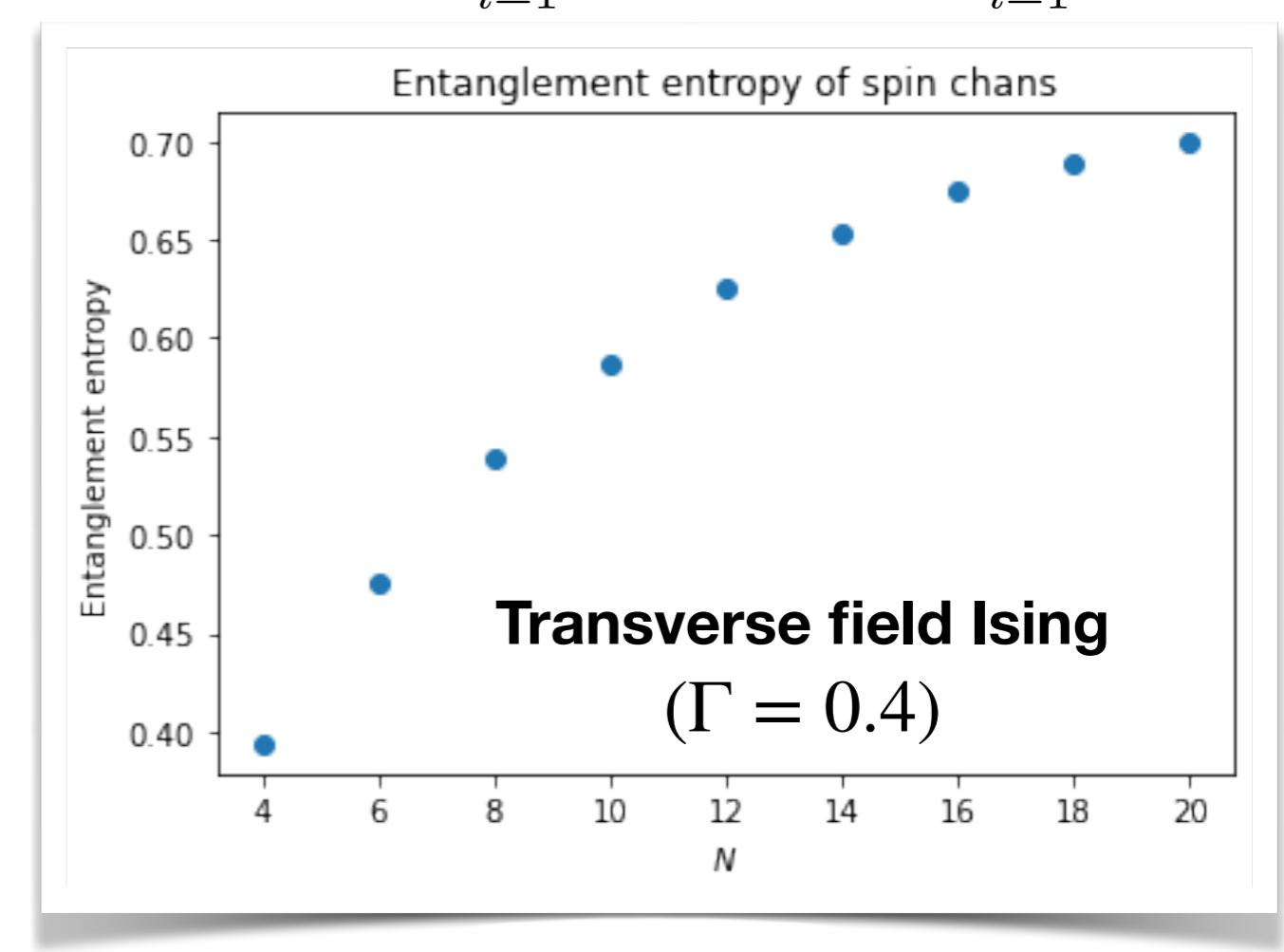
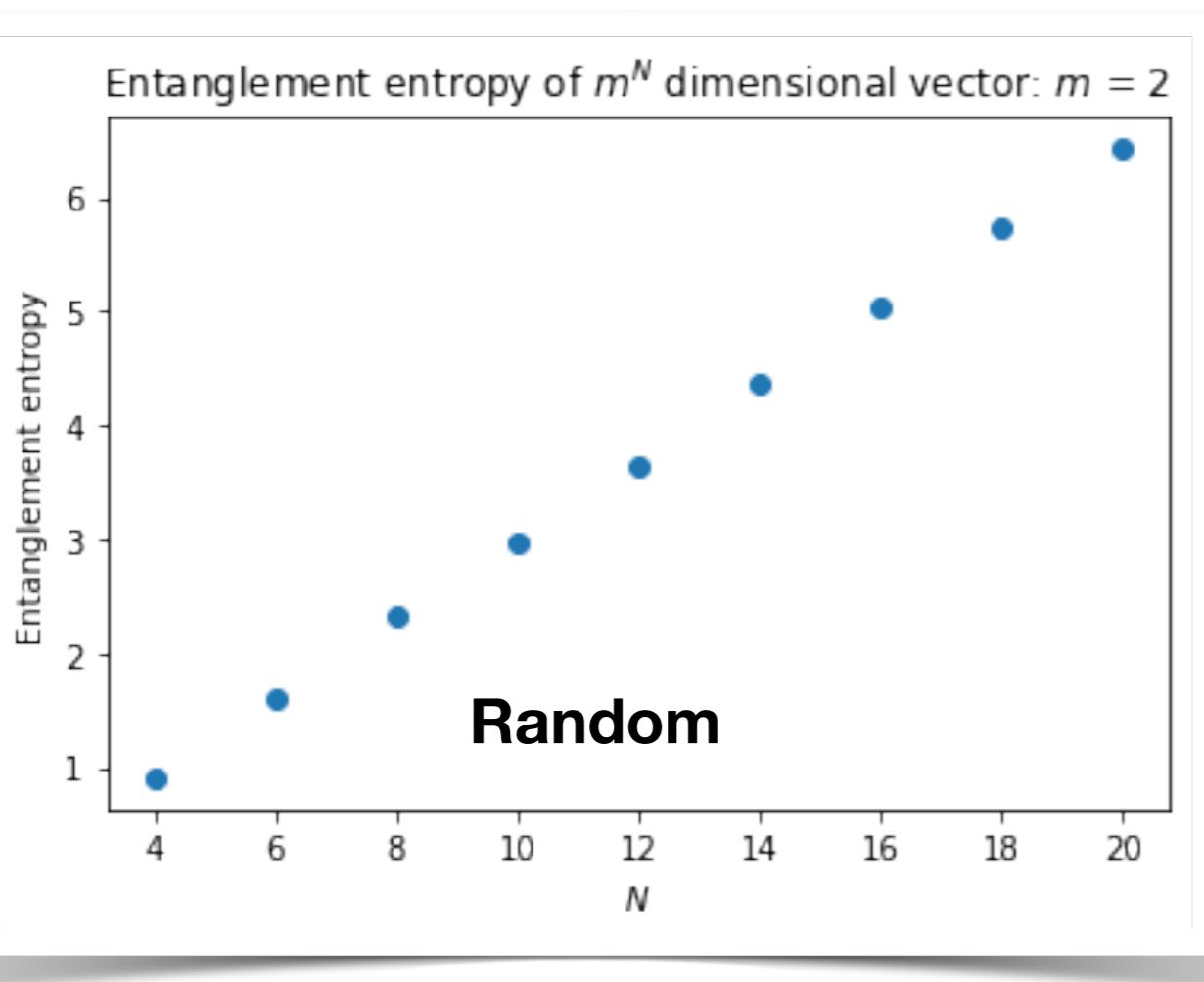
cf. free fermion

$$S \propto L^{d-1} \log L$$

For $d \geq 2$, leading contribution satisfies area law even for gapless (critical) systems.

Examples of entanglement entropy scalings

$$\vec{v} \in \mathbb{C}^{2^N}$$



Random vector: Volume low
Ground state: Area low

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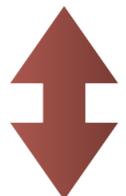
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Data compression of tensors (vectors)

Eg. General wave function:

$$|\Psi\rangle = \sum_{\{i_1, i_2, \dots, i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

Coefficient vector can represent any points in the Hilbert space.

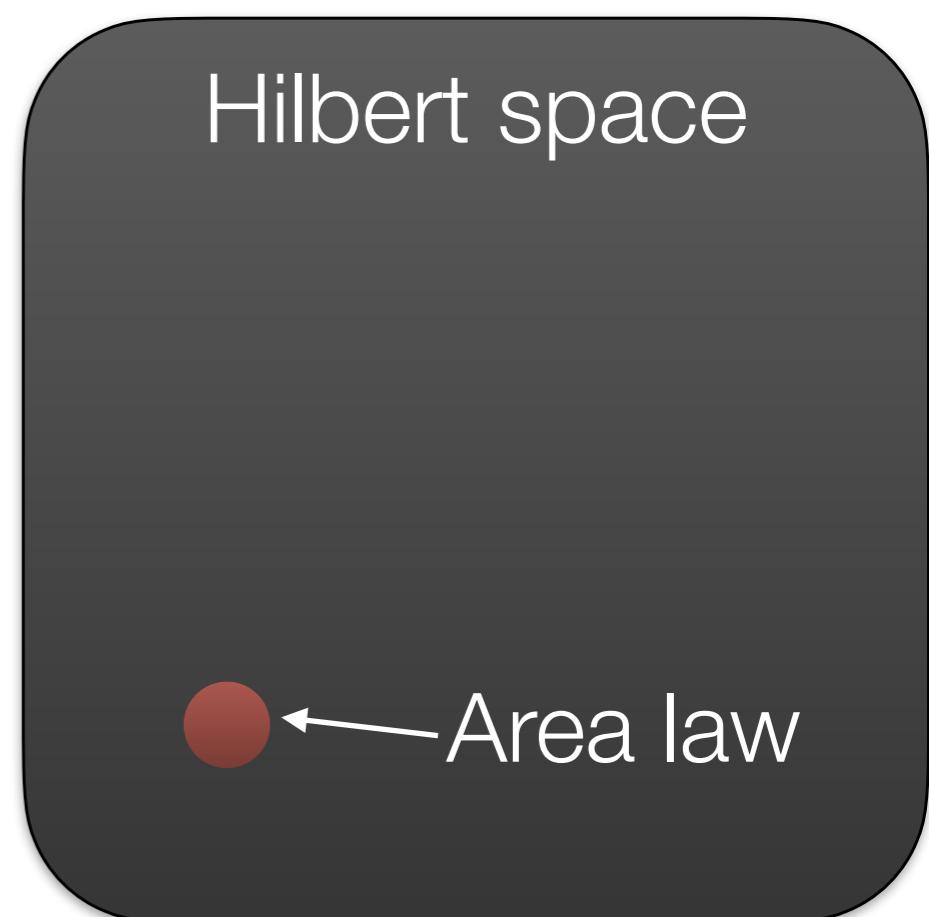


Ground states satisfy **the area law**.

- In order to represent the ground state **accurately**, we might not need all of a^N elements.
- Data compression by tensor decomposition:

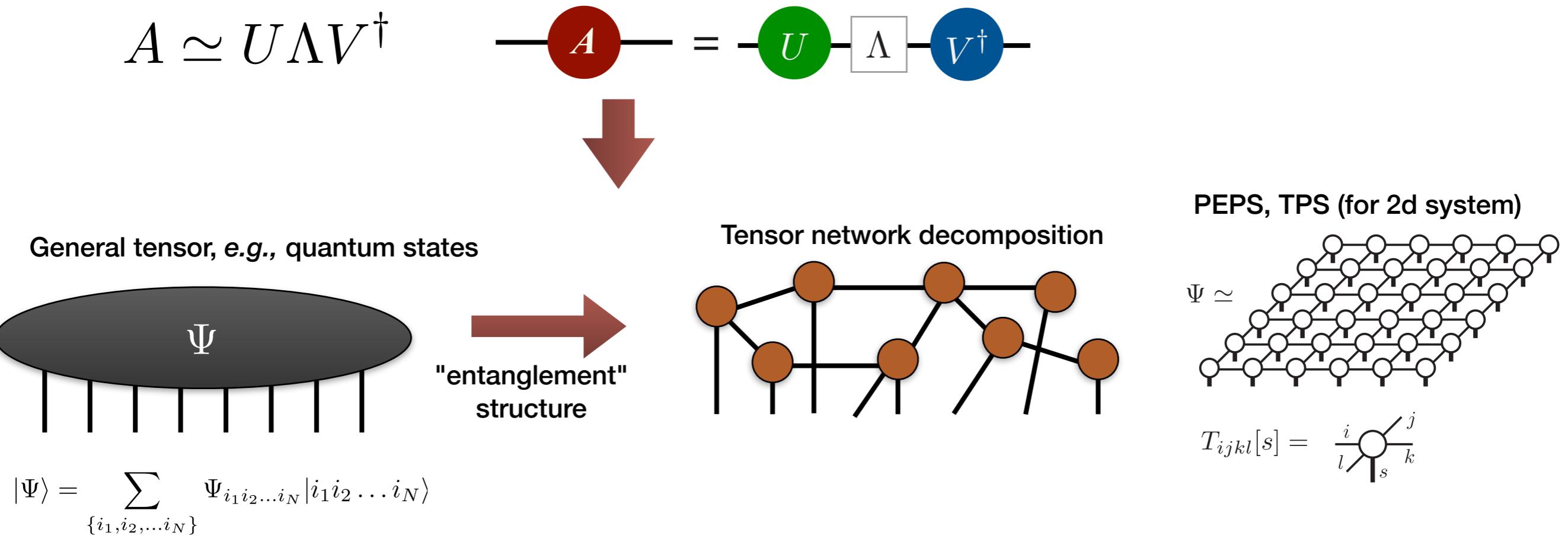
Tensor network decomposition

***Same idea holds for any tensors.**



Tensor network state for quantum many-body system

Generalization of the low-rank approximation of matrices to tensors



By choosing a "good" network, we can express G.S. wave function efficiently.

ex. TPS: # of elements $\sim ND^4$

D : dimension of the tensor T

Exponential → Linear

Good reviews:

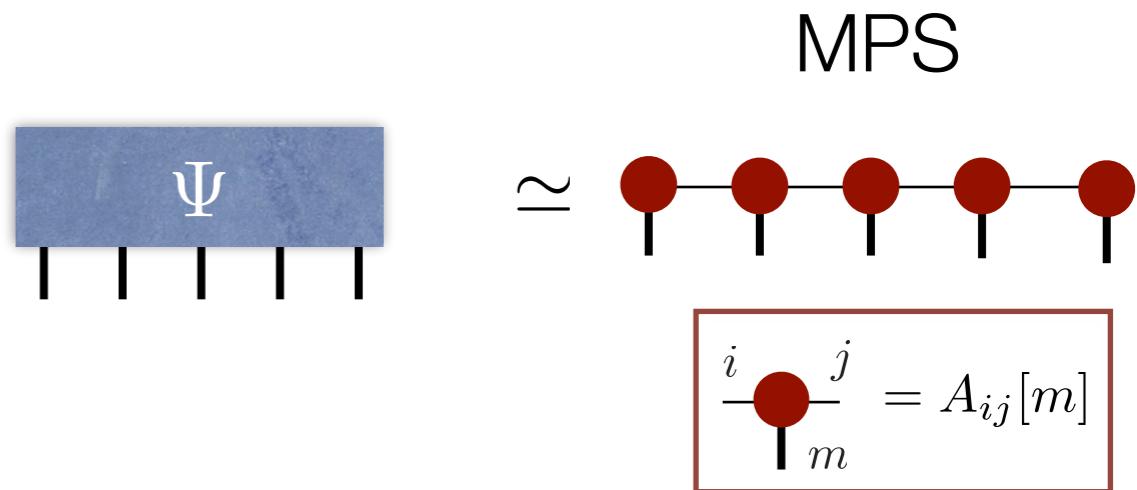
Matrix product state (MPS)

(U. Schollwöck, Annals. of Physics **326**, 96 (2011))
(R. Orús, Annals. of Physics **349**, 117 (2014))

$$|\Psi\rangle = \sum_{\{i_1, i_2, \dots, i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

$$\Psi_{i_1 i_2 \dots i_N} \simeq A_1[i_1] A_2[i_2] \cdots A_N[i_N]$$

$A[i]$: Matrix for state i



Note:

- MPS is called "tensor train decomposition" in applied mathematics
(I. V. Oseledets, SIAM J. Sci. Comput. **33**, 2295 (2011))
- A product state is represented by MPS with 1×1 "Matrix" (scalar)

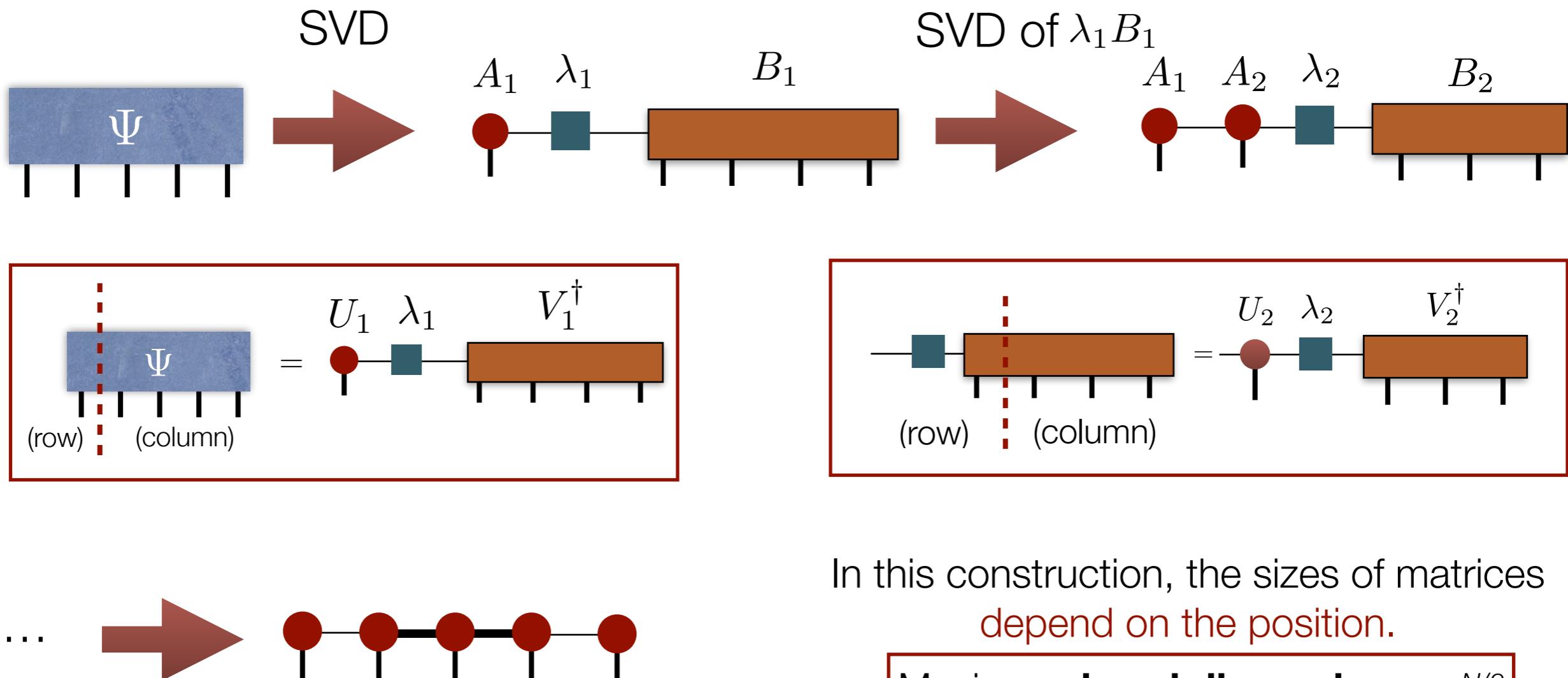
$$|\Psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots$$

$$\Psi_{i_1 i_2 \dots i_N} = \phi_1[i_1] \phi_2[i_2] \cdots \phi_N[i_N]$$

$$\phi_n[i] \equiv \langle i | \phi_i \rangle$$

Matrix product state without approximation

General vectors can be represented by MPS exactly through successive Schmidt decompositions

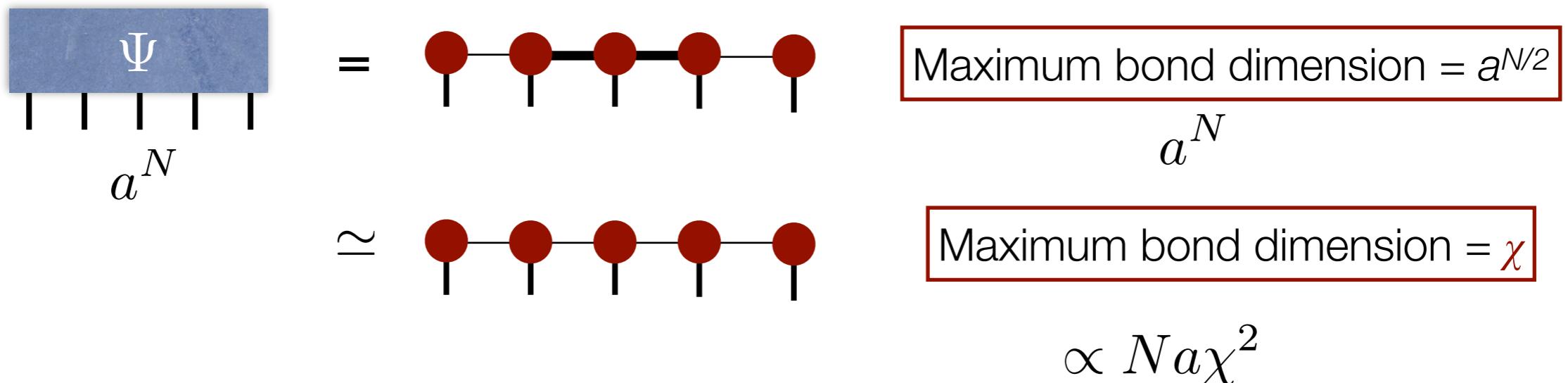


In this construction, the sizes of matrices depend on the position.

Maximum **bond dimension** = $a^{N/2}$

At this stage, **no data compression**.

Matrix product state: Low rank approximation

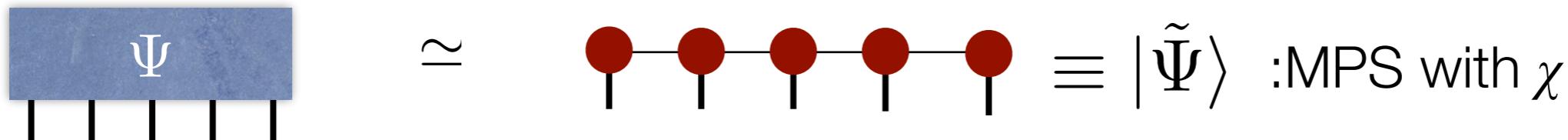


If the entanglement entropy of the system is **O(1)** (independent of N), matrix size " χ " can be small for accurate approximation.

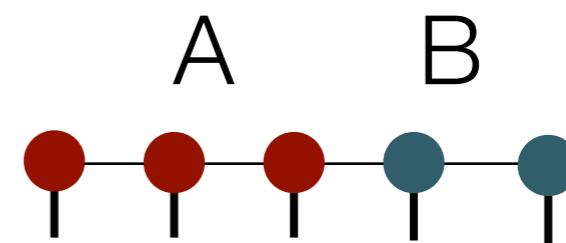
→ MPS is good for gapped 1d systems.

On the other hand, if the EE increases as increase N , " χ " must be increased to keep the same accuracy.

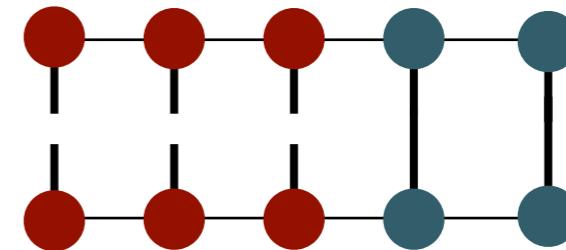
Upper bound of Entanglement entropy



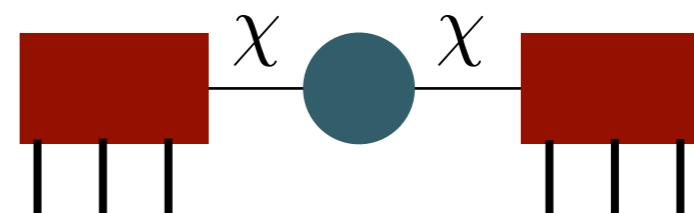
→ Reduced density matrix of region A:



$$\rho_A = \text{Tr}_B |\tilde{\Psi}\rangle\langle\tilde{\Psi}| =$$



★ Structure of ρ_A :

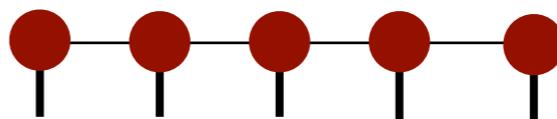


$$\text{rank } \rho_A \leq \chi$$

$$S_A = -\text{Tr } \rho_A \log \rho_A \leq \log \chi$$

Required bond dimension in MPS representation

$$S_A = -\text{Tr } \rho_A \log \rho_A \leq \log \chi$$



The upper bound is independent of the "length".

length of MPS \Leftrightarrow size of the problem

$$N \quad a^N$$

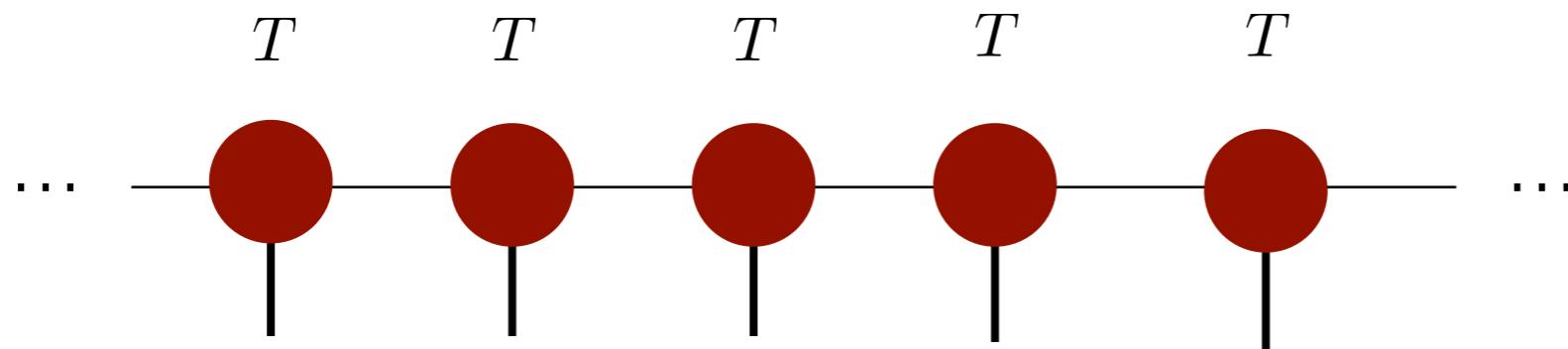


EE of the original vector	Required bond dimension in MPS representation
$S_A = O(1)$	$\chi = O(1)$
$S_A = O(\log N)$	$\chi = O(N^\alpha)$
$S_A = O(N^\alpha)$	$\chi = O(c^{N^\alpha})$

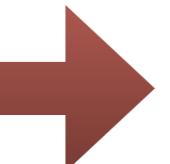
$$(\alpha \leq 1)$$

MPS for infinite chains

By using MPS, we can write the wave function of a translationally invariant **infinite chain**



Infinite MPS (iMPS) is made by repeating T infinitely.

Translationally invariant system  T is independent of positions!

Point!

If the entanglement entropy of a certain state satisfies the area law, we efficiently approximate infinite system with a finite size matrix (tensor) T .

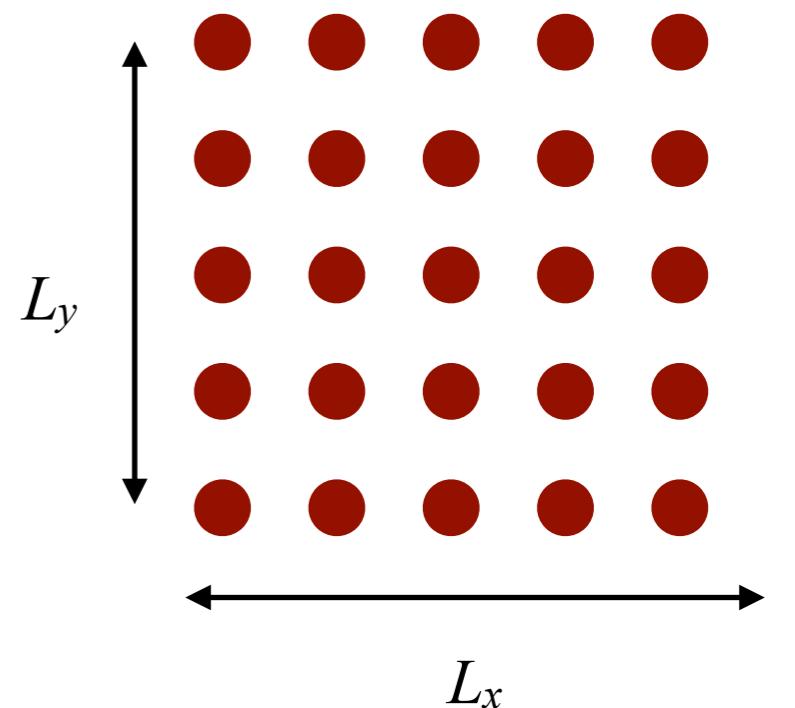
Higher dimensional system

Transverse field Ising model on **square lattice**:

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_i^z S_j^z - h \sum_{i=1}^N S_i^x$$

$\sum_{\langle i,j \rangle}$:Sum over the nearest neighbor pair

Two-dimensional array



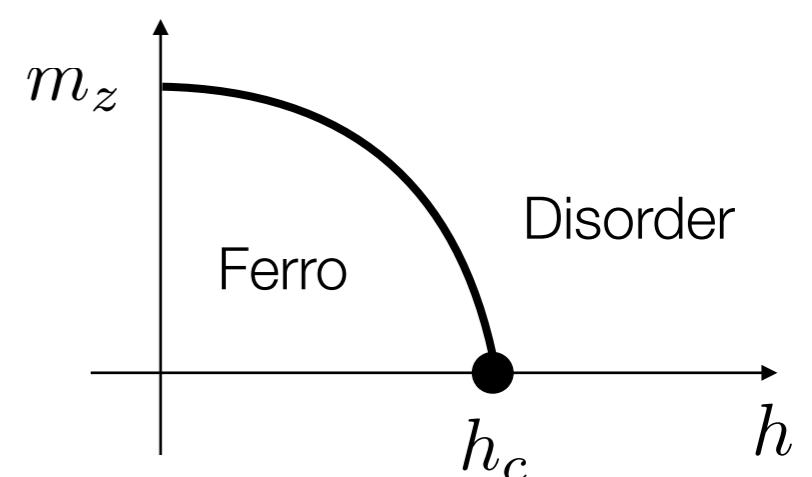
Area law

Even in ferro and disordered phases,
the entanglement entropy depends on size N .

$$S_A \sim \sqrt{N} = L$$

$$N = L_x \times L_y$$

Phase diagram

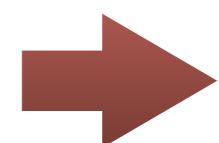


MPS for two-dimensional system

When we apply MPS representation for a square lattice system:

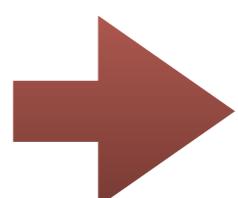
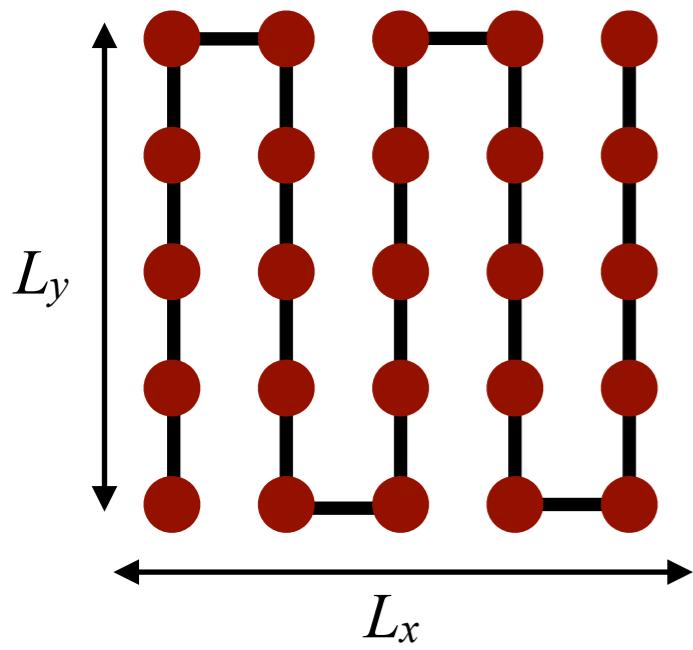
Setting **(1)** $S_A \leq L_x \log \chi$:Satisfying area law?

Setting **(2)** $S_{A'} \leq \log \chi$:Break down of the area law!



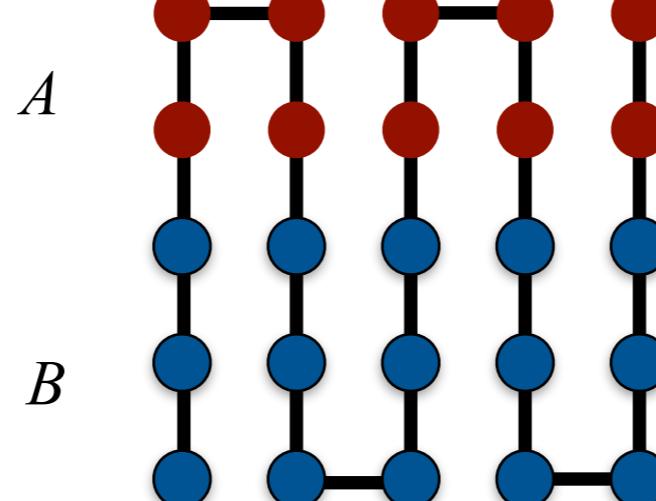
MPS cannot cover the area law of the entanglement entropy in higher ($d = 2, 3, \dots$) dimensions.

Possible MPS
(Snake form)

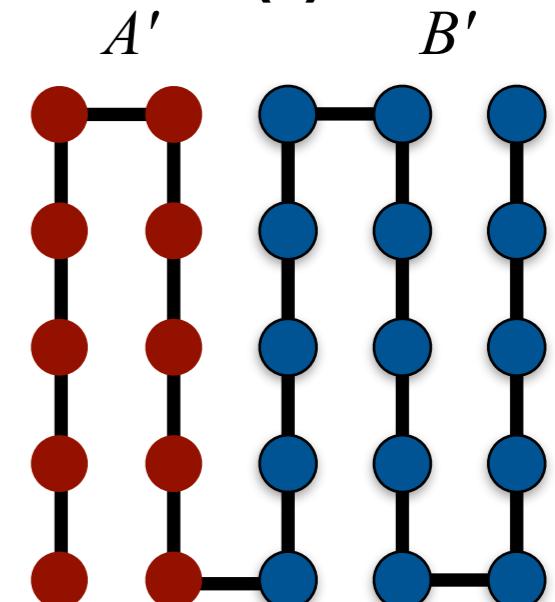


Two settings of **system** and **environment**

(1)



(2)



MPS for two-dimensional system: comment

MPS can treat "rectangular" or "quasi one dimensional" lattice.

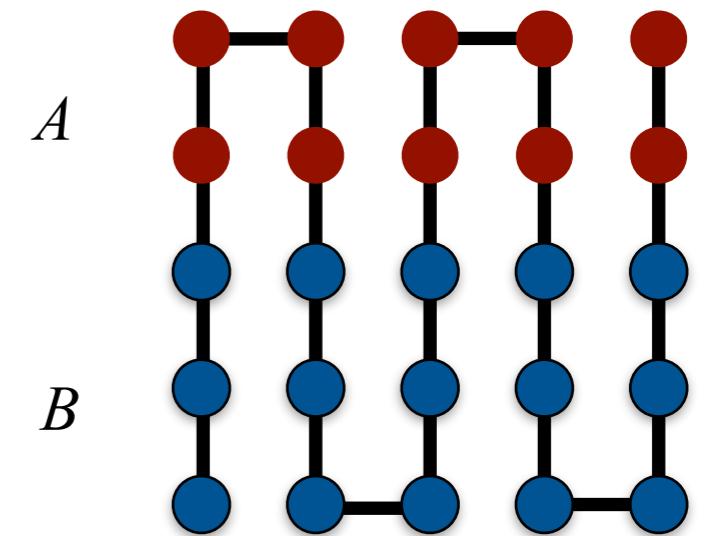
In setting (1), MPS can satisfy the area law **partially**.

→ We can increase L_x easily with keeping L_y constant.

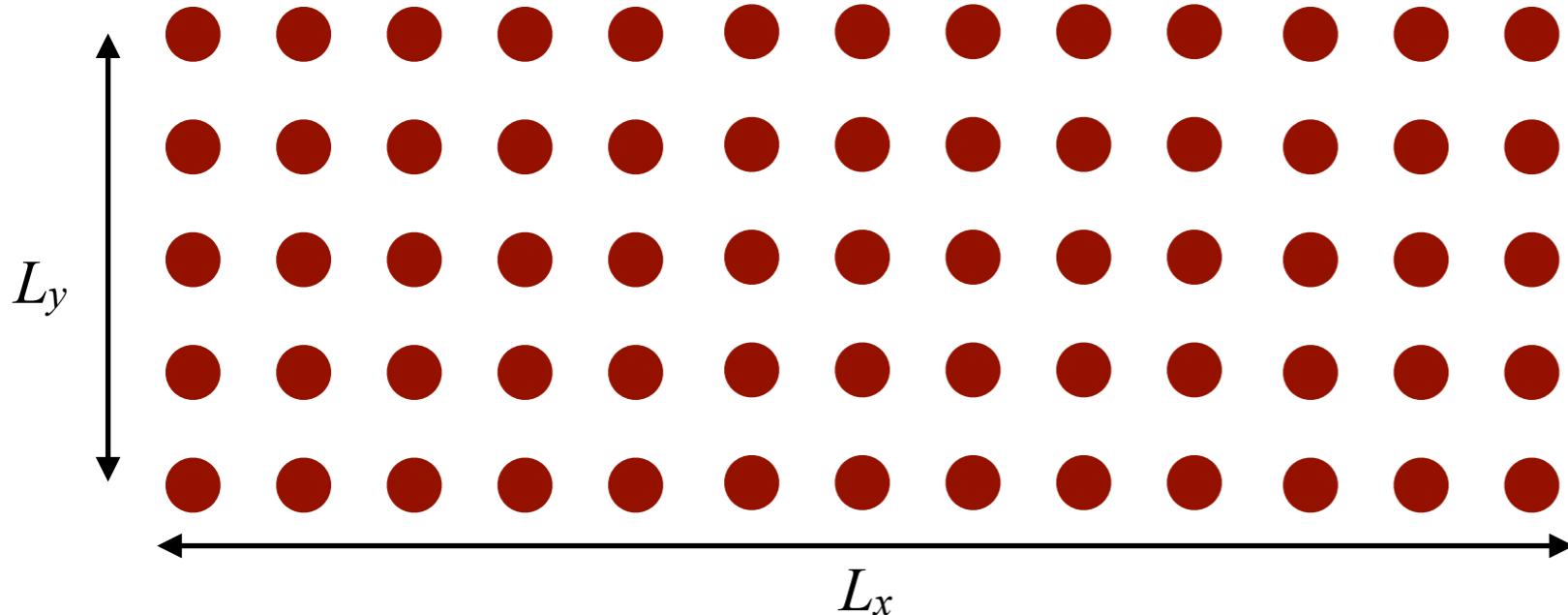
$$\chi = O(e^{L_y})$$

$$L_y \lesssim 10, L_x \gg L_y$$

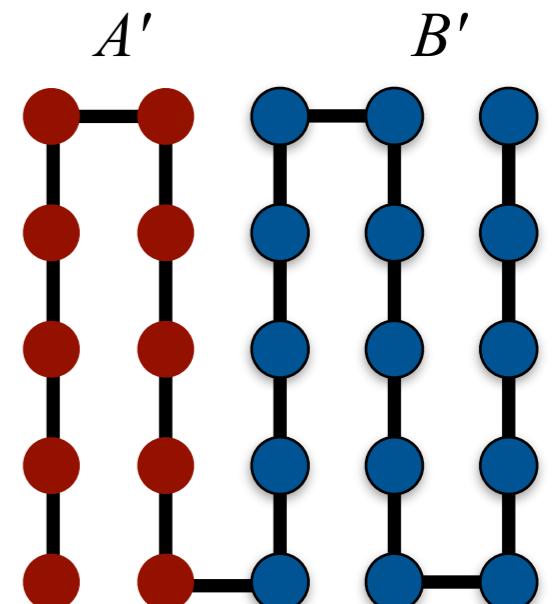
(1) $S_A \leq L_x \log \chi$



Quasi one dimensional system ("strip" or "cylinder")



(2) $S_{A'} \leq \log \chi$



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Entanglement entropy in higher dimensions

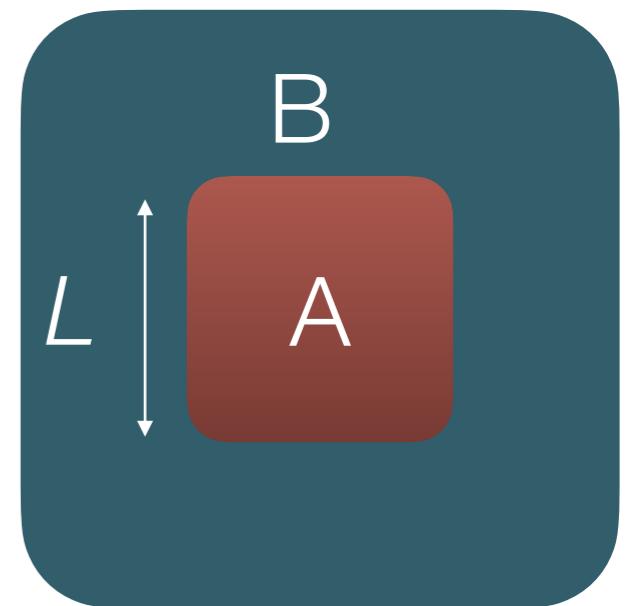
Ground state wave functions:

For a lot of ground states, EE is proportional to its area.

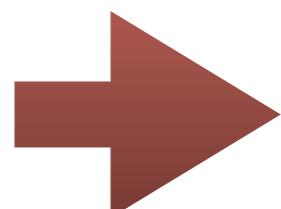
J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys, 277, **82** (2010)

Area law:

$$S = -\text{Tr}(\rho_A \log \rho_A) \propto L^{d-1}$$



In d=1, MPS satisfies the area law.



Q. What is a simple generalization of MPS to $d > 1$?

A. It is a Tensor Product State (TPS)!

Tensor product states (TPS)

TPS (Tensor Product State) (AKLT, T. Nishino, K. Okunishi, ...)

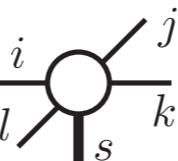
PEPS (Projected Entangled-Pair State)

(F. Verstraete and J. Cirac, arXiv:cond-mat/0407066)

Ex. : Square lattice TPS

Network consist of 4+1-leg tensors

local degree : s

$$T_{ijkl}[s] = \begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{array}$$


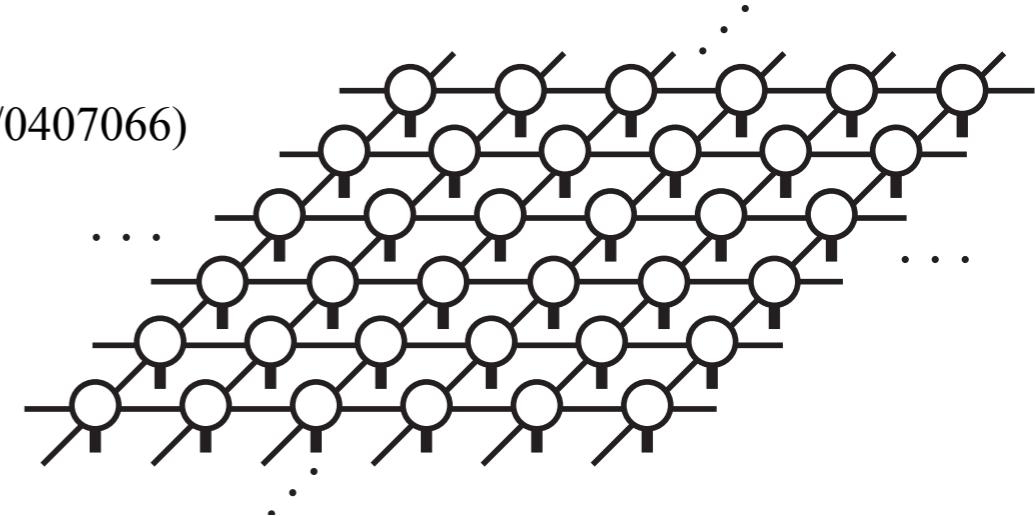
Virtual degrees : i, j, k, l

Dimension of each indices = **bond dimension (D)**

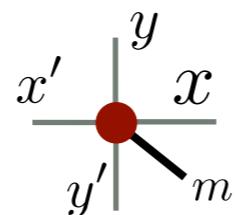
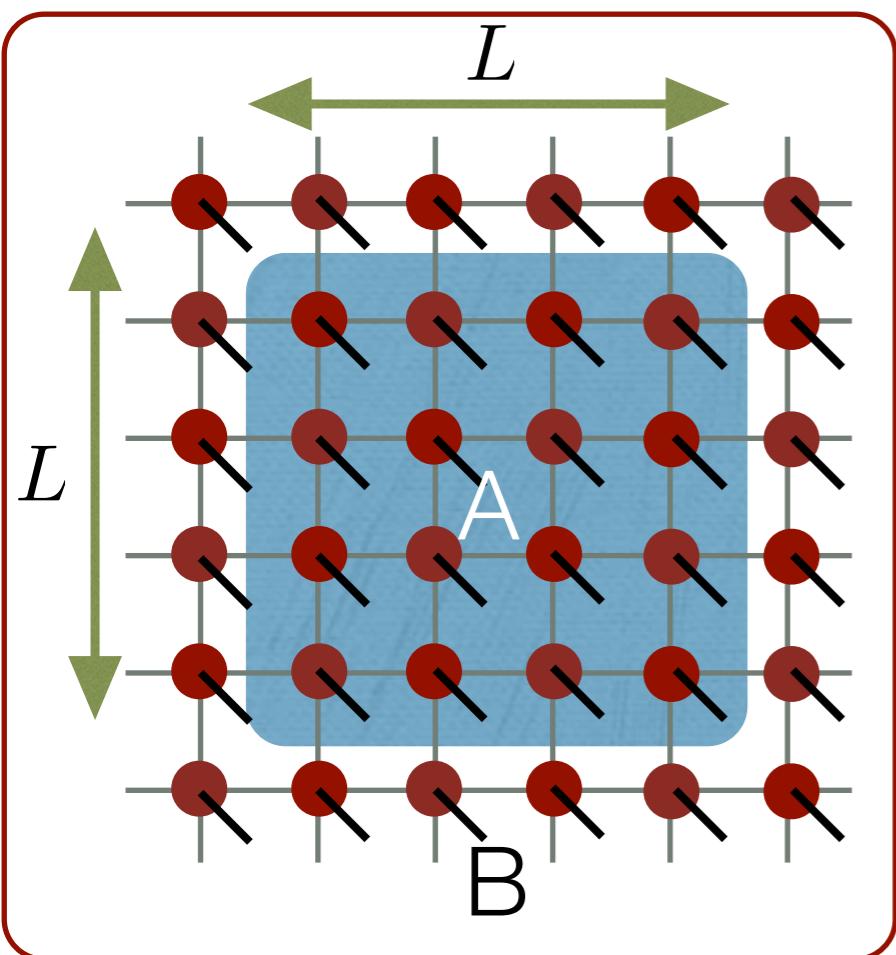
It determines the accuracy of the approximated wavefunction. ($D \rightarrow \infty$ it becomes exact.)

As we will see, TPS satisfy the area law of the entanglement entropy.

- $S \leq L^{d-1} \log D \propto L^{d-1}$
 - Finite D give us an accurate approximation of the low energy states.
 - We can treat even **infinite system** directly with a finite D : **iTPS**



Entanglement entropy of TPS (PEPS)



Bond dimension = D

of bonds connecting regions A and B

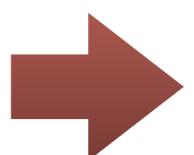
$$N_c(L) = 4L \quad (\text{square lattice})$$

$$N_c(L) = 2dL^{d-1} \quad (\text{d-dimensional hyper cubic lattice})$$

$$\text{rank } \rho_A \leq D^{N_c(L)} \sim D^{2dL^{d-1}}$$

$$S_A = -\text{Tr } \rho_A \log \rho_A \leq 2dL^{d-1} \log D$$

TPS can satisfy the area law even for $d > 1$.



We can efficiently approximate vectors in higher dimensional space by TPS.

* Similar to the MPS in 1d, TPS can approximate infinite system!

Tensor product states for infinite system: iTPS

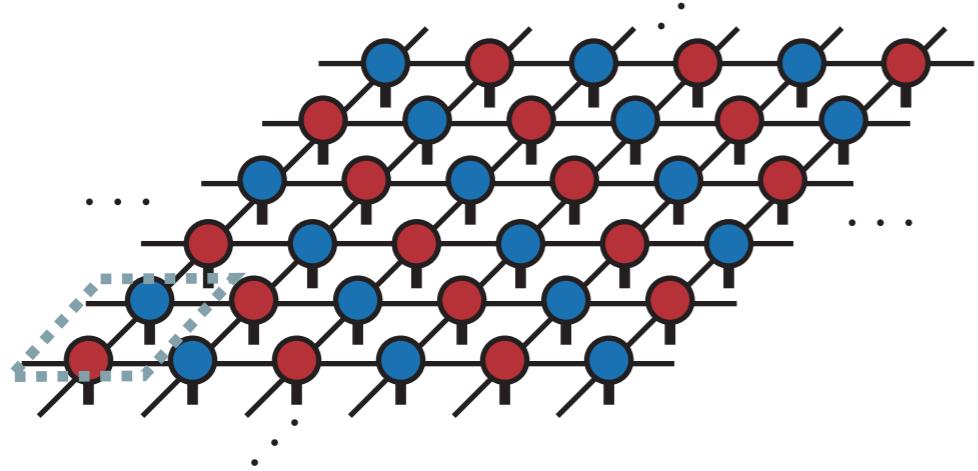
When the state has a translational invariance:

$$\underline{T}|\Psi\rangle = |\Psi\rangle$$

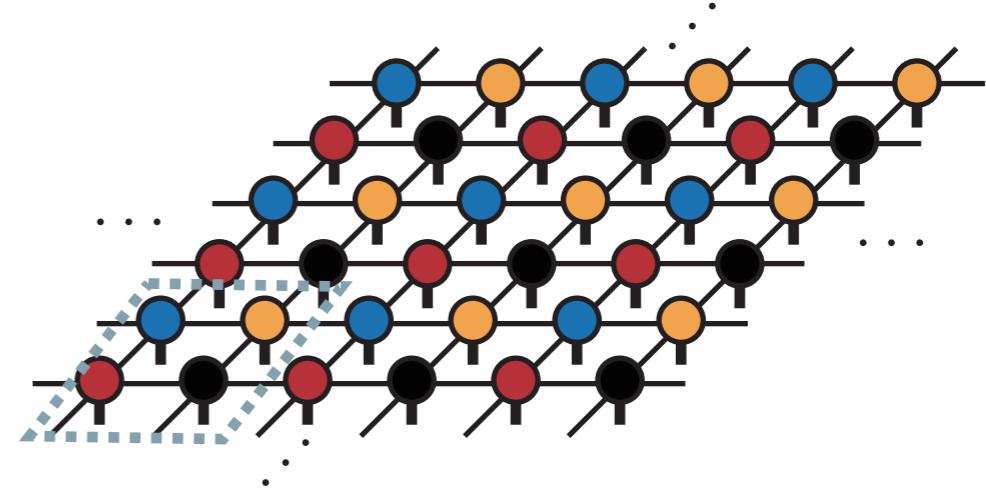
translation ↑
 No phase factor

Quantum state for the infinite system can be represented by repeating the identical tensors periodically.

→ We can represent infinite system by a finite degree of freedoms.



2-site unit cell



4-site unit cell

* A lot of interesting problems in quantum spin systems satisfy such translational symmetry.

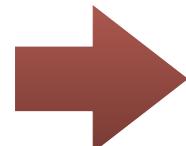
Difference between MPS and TPS

Cost of tensor network contraction:

d-dimensional cubic lattice $N = L^d$

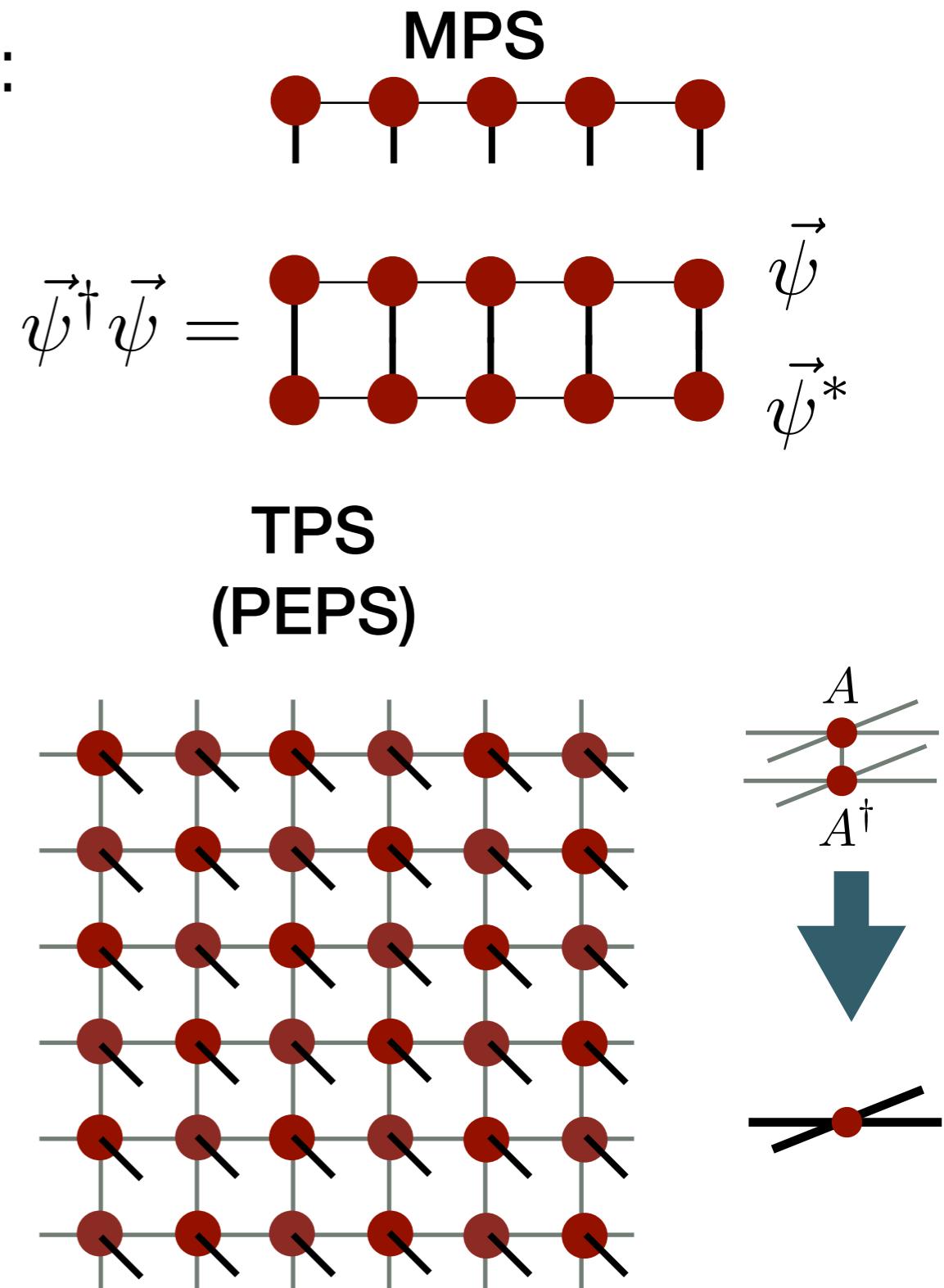
MPS: $O(N)$

TPS: $O(e^{L^{d-1}})$



It is **impossible** to perform exact contraction even if we know local tensors in the case of TPS.

In the case of TPS,
usually we **approximately**
calculate the contraction.



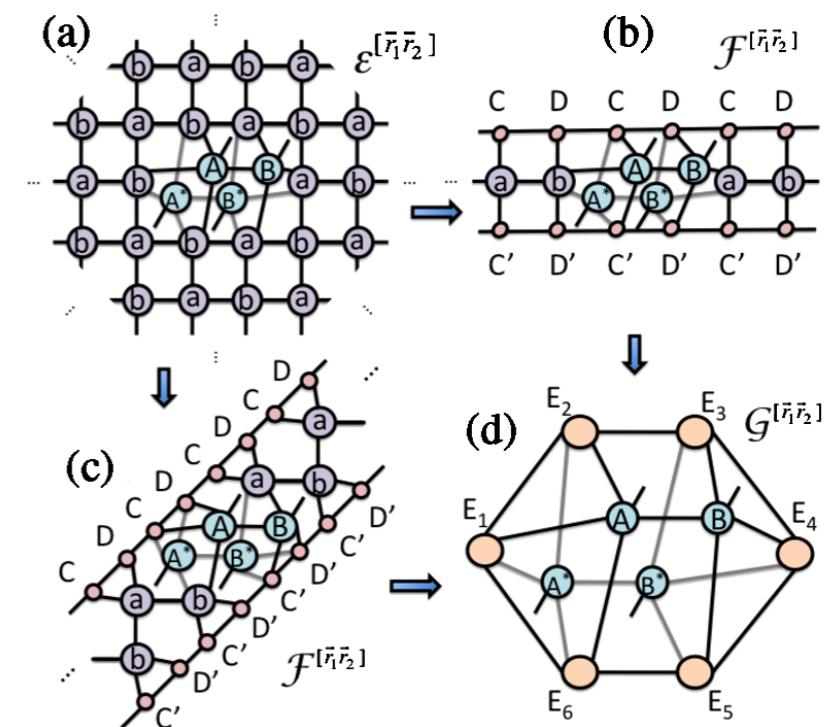
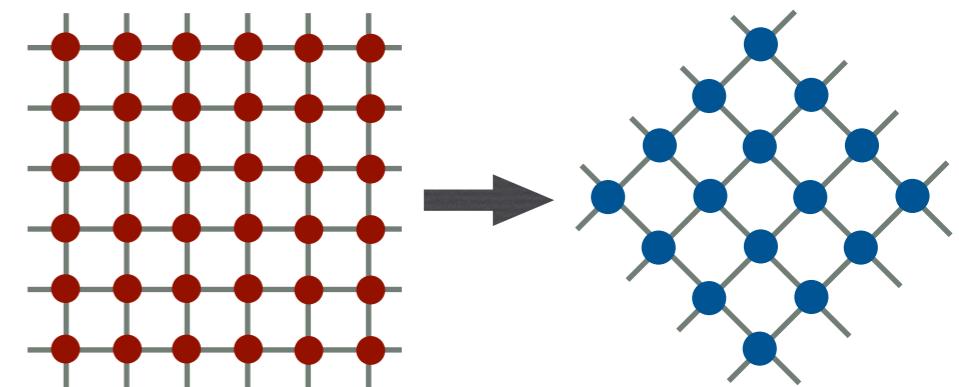
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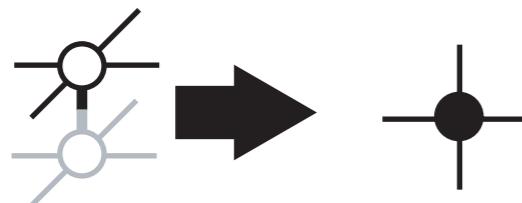
Contraction of iTPS

Methods for approximate contraction of iTPS:

- Tensor network renormalizations
 - TRG, HOTRG, SRG, TNR, loop-TNR, ...
- Boundary MPS
 - (Y. Hieida *et al* (1999) , J. Jordan *et al*, Phys. Rev. Lett. **101**, 250602 (2008))
- Corner transfer matrix
 - T. Nishino and K. Okunishi, JPSJ **65**, 891 (1996), R. Orús *et al*, Phys. Rev. B **80**, 094403 (2009).
- Single layer approaches
 - bMPS: H. J. Liao *et al*, PRL **118**, 137202 (2017), Z. Y. Xie *et al*, PRB **96**, 045128 (2017).
 - CTM: Chih-Yuan Lee *et al*, PRB **98**, 224414 (2018) .
- Mean-field environment
 - S. Jharomi and R. Orús, PRB **99**, 195105 (2019).



Corner transfer matrix (CTM) method for contraction

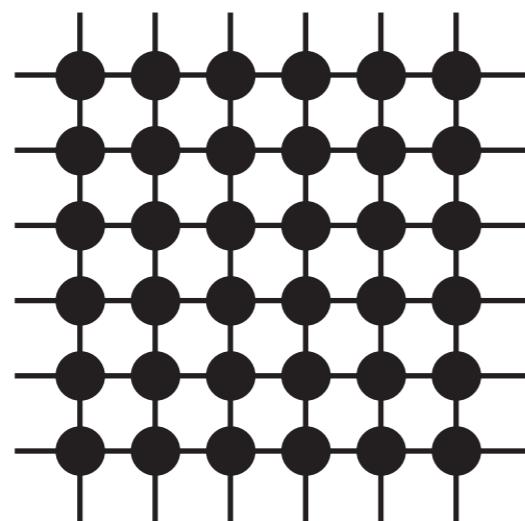


Bond-dimension: D

Bond-dimension: D^2

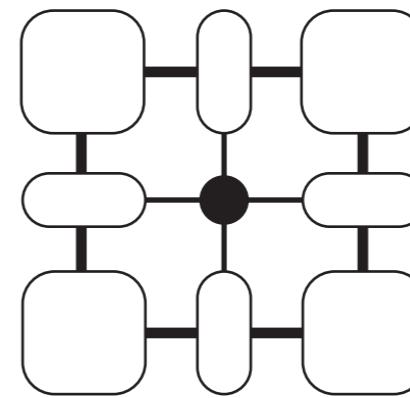
:

$\langle \Psi | \Psi \rangle = \dots$



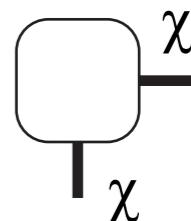
\dots

**Corner transfer matrix
Representation**

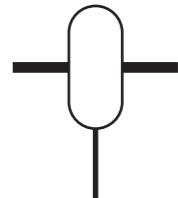


\approx

Corner transfer matrix

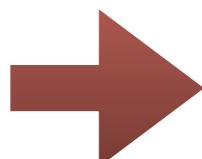


Edge tensors



Approximated representation of infinite environment with bond-dimension χ corner transfer matrices

Corner transfer matrices are calculated with the cost $O(\chi^2 D^6)$, $O(\chi^3 D^4)$

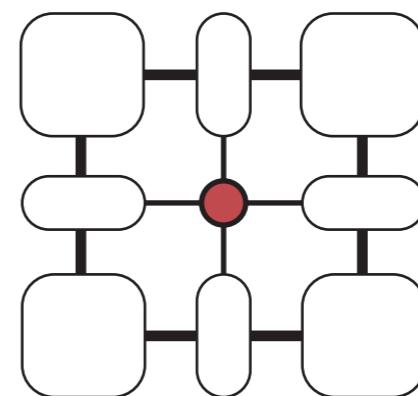
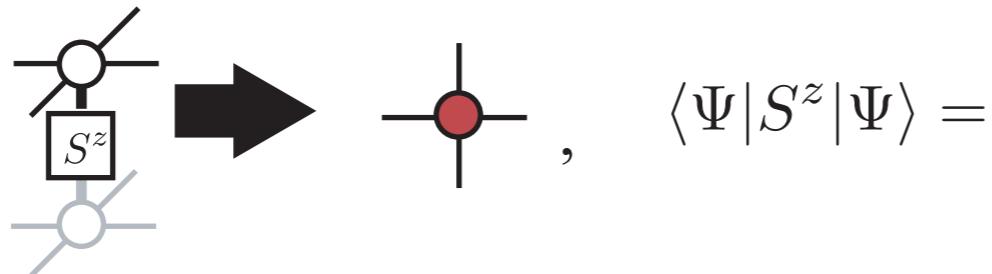


- * χ should be sufficiently large so that physical quantities converge.
- * Usually, such χ scales as $O(D^2)$, thus, the total contraction cost is $O(D^{10})$

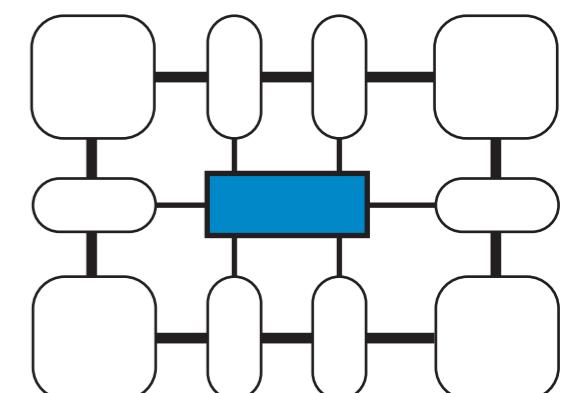
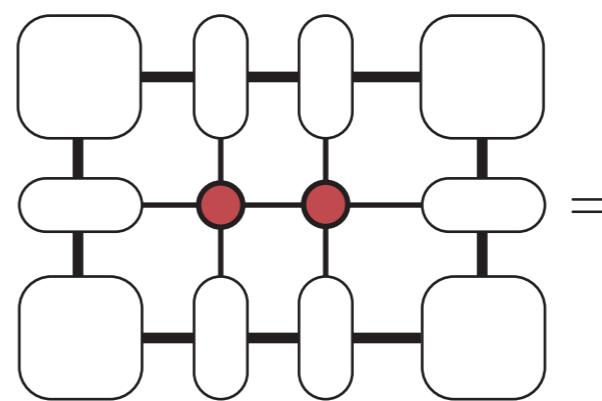
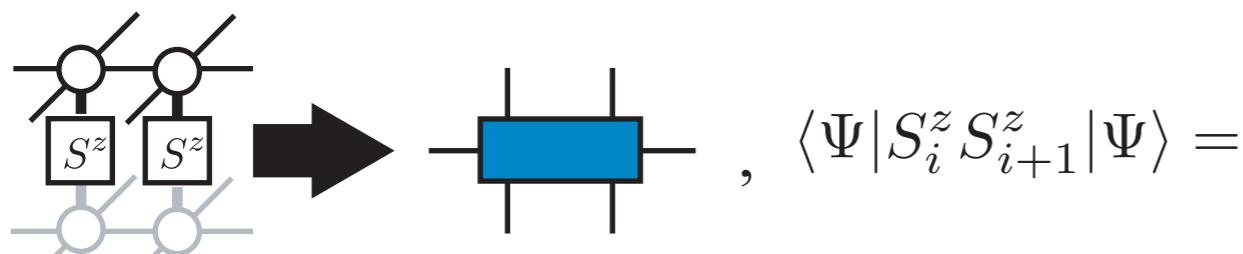
Physical quantities by CTMs

We can calculate physical quantities by CTM environments

1-site quantity:



2-site quantity:



* The computation cost increases when the size of the diagram is enlarged.

- Long-range correlation function along the diagonal direction.
- Many-body correlations on a larger cluster.

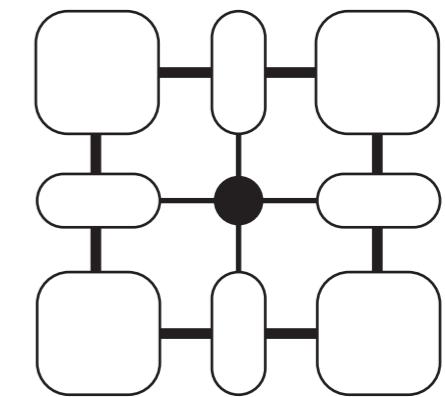
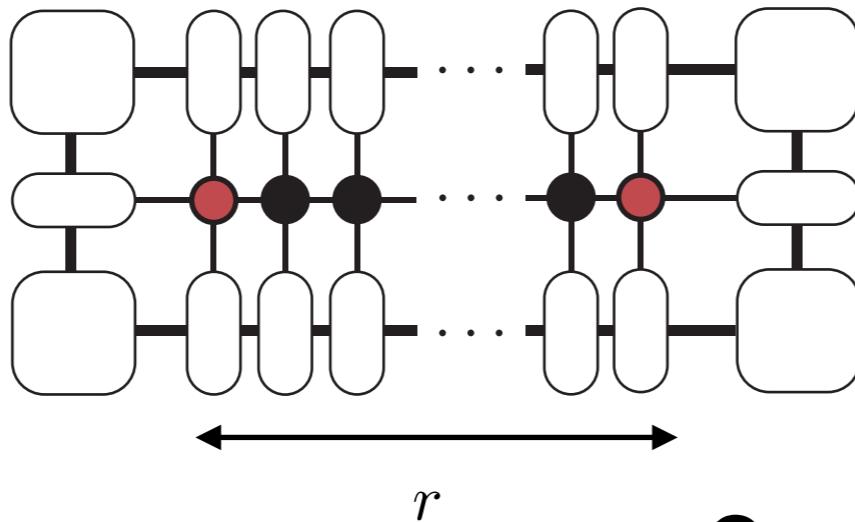
Correlation length with CTM

We can also calculate **correlation lengths**.

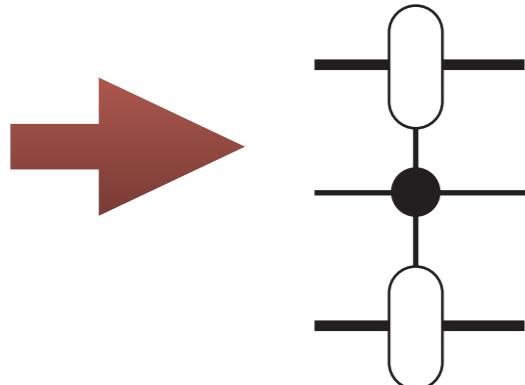
CTM environment

Correlation function

$$\langle \Psi | S_i^z S_{i+r}^z | \Psi \rangle =$$



Transfer matrix



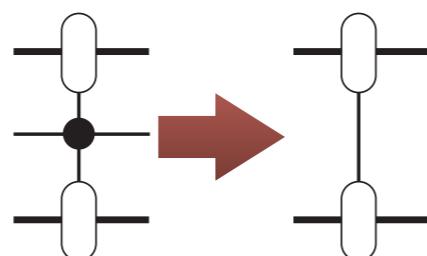
Eigenvalues: λ_i

$$|\lambda_0| \geq |\lambda_1| \geq |\lambda_2| \geq \dots$$

Correlation length

$$\frac{1}{\xi} = -\ln \frac{|\lambda_1|}{|\lambda_0|}$$

* CMT represents the infinite environment. So we can **neglect the center tensor**.



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Expected entanglement scaling for spin systems

Table 1

Entanglement entropy scaling for various examples of states of matter, either disordered, ordered, or critical, with smooth boundaries (no corners).

Physical state	Entropy	Example
Gapped (brok. disc. sym.)	$aL^{d-1} + \ln(\deg)$	Gapped XXZ [143]
$d = 1$ CFT	$\frac{c}{3} \ln L$	$s = \frac{1}{2}$ Heisenberg chain [21]
$d \geq 2$ QCP	$aL^{d-1} + \gamma_{\text{QCP}}$	Wilson–Fisher O(N) [136]
Ordered (brok. cont. sym.)	$aL^{d-1} + \frac{n_G}{2} \ln L$	Superfluid, Néel order [147]
Topological order	$aL^{d-1} - \gamma_{\text{top}}$	\mathbb{Z}_2 spin liquid [159]

(Nicolas Laflorencie, Physics Reports **646**, 1 (2016))

cf. free fermion

$$S \propto L^{d-1} \log L$$

For $d \geq 2$, leading contribution satisfies area law
even for gapless (critical) systems.

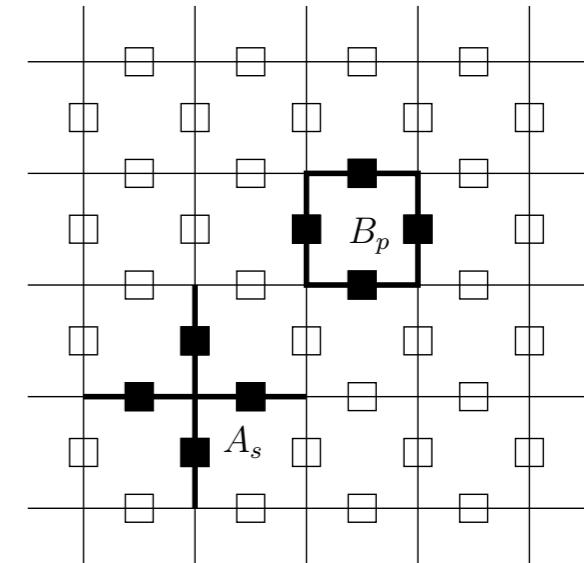
Example: Ground state represented by iTPS

Toric code model

(A. Kitaev, Ann. Phys. **303**, 2 (2003)).

$$\mathcal{H} = - \sum_s A_s - \sum_p B_p$$

$$A_s = \prod_{j \in \text{star}(s)} \sigma_j^x \quad B_p = \prod_{j \in \partial p} \sigma_j^z.$$



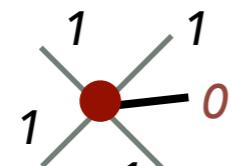
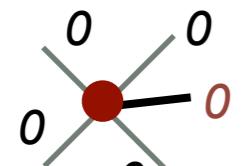
Its ground state is so called Z_2 spin liquid state.

"Spin liquid" is a novel phase different from conventional magnetic orders.

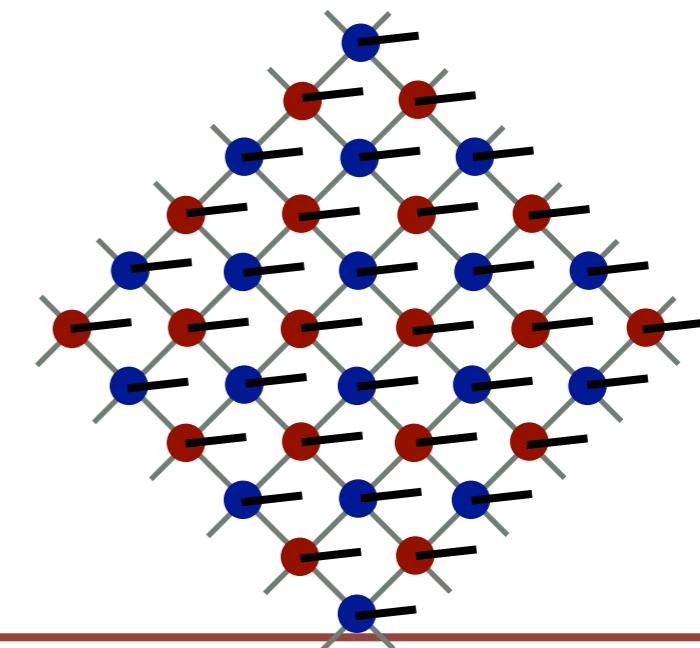
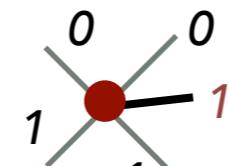
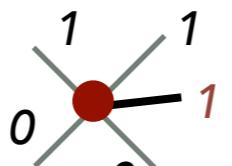
It can be represented by $D=2$ TPS.

(F. Verstraete, et al, Phys. Rev. Lett. **96**, 220601 (2006)).

0,1: eigenstate of σ_x



(Non-zero elements of tensor)



Example: Loop gas state for gapless Kitaev SL

Kitaev model

$$\mathcal{H} = - \sum_{\gamma, \langle i,j \rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma \quad \gamma : \text{bond direction}$$

A. Kitaev, Annals of Physics 321, 2 (2006)

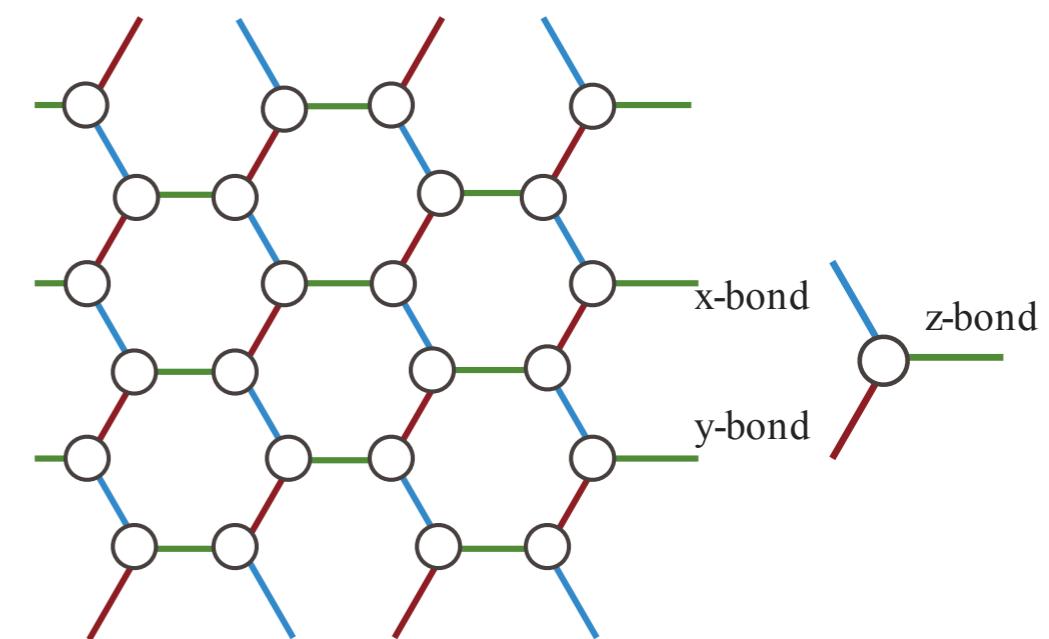
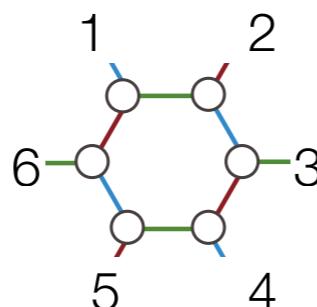
Ground states are spin liquids

The ground state is in the "vortex free" sector.

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$$[\mathcal{H}, W_p] = 0, [W_p, W_{p'}] = 0$$

vortex free = $\forall p, W_p = 1$



Anisotropic region (A) : gapped spin liquid

- Excitations of Majorana fermions has finite gap.
- It is adiabatically connected to the toric code.

Isotropic region (B) : gapless spin liquid

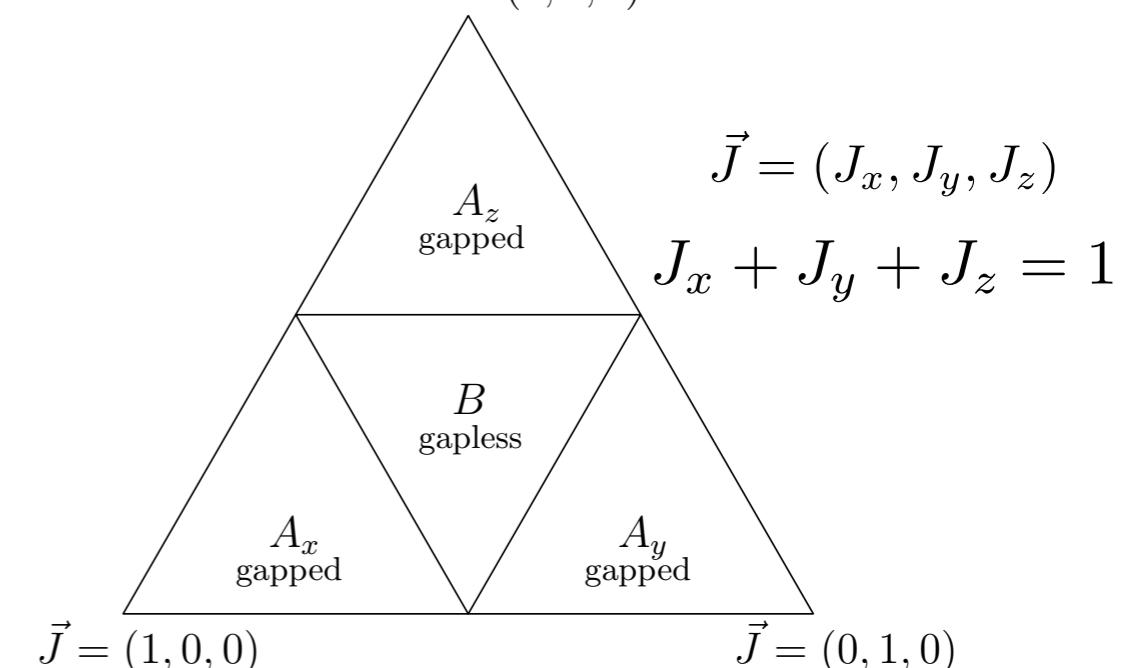
- Majorana fermions shows gapless excitation.
- The flux excitations is gapped.

G.S. Phase diagram

$$\vec{J} = (0, 0, 1)$$

$$\vec{J} = (J_x, J_y, J_z)$$

$$J_x + J_y + J_z = 1$$



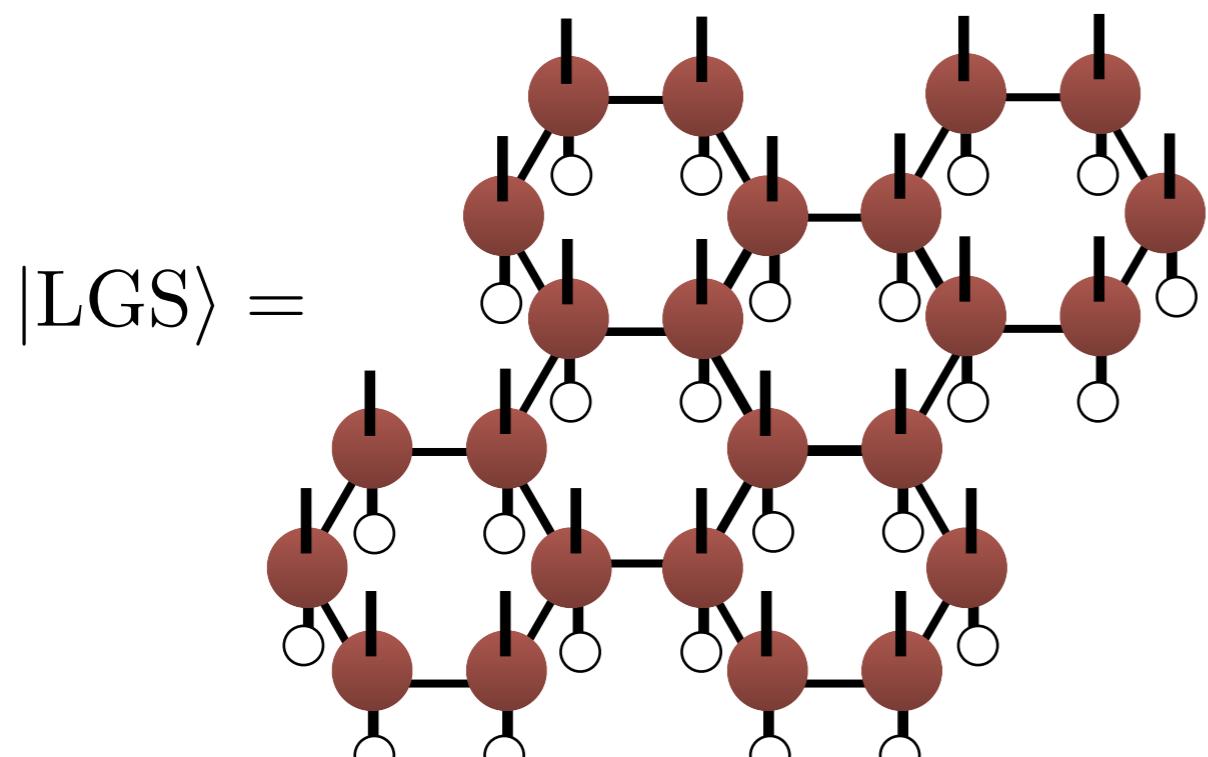
Example: Loop gas state for gapless Kitaev SL

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL, **123** 087203 (2019).

A simple **vortex free state** corresponding to the **isotropic Kitaev model**:

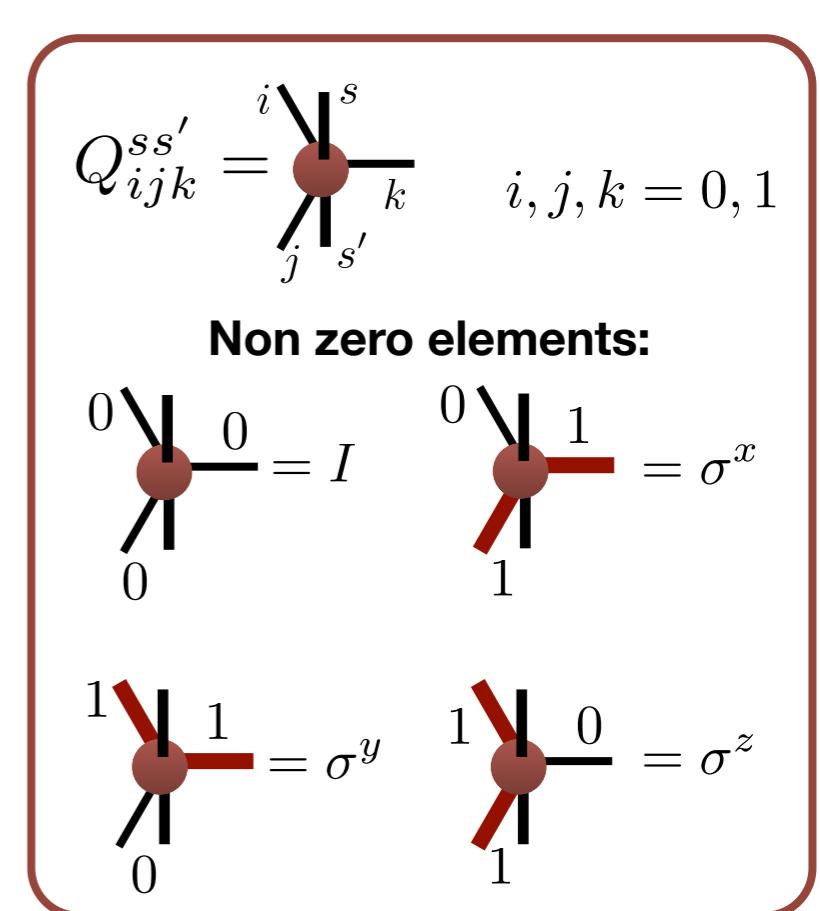
$$|\text{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$$

Ferromagnetic state pointing (1,1,1) direction.



$D=2$, TPS

$|111\rangle =$



This LGS is critical,
with the Ising CFT universality.

Systematic improvement with local dimer excitations

*n*th-order string gas state (SGS)

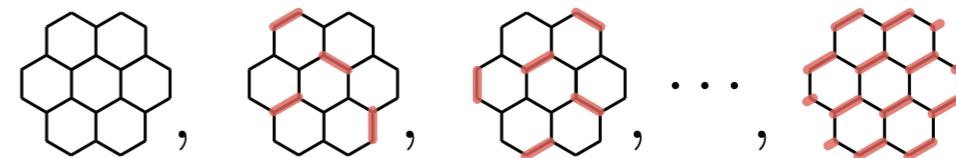
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

$$|\psi_n\rangle = \left[\prod_i^n \hat{R}_{DG}(\phi_i) \right] |\text{LGS}\rangle$$

($|\psi_n\rangle$ is represented by $D = 2^n$ iTPS.)

$\{\phi_i\}$: variational parameters

\hat{R}_{DG} introduces dimer excitations:



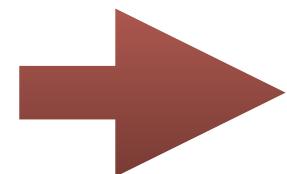
— : local dimer $S_i^\gamma S_j^\gamma$ ϕ_i determines density of the dimers

	$ \psi_0\rangle = \text{LGS}\rangle$	$ \psi_1\rangle$	$ \psi_2\rangle$	Exact
D	2	4	8	
# of	0	1	2	
E/J	-0.16349	-0.19643	-0.19681	-0.19682
$\Delta E/E_{\text{ex}}$	0.17	0.02	0.0007	-

By LGS and SGS, we can accurately represent the gapless Kitaev spin liquid qualitatively and quantitatively!

iTPS as variational wave function

A lot of two-dimensional spin systems **satisfy** the area law of the entanglement entropy.



It indicate, iTPS can be good variational wave function for infinite systems.

However, **optimization** of iTPS for a given Hamiltonian is not an easy task.

Difficulties:

- Optimization of infinitely repeated tensors a **highly non-linear problem**.
- Contraction of iTPS is performed **only approximately**.

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Typical optimization methods for iTPS

1. Imaginary time evolution

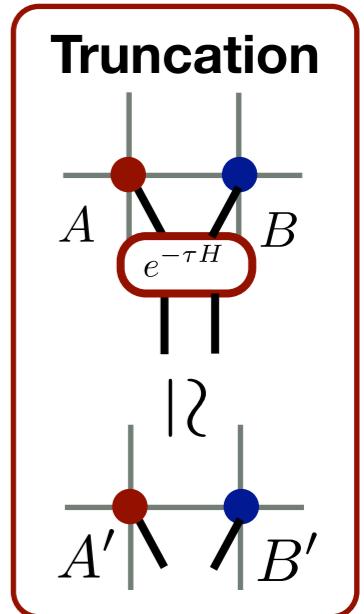
$$\lim_{M \rightarrow \infty} (e^{-\tau \mathcal{H}})^M |\psi\rangle = \text{ground state}$$

Suzuki-Trotter decomposition: $e^{-\tau H} \simeq e^{-\tau H_x} e^{-\tau H_y} e^{-\tau H'_x} e^{-\tau H'_y} + O(\tau^2)$

* By operating the time evolution operator,
the bond dimension increases from original D.



We need a “truncation.”



cf. iTEBD for iMPS

- **Full update** : consider global environment → Accurate but higher cost ($O(D^8) \sim O(D^{10})$)
- **Simple update**: consider only local environment → lower cost ($O(D^5)$)

2. Variational optimization

$$\min_A E(A) = \min_A \frac{\langle \Psi(A) | \hat{H} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle}$$

P. Corboz, Phys. Rev. B **94**, 035133 (2016).

L. Vanderstraeten *et al*, Phys. Rev. B **94**, 155123 (2016).

H.-J. Liao *et al*, Phys. Rev. X **9**, 031041 (2019).

cf. DMRG or VUMPS for MPS

Truncations in ITE

- Full update

Minimize the difference between two wave functions:

$$||\Psi\rangle - |\Psi'\rangle||^2 = \langle\Psi|\Psi\rangle + \langle\Psi'|\Psi'\rangle - 2\text{Re} \langle\Psi|\Psi'\rangle$$

$|\Psi\rangle$: wave function (after ITE)

$|\Psi'\rangle$: wave function after truncation

- Ideal approximation for finite TPS
- We need tensor network contractions, $O(D^8) \sim O(D^{10})$

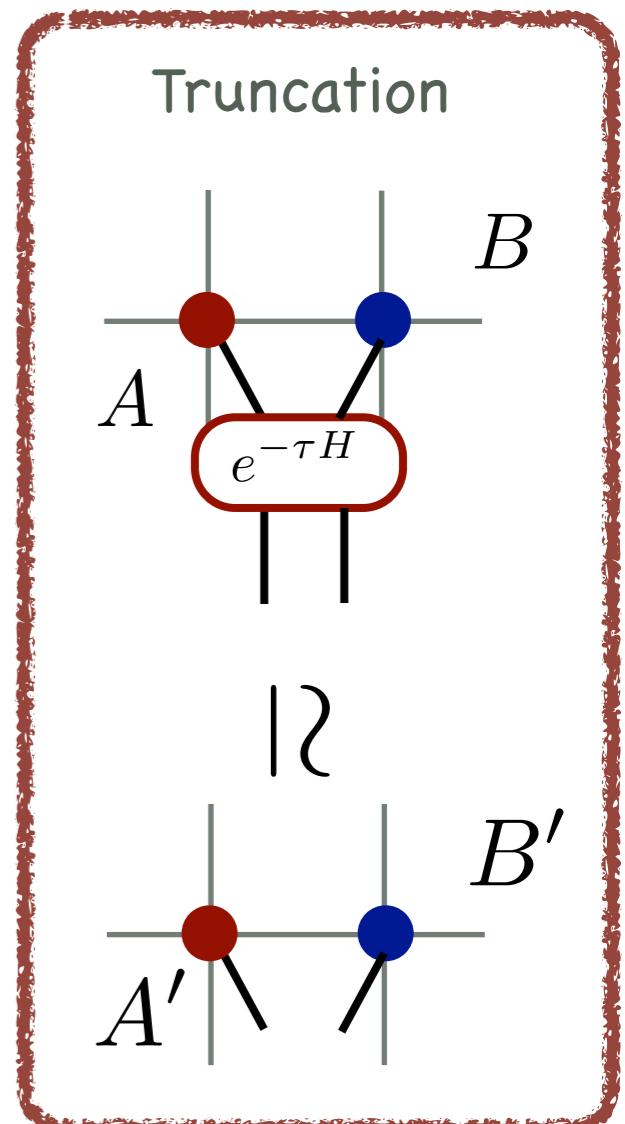
- Simple update

(H. G. Jiang *et al*, Phys. Rev. Lett. **101**, 090603 (2008))

Truncation by using local information

- Low computation cost : $O(D^5)$

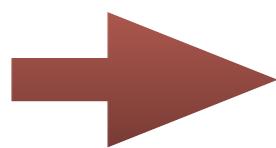
- iTPS tends to represent only short range correlations



Additional approximation for infinite system

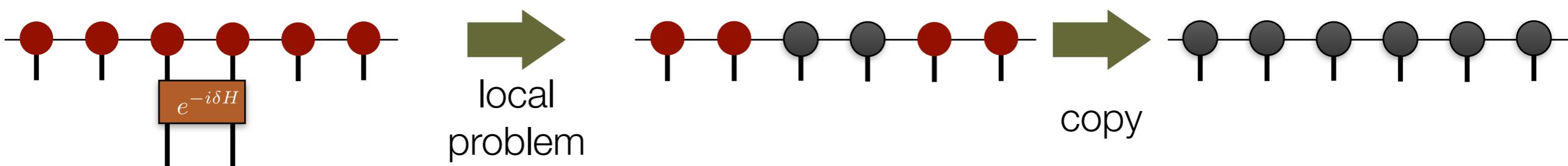
Even in full update, we actually consider iTPS **locally**:

We evaluate $||\Psi\rangle - |\tilde{\Psi}\rangle||^2 = \langle\Psi|\Psi\rangle + \langle\tilde{\Psi}|\tilde{\Psi}\rangle - 2\text{Re}\langle\Psi|\tilde{\Psi}\rangle$
with fixing environment (CTMs).



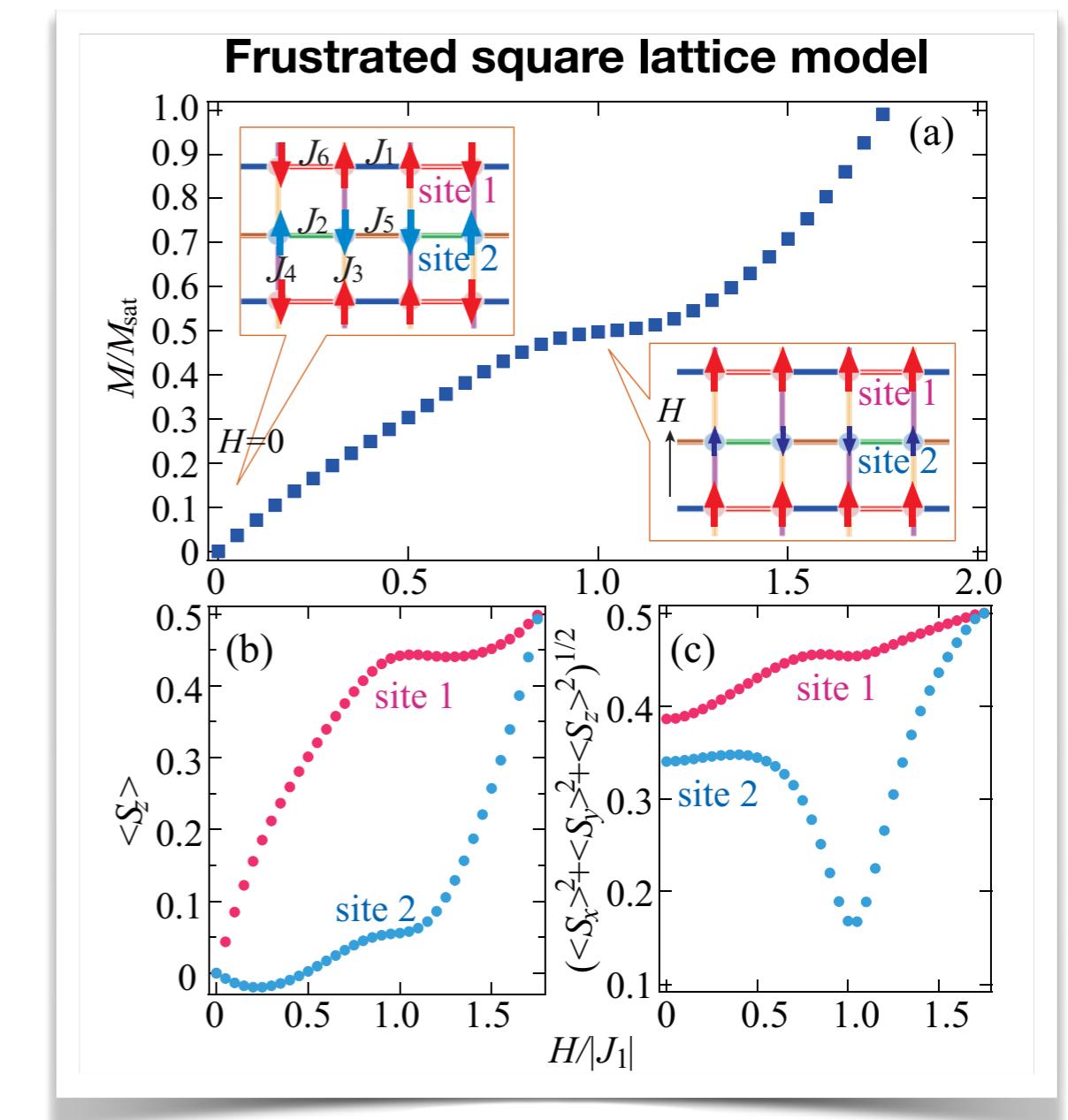
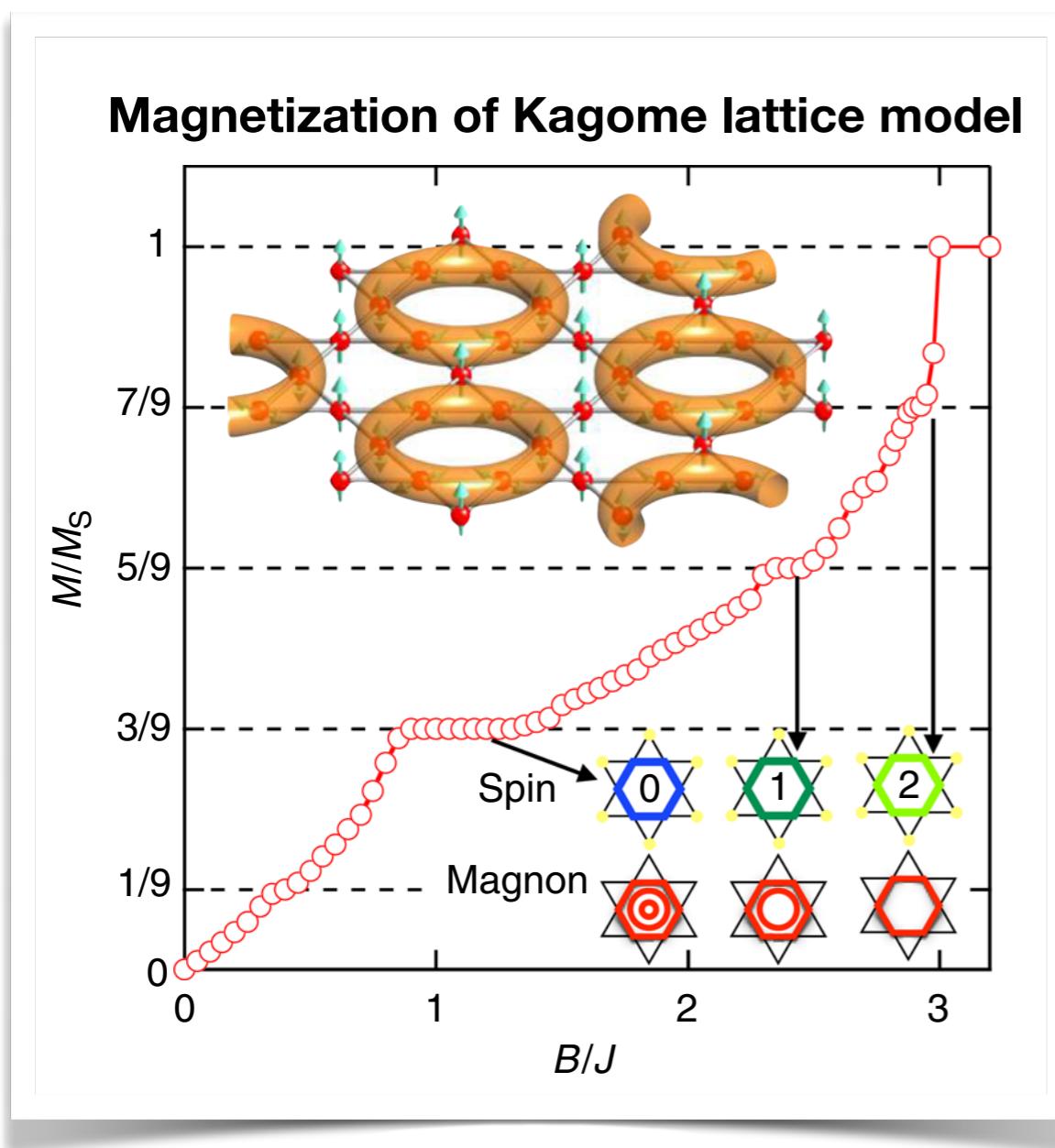
Then, from **translational invariance** of the iTPS,
we **copy** the "local" solution to whole system.

Thus, in the case of infinite systems,
it is **not the ideal projection** (truncation) of ITE.



Application to quantum many-body systems

Examples: Frustrated spin systems (We can not apply QMC due to the sing problem.)



Ground state calculation of a Kitaev material

T. Okubo, K. Shinjo, Y. Yamaji et al, Phys. Rev. B **96**, 054434 (2017).

Strong spin-orbit interaction →

Kitaev interaction in real compound

G.Jackeli, et al., PRL 102, 017205 (2009)

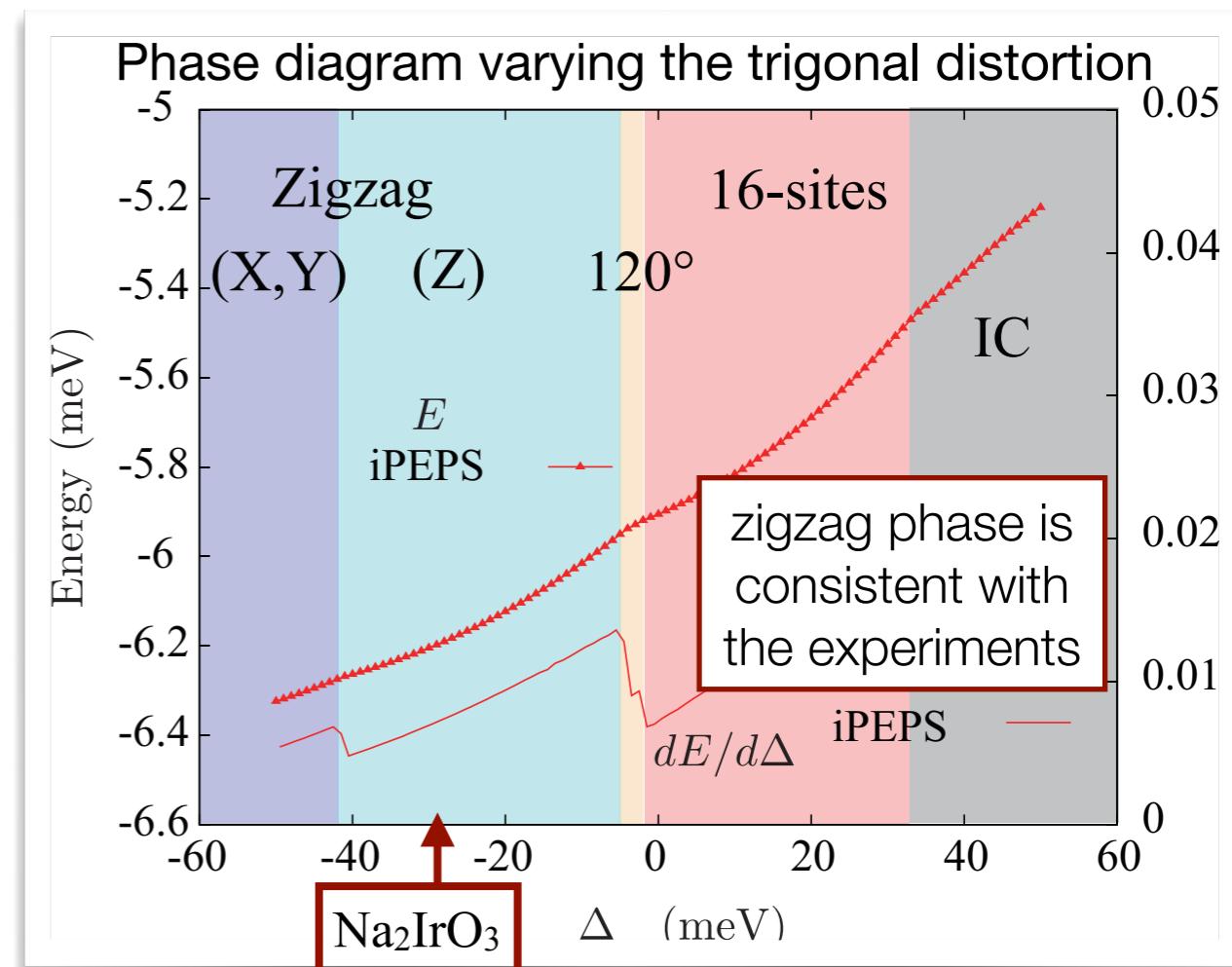
ab initio spin Hamiltonian for Na_2IrO_3

(Y. Yamaji et al. Phys. Rev. Lett. **113**, 107201(2014))

Kitaev + Heisenberg + Off-diagonal interactions
+
2nd and 3rd nearest neighbor interactions

Ground state of infinite system
calculated by using iTPS

- Due to additional interactions, GS is a magnetically ordered state, instead of the spin liquid.
- In this case, iTPS calculation correctly captured such magnetically ordered GS of the *ab initio* Hamiltonian.



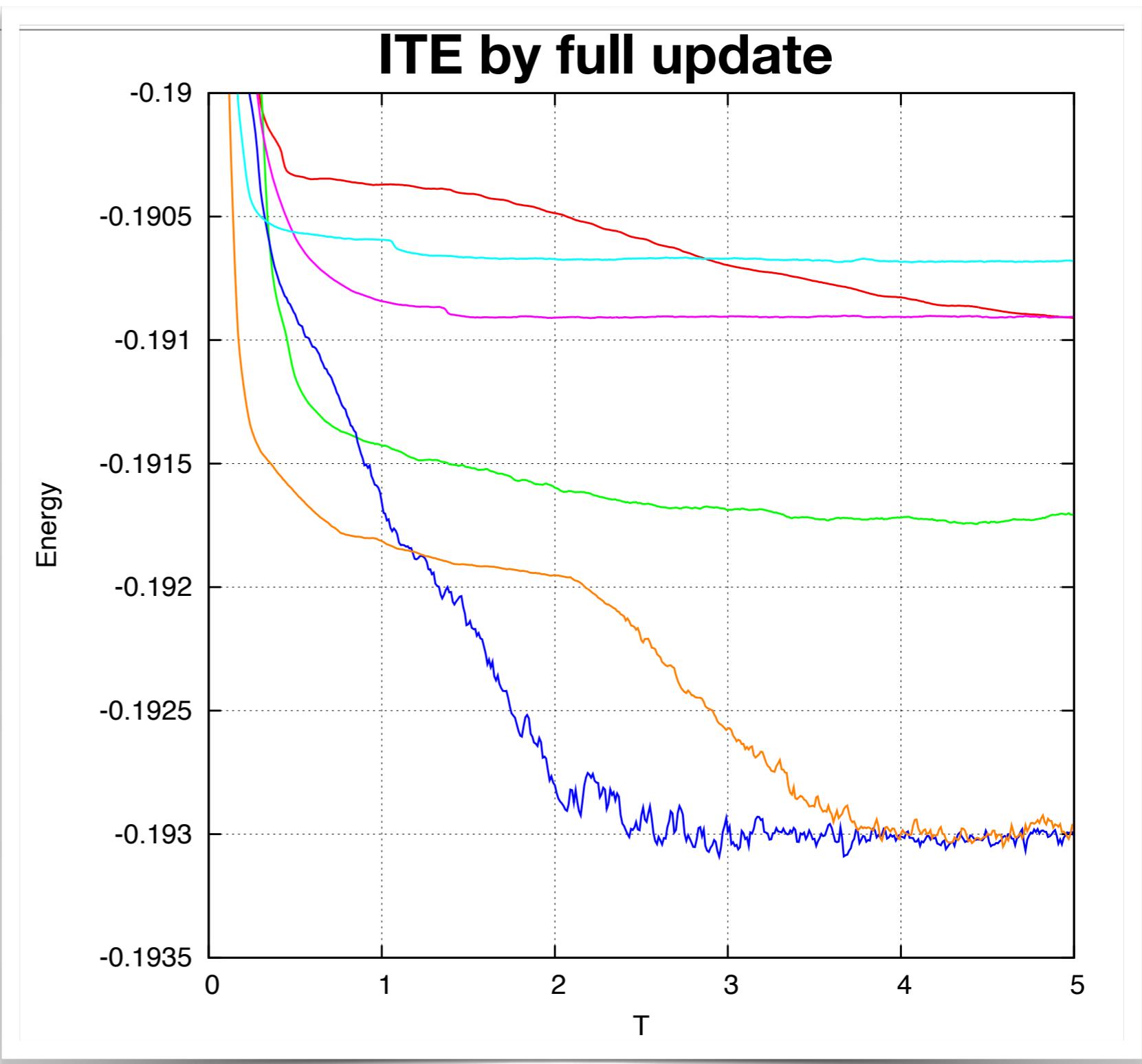
Importance of variational optimization

Problems in imaginary time evolution

- Quantum states obtained by ITE tend to be biased by initial states.
 - It is not easy to obtain a quantum spin liquid (QSL) state even in the case of Kitaev model, whose GS is exact QSL.
(cf. Kaneko's symposium talk)
 - For frustrated spin systems, it is also difficult to obtain the GS among several candidates of magnetically ordered states with small energy differences.
- Due to the projection onto iTPS, energy can increase along ITE.
 - It might be troublesome to pick up the lowest energy state.

Example: isotropic Kitaev model

ITE from random TPS
converges several
metastable states!



More sophisticated optimization: variational optimization

Variational method:

(P. Corboz, Phys. Rev. B **94**, 035133 (2016))

(L. Vanderstraeten, et al., Phys. Rev. B **94**, 155123 (2016))

(H.-J. Liao *et al*, Phys. Rev. X **9**, 031041 (2019).)

minimize cost function: $F = \frac{\vec{\psi}^\dagger (\mathcal{H} \vec{\psi})}{\vec{\psi}^\dagger \vec{\psi}}$

Advantage:

- Energies **strictly decrease along optimization**.
- It seems to avoid to be trapped at local minimum for several models.

Disadvantage:

How to calculate the derivative of F for iTPS?

- CTM with **systematic summation**
- Automatic differentiation of F . (It is highly recommended.)

Variational optimization by CTMRG

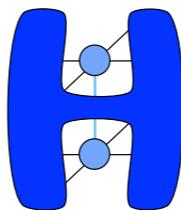
(P. Corboz, Phys. Rev. B 94, 035133 (2016))

"Minimize Energy directly" $\min_A E(A) = \min_A \frac{\langle \Psi(A) | \hat{H} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} = \min_{\vec{A}} \frac{\vec{A}^\dagger \mathbf{H} \vec{A}}{\vec{A}^\dagger \mathbf{N} \vec{A}}$

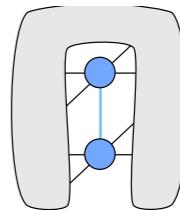
A : local tensor of iTPS

Diagrams:

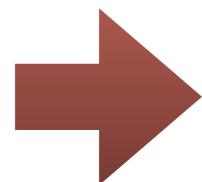
$$\vec{A}^\dagger \mathbf{H} \vec{A} =$$



$$\vec{A}^\dagger \mathbf{N} \vec{A} =$$



Solve generalized eigenvalue problem



$$\frac{\partial}{\partial \vec{A}^\dagger} \left(\frac{\vec{A}^\dagger \mathbf{H} \vec{A}}{\vec{A}^\dagger \mathbf{N} \vec{A}} \right) = 0, \quad \rightarrow \quad \mathbf{H} \vec{A} = E \mathbf{N} \vec{A}.$$

$$= E$$

CTM representation of H "matrix":

(P. Corboz, Phys. Rev. B 94, 035133 (2016))

$$\langle \Psi | \hat{H} | \Psi \rangle = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \dots$$

Blue tensors contain infinite sum of the local hamiltonian.

$$\text{Diagram 1} = \text{Diagram 1a} + \text{Diagram 1b} + \text{Diagram 1c} + \text{Diagram 1d} + \dots$$
$$\text{Diagram 2} = \text{Diagram 2a} + \text{Diagram 2b} + \text{Diagram 2c} + \dots$$

Applications: S=1/2 Heisenberg model

Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

GS energy (from QMC):

$$E = -0.6694421(4)$$

A. W. Sandvik, AIP Conf. Proc. No. 1297, pp. 135 (2010)

Spontaneous magnetization

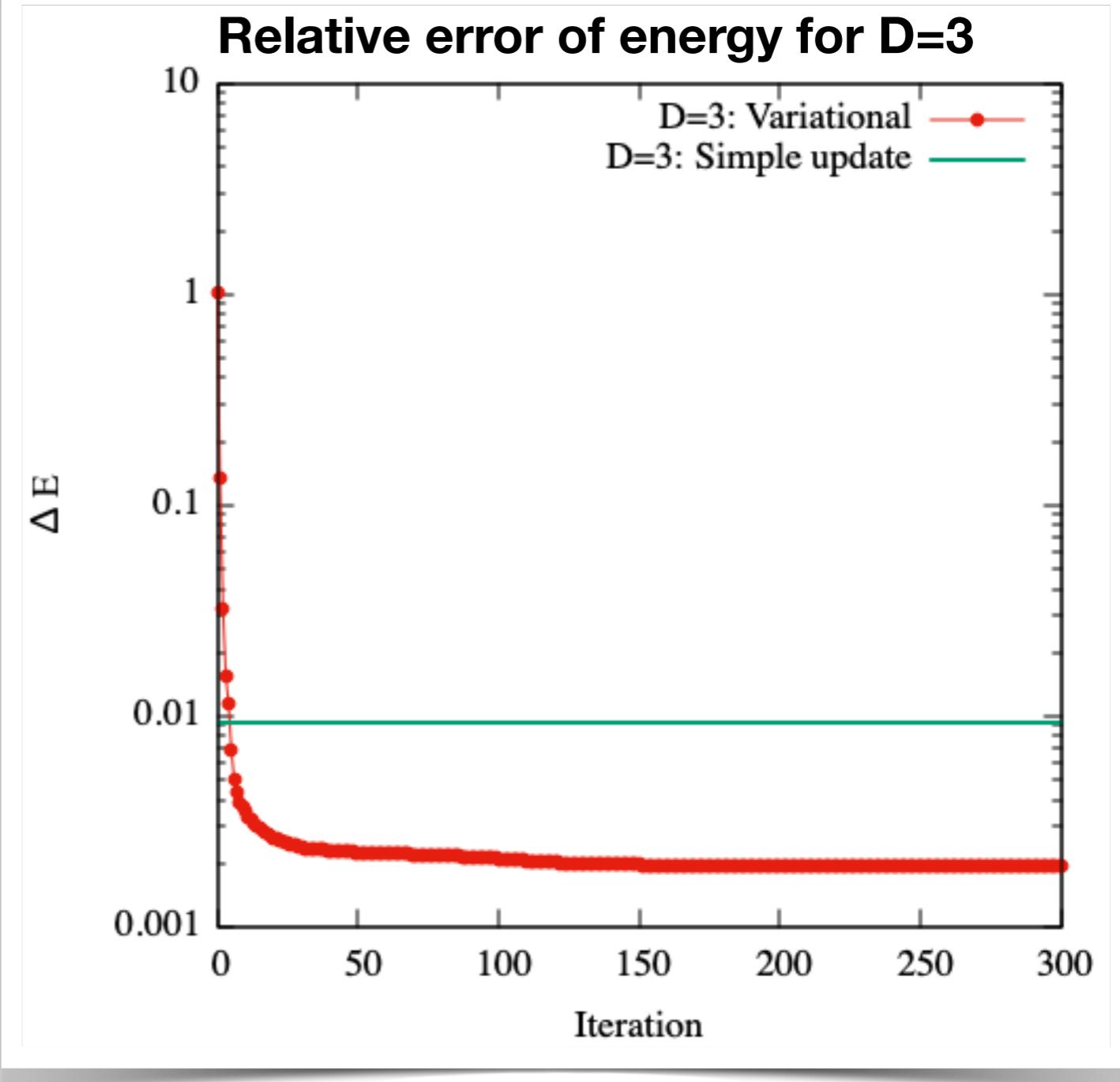
$$m_s = 0.3074$$

For D=3 iTPS

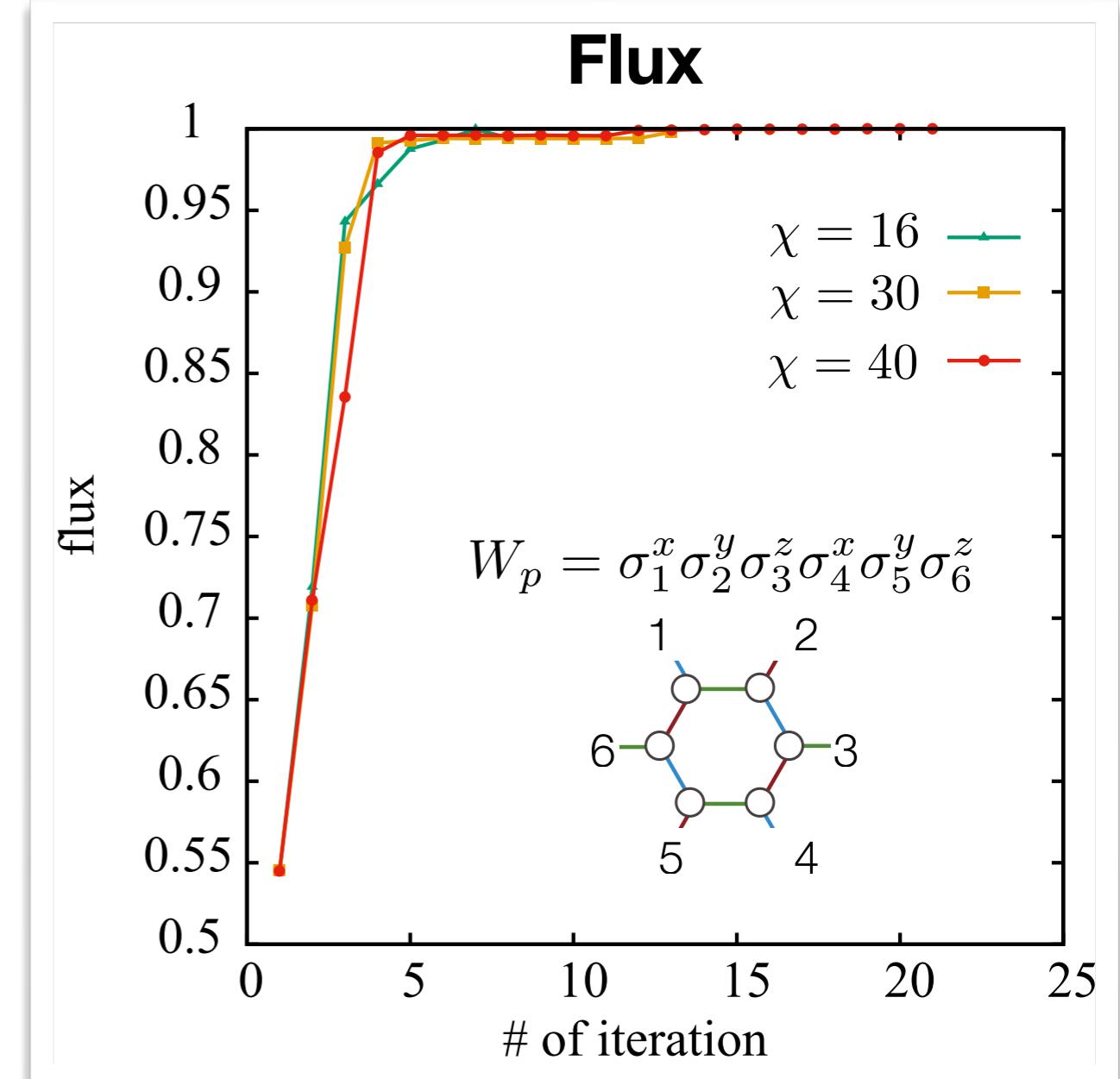
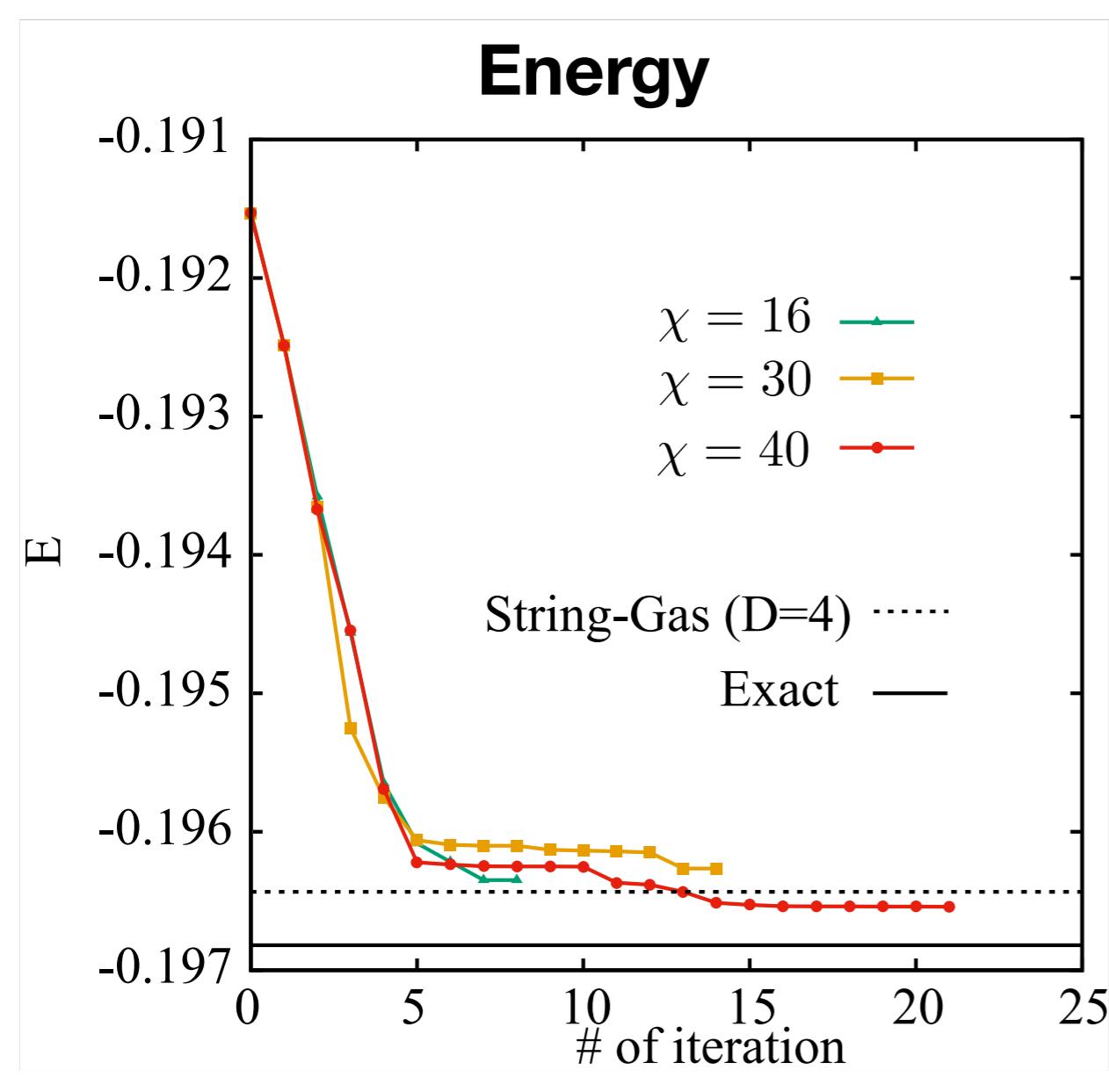
$$m_s = 0.3769 \text{ (Simple update)}$$

$$m_s \approx 0.35 \quad \text{(Full update from P. Corboz, Phys. Rev. B 94, 035133 (2016))}$$

$$m_s = 0.3393 \text{ (Variational)}$$



Applications: pure Kitaev model (D=4, 2-site unit)



Even if we start from a ferromagnetic state,
we obtain accurate Kitaev spin liquid by variational optimization.

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Finite temperature: Partition function

Partition function

$$Z = \text{Tr } e^{-\beta \mathcal{H}}$$

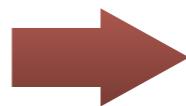
Density matrix

$$\rho(\beta) = \frac{1}{Z} e^{-\beta \mathcal{H}}$$

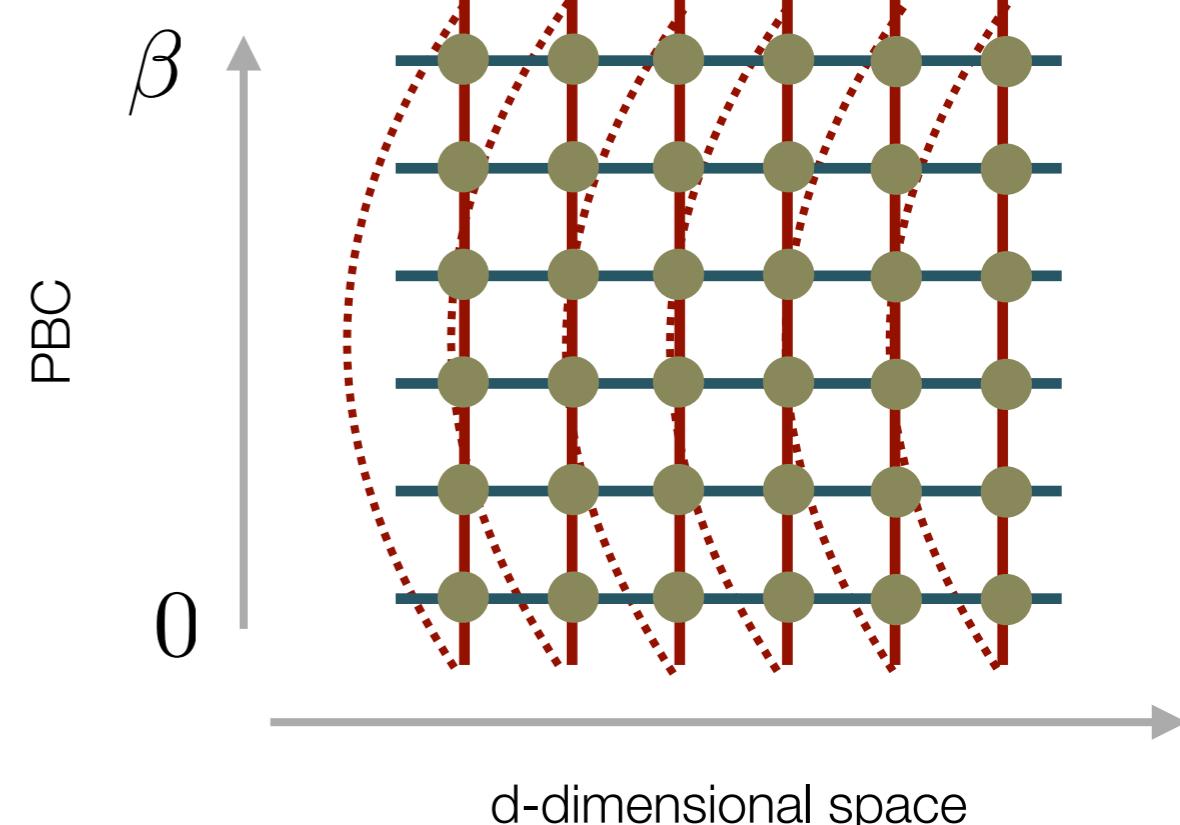
Expectation value

$$\langle \hat{O} \rangle_\beta = \text{Tr}[\rho(\beta) \hat{O}]$$

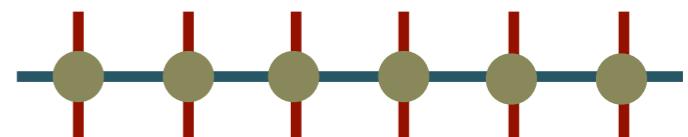
Suzuki-Trotter
decomposition



Z: d+1 dim. tensor network

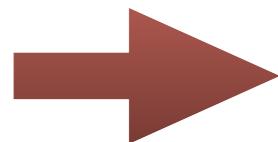


Imaginary time evolution operator: $e^{-\tau \mathcal{H}}$
PEPO (MPO) representation



Simplest approach: calculate partition function

Calculation of the partition function = contraction of d+1 classical TN.



We can use methods for classical systems

- Tensor network renormalizations
 - TNR for **1d quantum** (e.g. G. Evenly and G. Vidal, PRL 115, 200401(2015))
 - HOTRG, HOSRG **for 2d quantum** (e.g. Z.Y. Xie *et al*, PRB **86**, 045139 (2012))

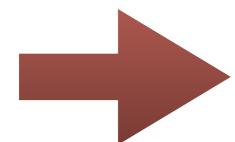
Disadvantages:

- Real space renormalization type calculation is less accurate than CTMRG type method.
 - However, CTMRG is not efficient for 3d ((2+1)d) systems.
 - For 3d, it requires $O(D^{11})$ computation cost.
 - When we use ATRG (D. Adachi, TO, *et al.*, PRB 102, 054432 (2019)), it is reduced to $O(D^7)$.

More efficient method?

Typical pure state?

In the case of small clusters, **TPQ method** is often used.



TPQ states:

expectation values calculated from one pure state
are almost same with the thermal average.

Cf, finite temperature Lanczos

Can we approximate TPQ state by TNS?

In my opinion, approximation by TNS, e.g. MPS, is **not efficient**.

Because,

- The entanglement entropy of TPQ state shows **the volume law**.
- Random initial state for $\beta=0$ is hard to treat for infinite system.

*For a finite-size system, alternatively, we can use METTS algorithm.

S. R. White PRL **102**, 190601 (2009)

(It is based on random sampling of pure states represented by MPS)

Tensor network representation of density matrix

Another way for calculating thermal properties:



Approximate **the density matrix** accurately

Possible two representations of the density matrix as TNs.

1. Represent it **by TPO directly**.

- e.g., A. Kshetrimayum et al, PRL **122**, 070502 (2019)

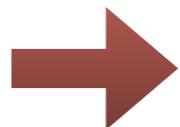
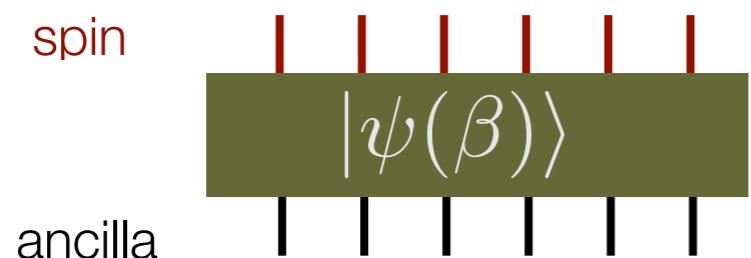
2. Represent it by **purification**, and represent the wavefunction as TPO.

- e.g., P. Czarnik et al, PRB **99**, 035115 (2019)

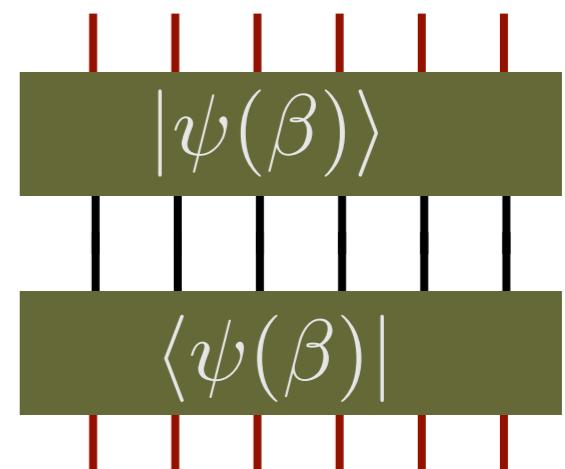
Purification: $\rho(\beta) \propto \text{Tr}_{\text{ancillas}} |\psi(\beta)\rangle\langle\psi(\beta)|$.

$|\psi(\beta)\rangle$: wave function in extended space (spin + ancilla)

spin



$\rho(\beta) =$



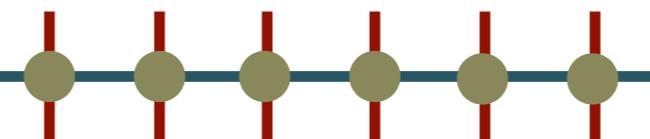
For both representations, we can use **the same algorithms** for the ITE of iTPS.

Pros and cons of two methods

1. Direct TPO representation

Pros: • Algorithm becomes simpler.

Cons: • Approximate density matrix may contain **negative (or complex) eigenvalues**.
• For full update, we need much cost than the case of purification.
(The cost depends on the definition of the distance.)

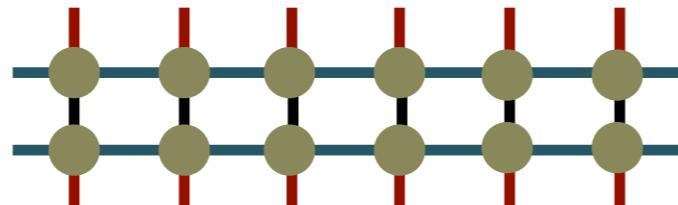
$$\rho(\beta) = \text{---|---|---|---|---|---}$$


2. Local purification

Pros: • The approximate density matrix is **positive semi-definite**.

Cons: • Optimization of ancilla digree of freedoms seems to be complex.
• **Bond dimensions can be much larger** than the direct representation.

Gemma De las Cuevas et al, New J. Phys. **15**, 123021 (2014)

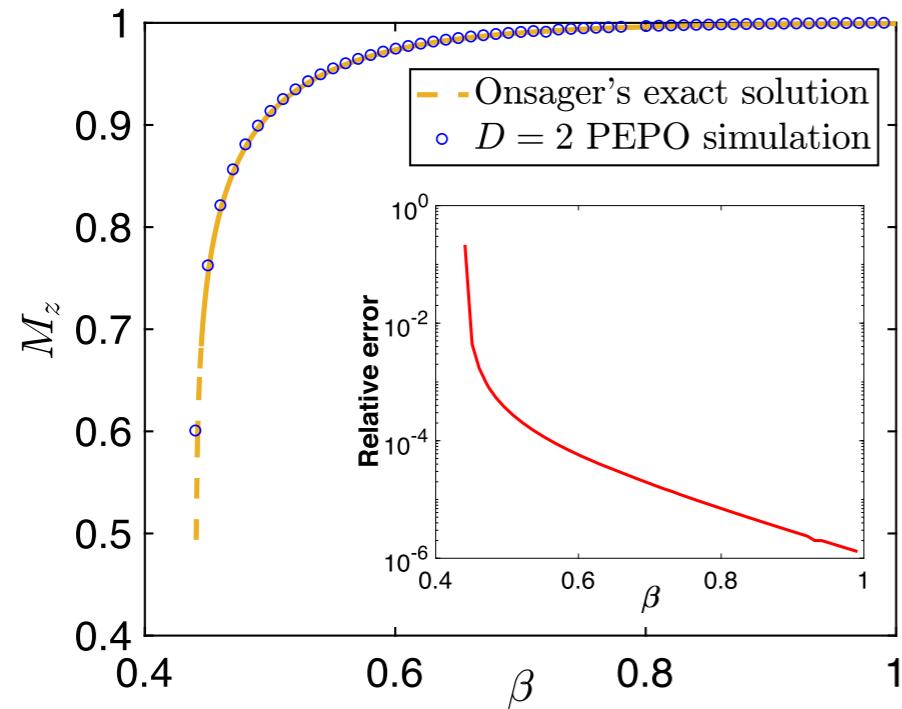
$$\rho(\beta) = \text{---|---|---|---|---|---}$$


Can we apply these methods to complicated problems?

Both method seem to work well for "easy" models

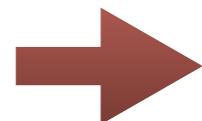
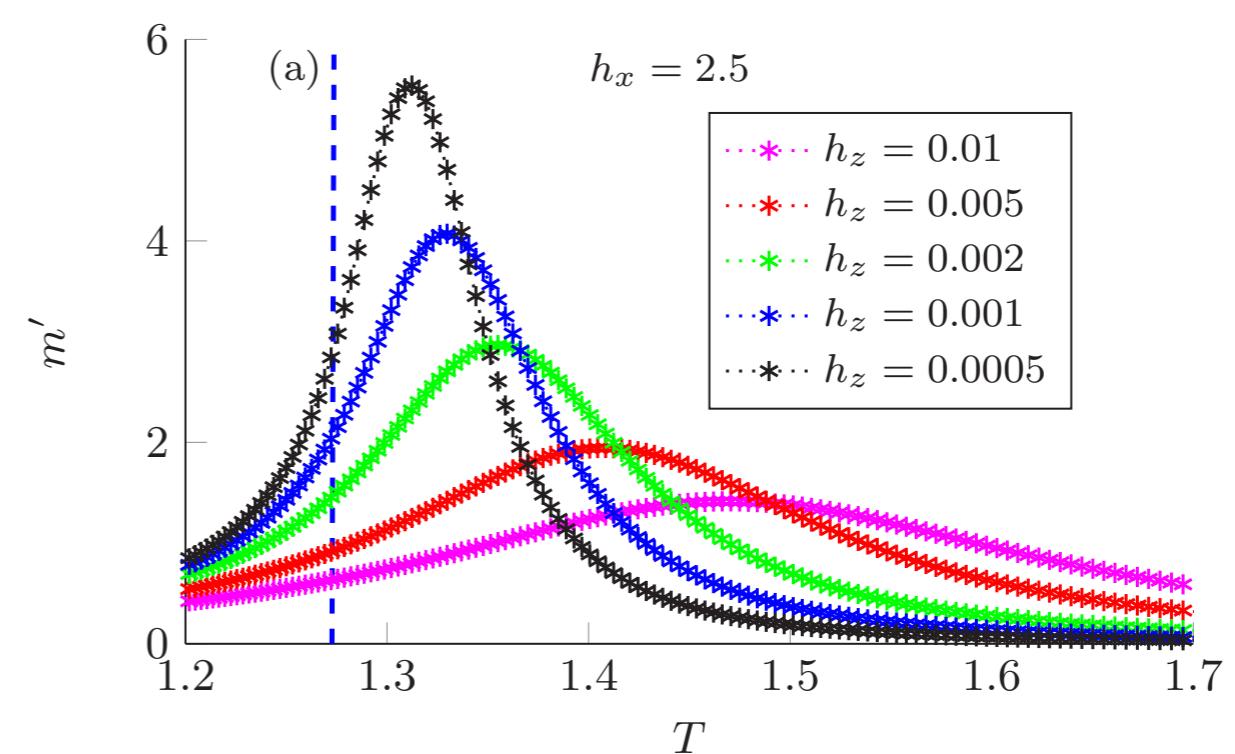
Ising model

A. Kshetrimayum et al, PRL **122**, 070502 (2019)



Transverse field Ising model

P. Czarnik et al, PRB **99**, 035115 (2019)



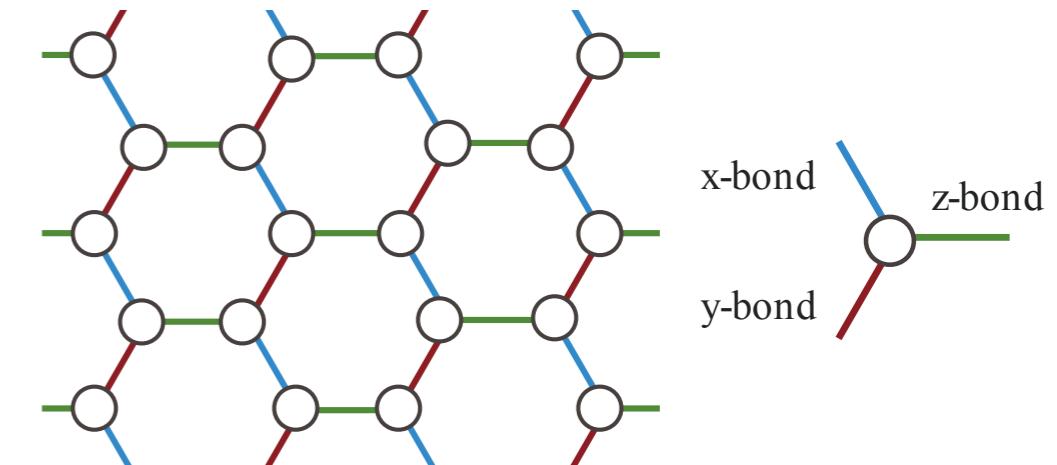
Can we apply them to "difficult" problems?

Application: Honeycomb lattice Kitaev Model

Kitaev model

A. Kitaev, Annals of Physics 321, 2 (2006)

$$\mathcal{H} = -K \sum_{\gamma, \langle i,j \rangle_\gamma} S_i^\gamma S_j^\gamma \quad \begin{matrix} \gamma : \text{bond direction} \\ \left(S = \frac{1}{2} \right) \end{matrix}$$



- Ground state is gapless **spin liquid**

It satisfies the vortex free condition:

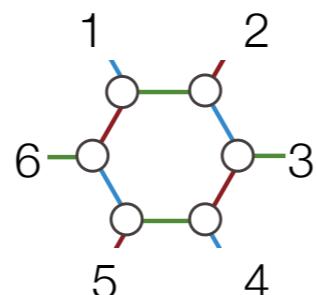
$$\forall p, W_p = 1$$

p : plaquette

$$\text{Flux: } W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

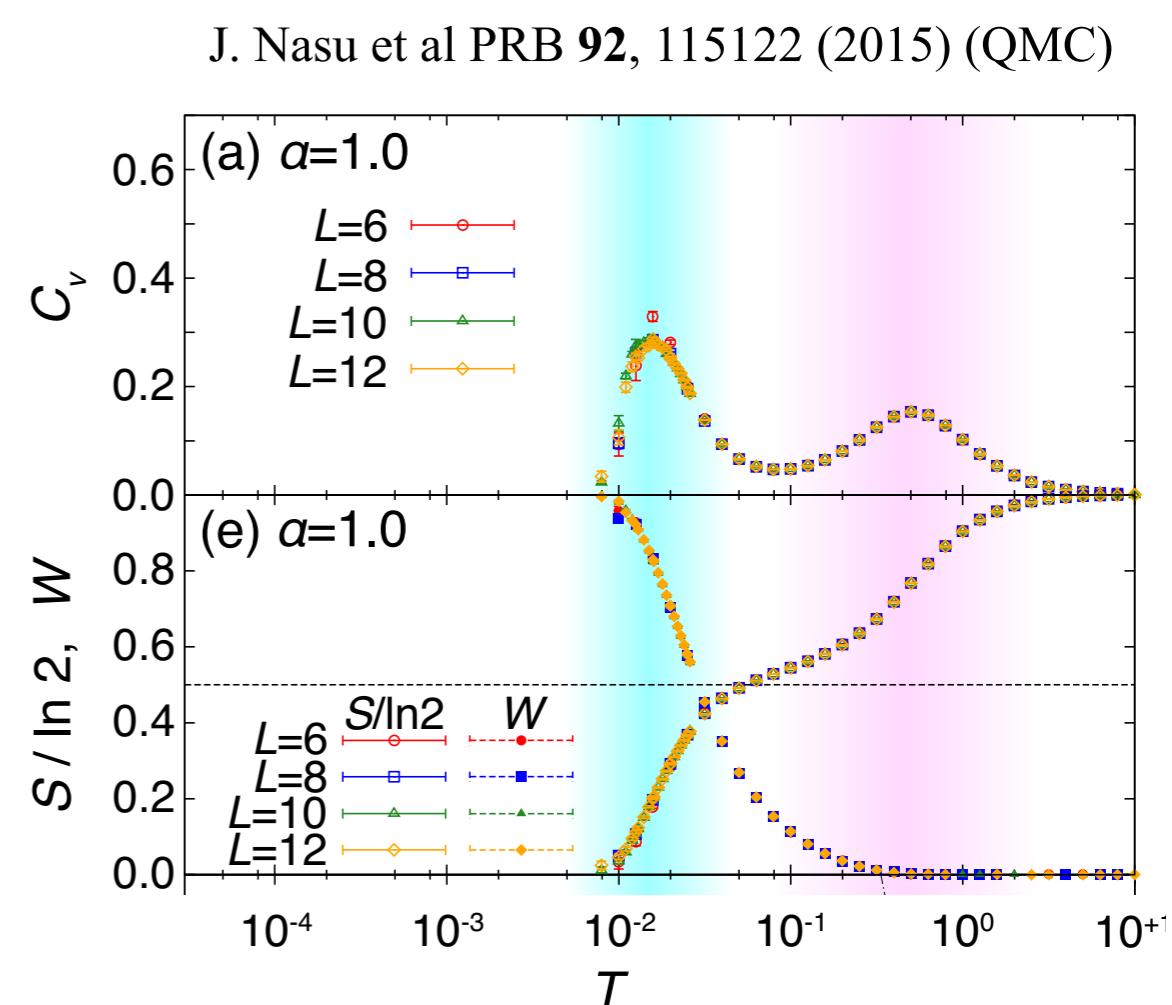
$$[\mathcal{H}, W_p] = 0, [W_p, W'_p] = 0$$

(cf. H.-Y. Lee, et al, PRL (2019))

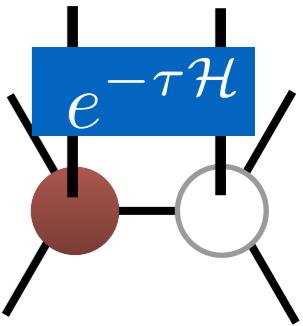


- At finite temperature, **double peaks** structure is expected in the specific heat.

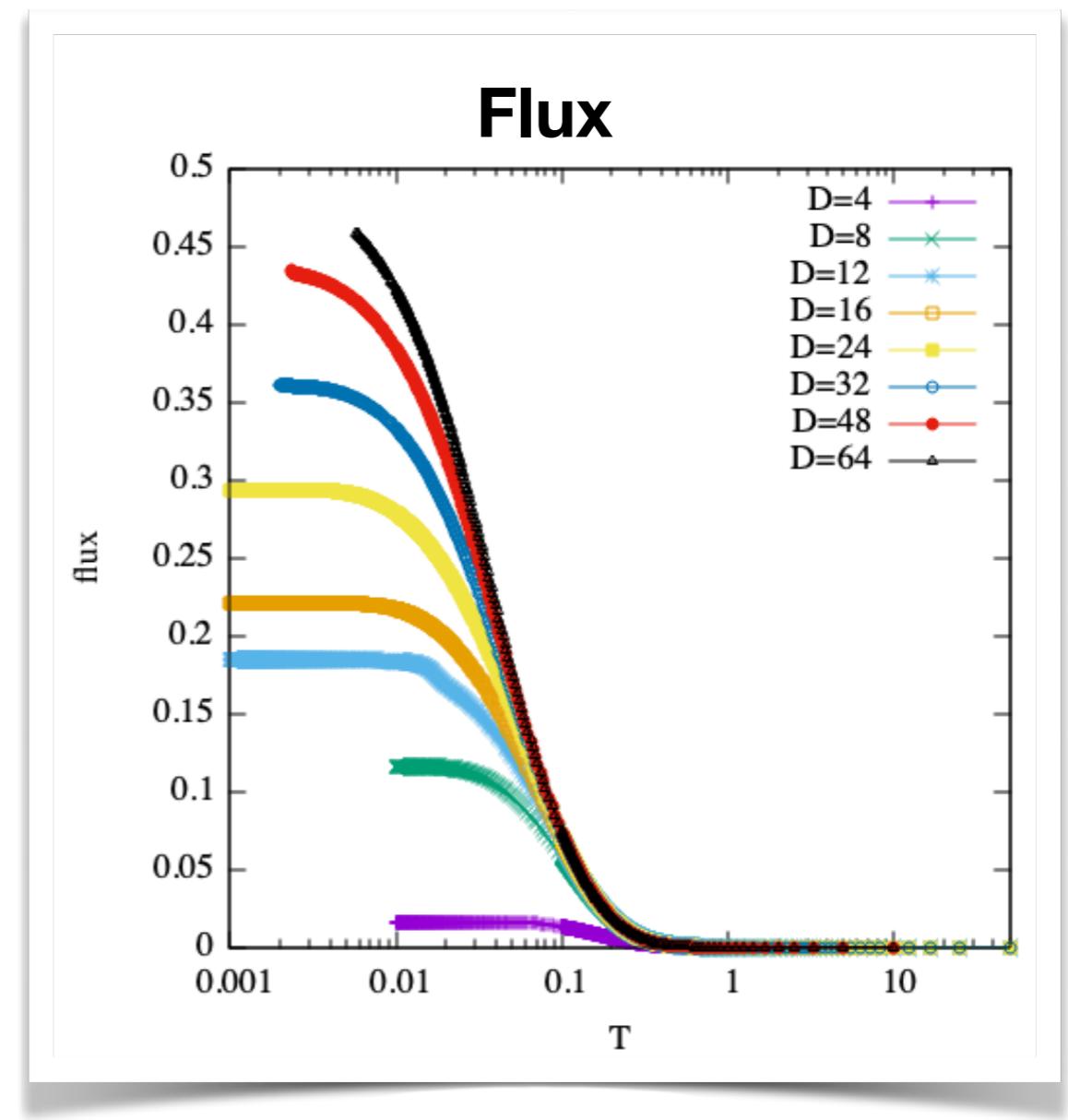
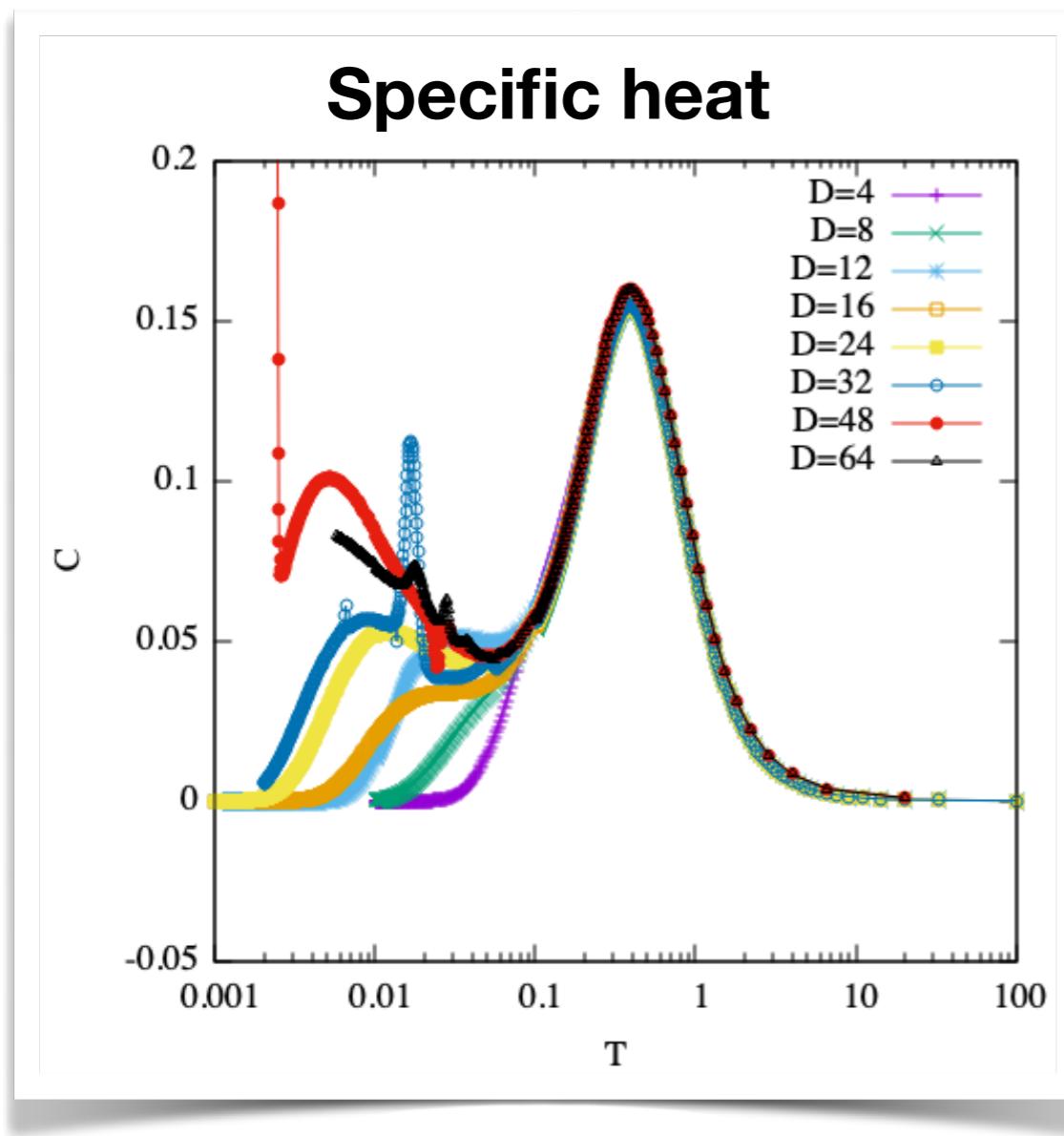
The low temperature peak corresponds to the development of the flux.



Can we reproduce it by iTPO method?



Results: specific heat and flux

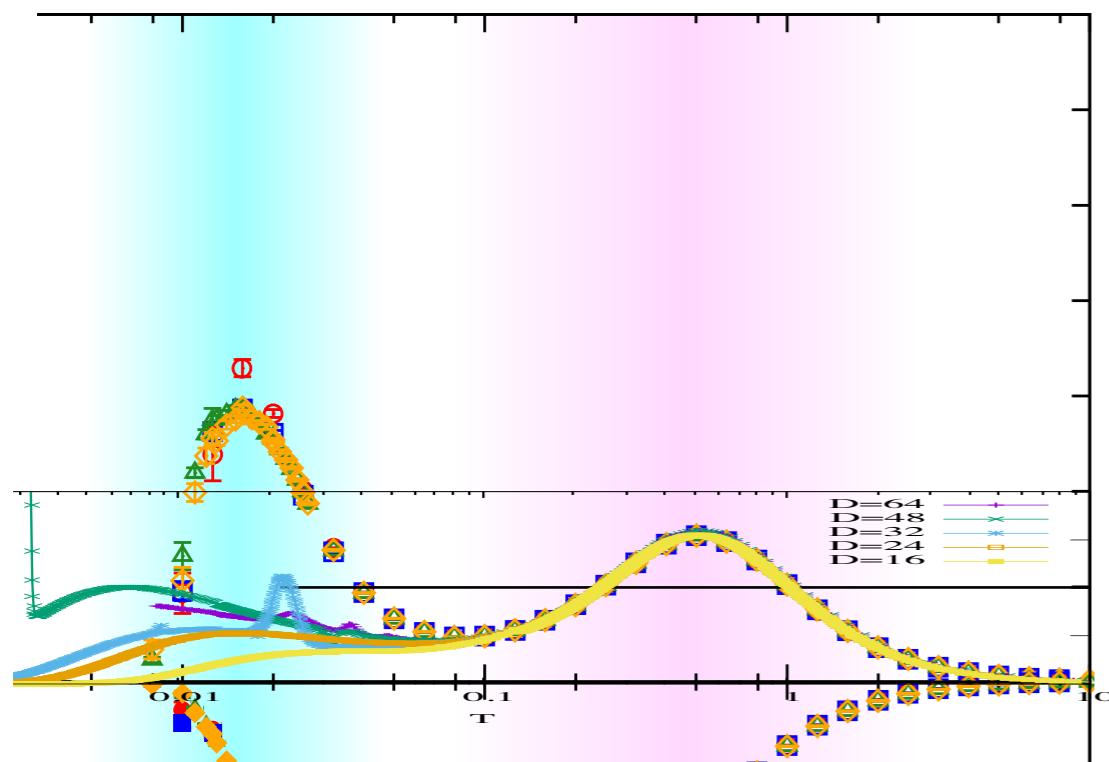


- Small D , we do not see two peak structure.
- As D is increased, the second peak becomes visible.
 - It corresponds to the increase of the flux.

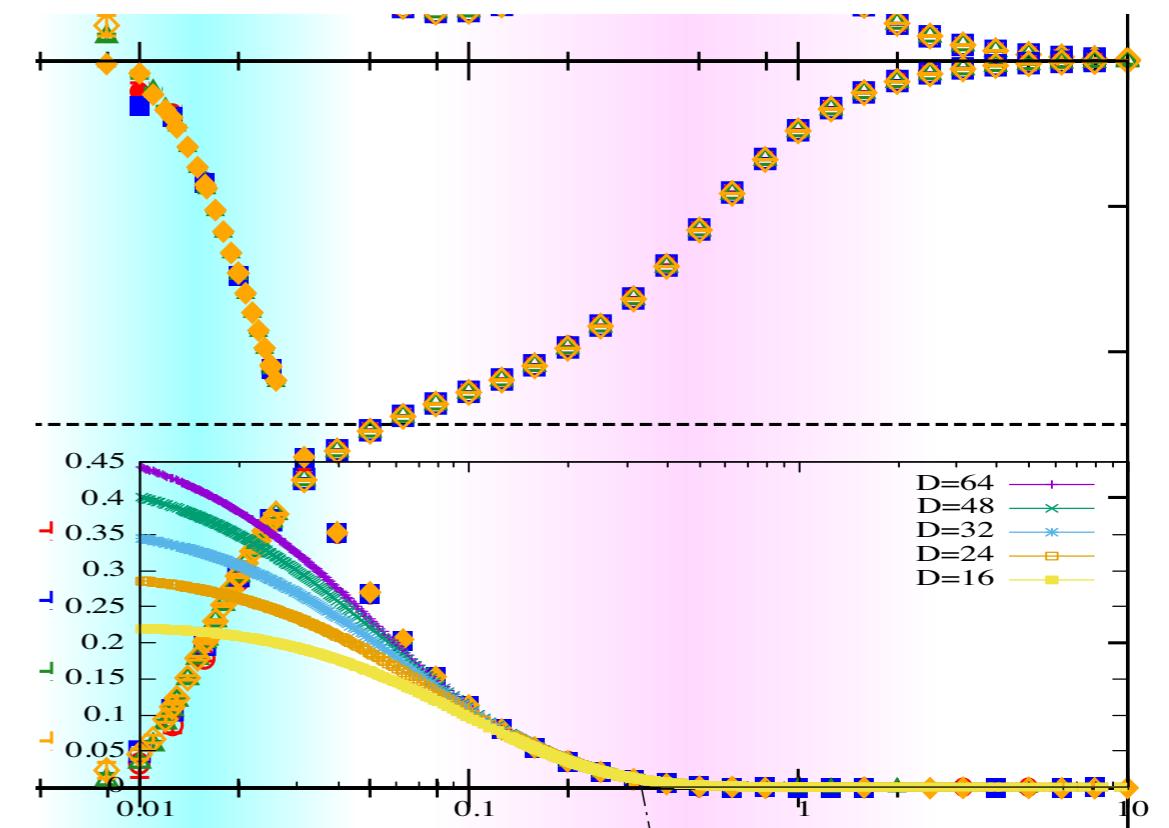
Comparison between iTPO and QMC

J. Nasu et al PRB **92**, 115122 (2015) (QMC)

Specific heat



Flux



Compared with QMC, TPO method could not capture the quantitative nature of Kitaev spin liquid at $T < 0.1$.

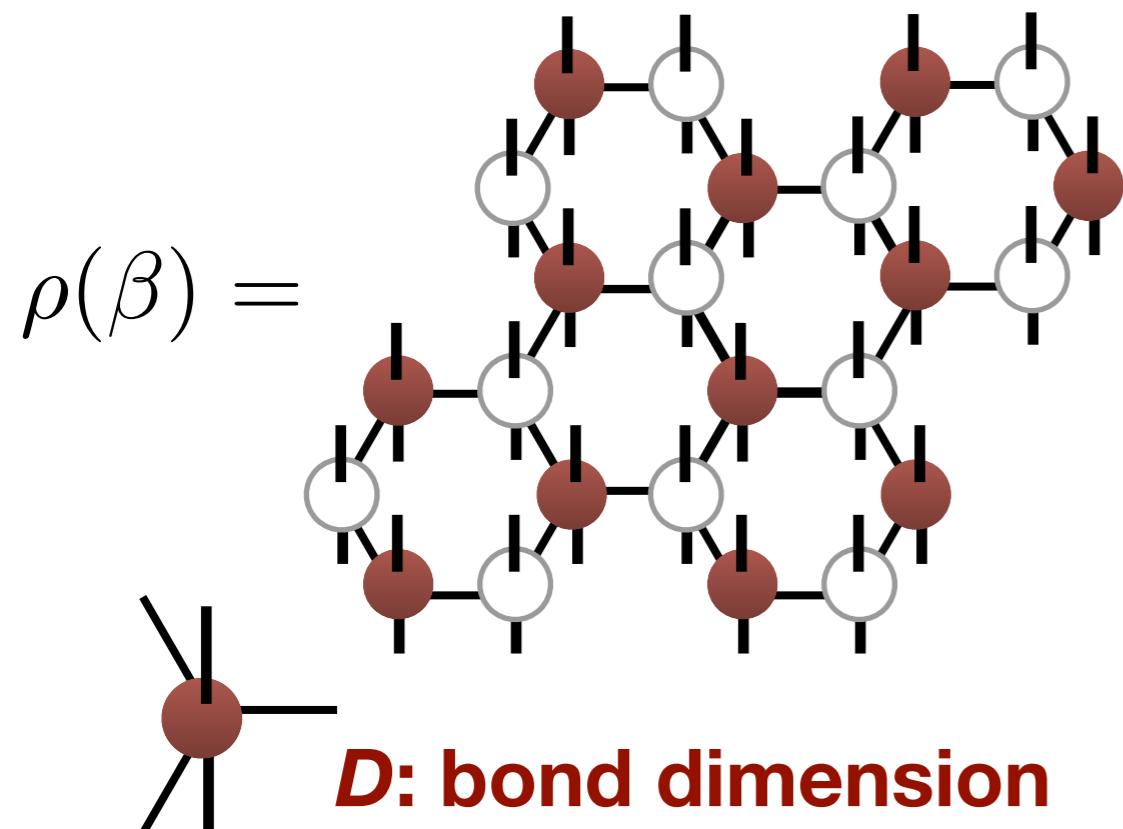
This is probably due to the difficulty of optimization for infinite TPS.

→ Finite temperature simulation for “difficult” problems is still challenging!

Importance of many-body correlations

Infinite TPO for a density matrix

$$\rho(\beta) = e^{-\frac{\beta}{2}\mathcal{H}} \rho(0) e^{-\frac{\beta}{2}\mathcal{H}}$$

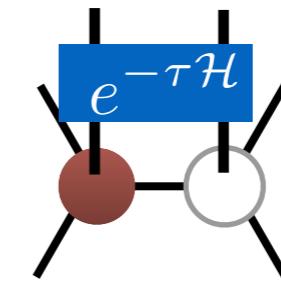


When we treat a larger cluster at each ITE step,
the specific heat is largely improved.

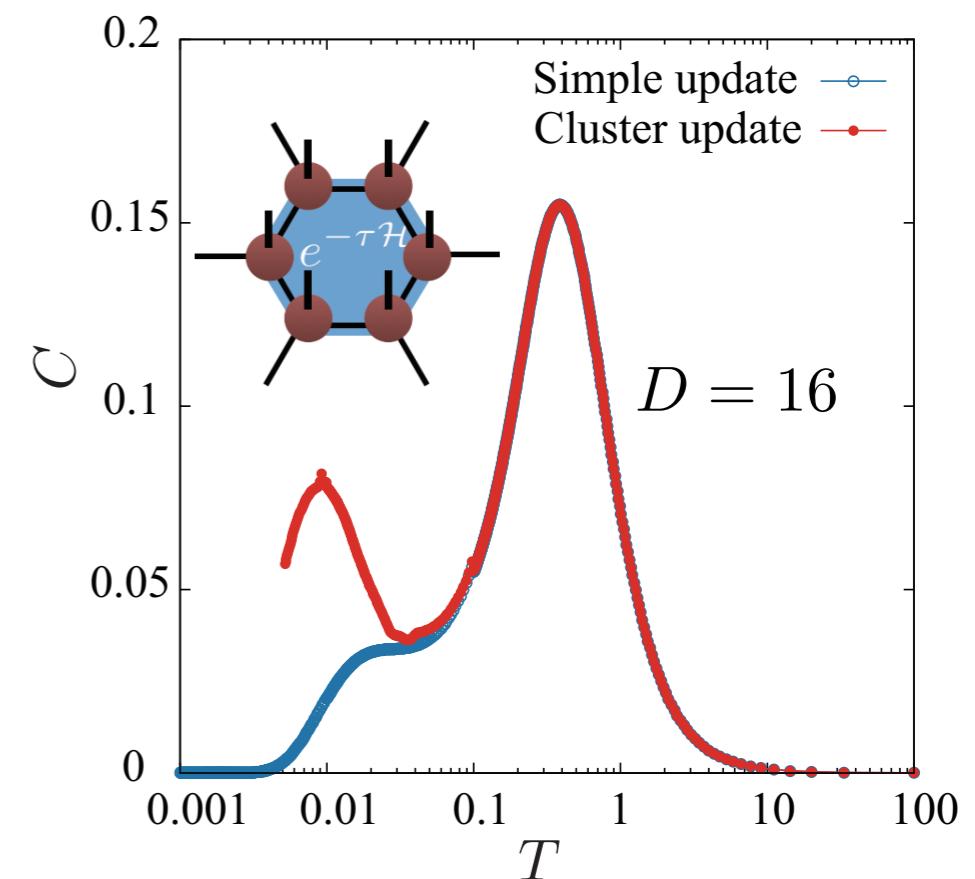
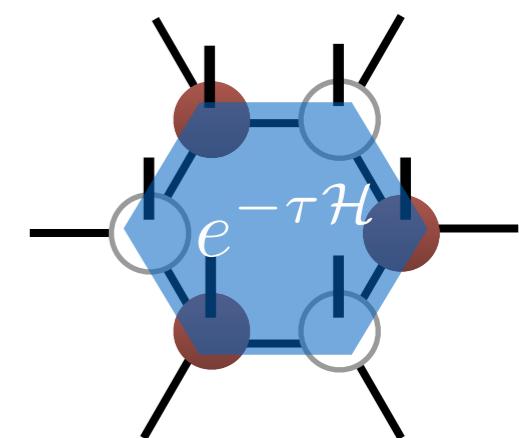
(T. Okubo, JPS meeting, September 2020)

Imaginary time evolution

Simple update



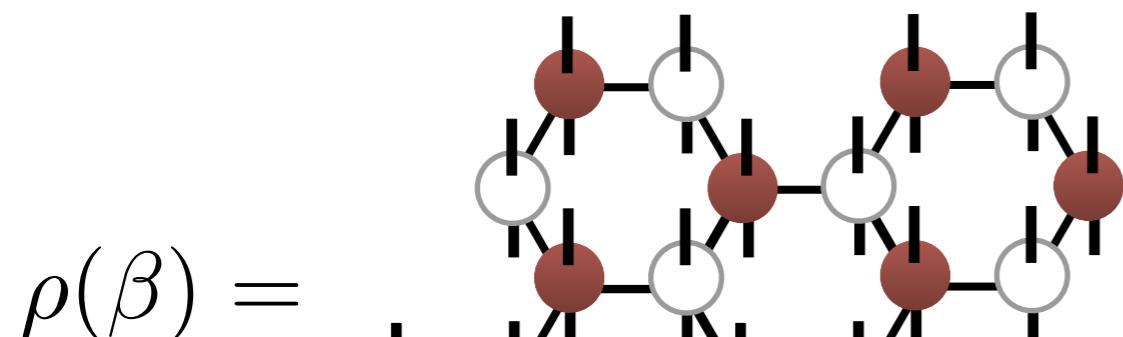
Cluster update



Importance of many-body correlations

Infinite TPO for a density matrix

$$\rho(\beta) = e^{-\frac{\beta}{2}\mathcal{H}} \rho(0) e^{-\frac{\beta}{2}\mathcal{H}}$$



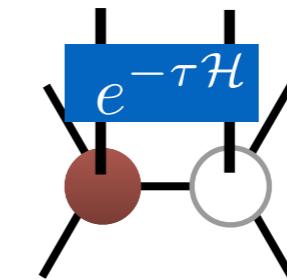
D: bond dimension

When we treat a larger cluster at each ITE step, the specific heat is largely improved.

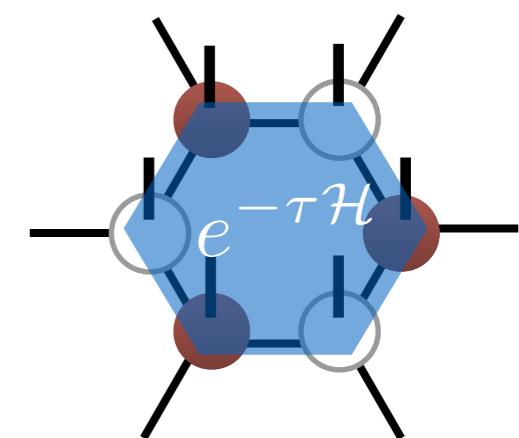
(T. Okubo, JPS meeting, September 2020)

Imaginary time evolution

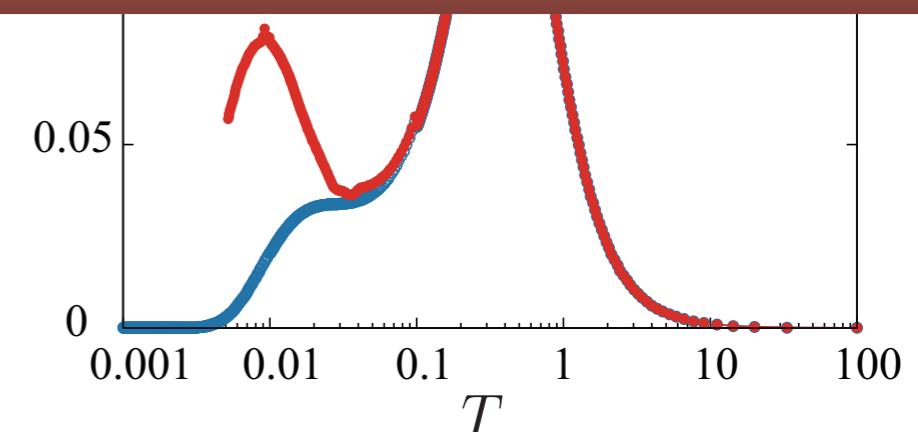
Simple update



Cluster update



Can we improve the treatment of many-body correlations in tensor network structure?



Summary

- By choosing the proper **tensor network structure**, ground state wave functions can be approximated accurately.
 - To search for good tensor networks, **the area law of the entanglement entropy** is important.
 - For one-dimensional quantum systems, matrix product states (**MPS**) works very well.
 - For two or higher-dimensional systems, MPS breaks down. In these cases, instead, **tensor product states** are good tensor networks.
- Owing to the **developments of algorithms and computers**, tensor network methods have become a powerful method to investigate **frustrated spin systems** in two dimensions.
- Optimization of iTPS is important to investigate (difficult) frustrated spin systems.
 - Variational optimization seems to be necessary to investigating non-trivial problems.
 - **Automatic differentiation** might be a good tool to implement VO.
- We can also apply the **.tensor network approach** to **finite temperature properties**.

Appendices

Application of MPS to eigenvalue problem

Calculation of minimum (or maximum) eigenvalue

Target vector space:

Exponentially large Hilbert space

$$\vec{v} \in \mathbb{C}^M \text{ with } M \sim a^N$$

+

Total Hilbert space is decomposed as
a product of "local" Hilbert space.

$$\mathbb{C}^M = \mathbb{C}^a \otimes \mathbb{C}^a \otimes \dots \otimes \mathbb{C}^a$$

Target matrix:

\mathcal{H} :Hermitian, square, and sparse

(Typically, only $O(M)$ ($=O(a^N)$) elements are finite.)

Notice:

We consider the situation where
we cannot store $O(M)$ variables in the memory.

Problem:

Find the smallest eigenvalue and its eigenvector

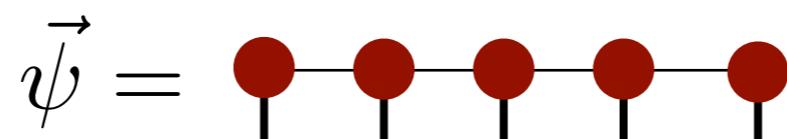
$$\mathcal{H}\vec{v}_0 = E_0\vec{v}_0$$

$$\rightarrow \min_{\vec{\psi} \in \mathbb{C}^M} \frac{\vec{\psi}^\dagger (\mathcal{H} \vec{\psi})}{\vec{\psi}^\dagger \vec{\psi}} \left(= \min_{|\psi\rangle} \frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle} \right)$$

Variational calculation using MPS:

Cost function: $F = \frac{\vec{\psi}^\dagger (\mathcal{H} \vec{\psi})}{\vec{\psi}^\dagger \vec{\psi}}$

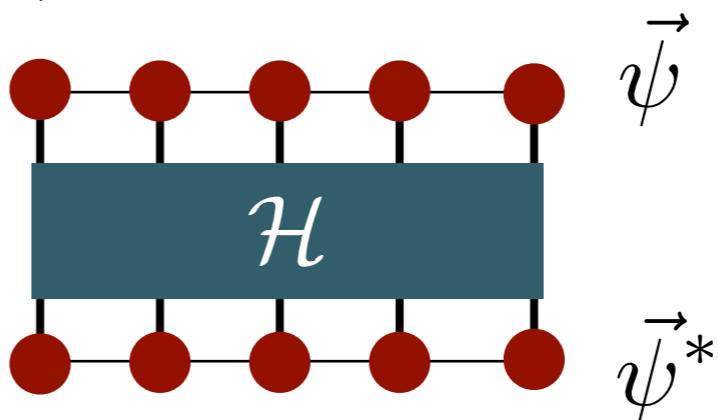
Find the MPS which minimizes F
by optimizing matrices in MPS.



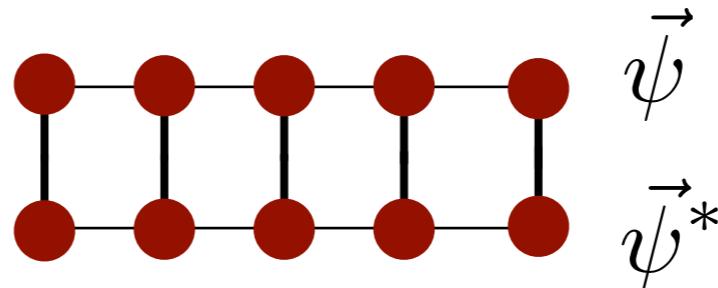
Problem in graphical representation

Cost function: $F = \frac{\vec{\psi}^\dagger (\mathcal{H} \vec{\psi})}{\vec{\psi}^\dagger \vec{\psi}}$

$$\vec{\psi}^\dagger (\mathcal{H} \vec{\psi}) =$$



$$\vec{\psi}^\dagger \vec{\psi} =$$



Find $A_i[\sigma_i] =$ which minimizes F .

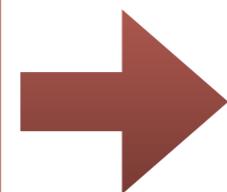
Iterative optimization

(F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004))

Local optimization problem when we focus on a "site" i :

Minimize

$$F = \frac{\vec{\psi}^\dagger (\mathcal{H} \vec{\psi})}{\vec{\psi}^\dagger \vec{\psi}} = \frac{A_i^\dagger (\tilde{\mathcal{H}}_i A_i)}{A_i^\dagger (\tilde{N}_i A_i)}$$

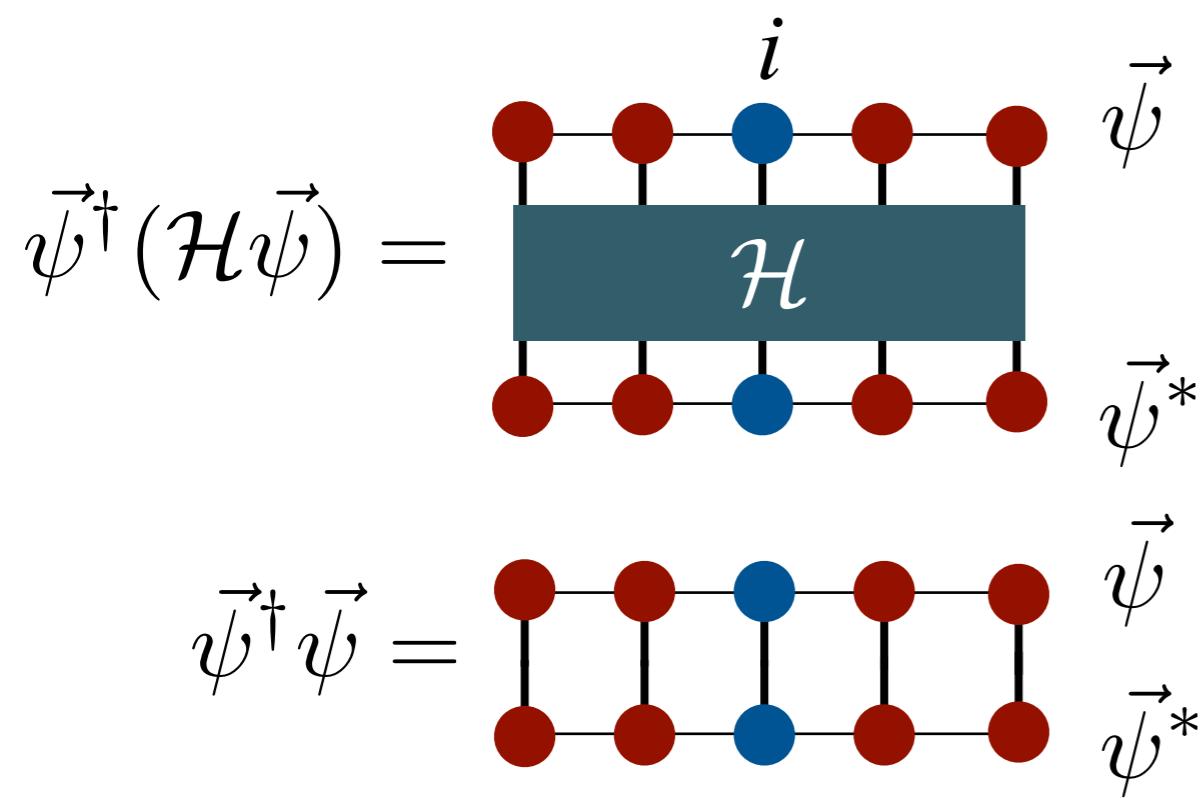


Solve generalized eigenvalue problem

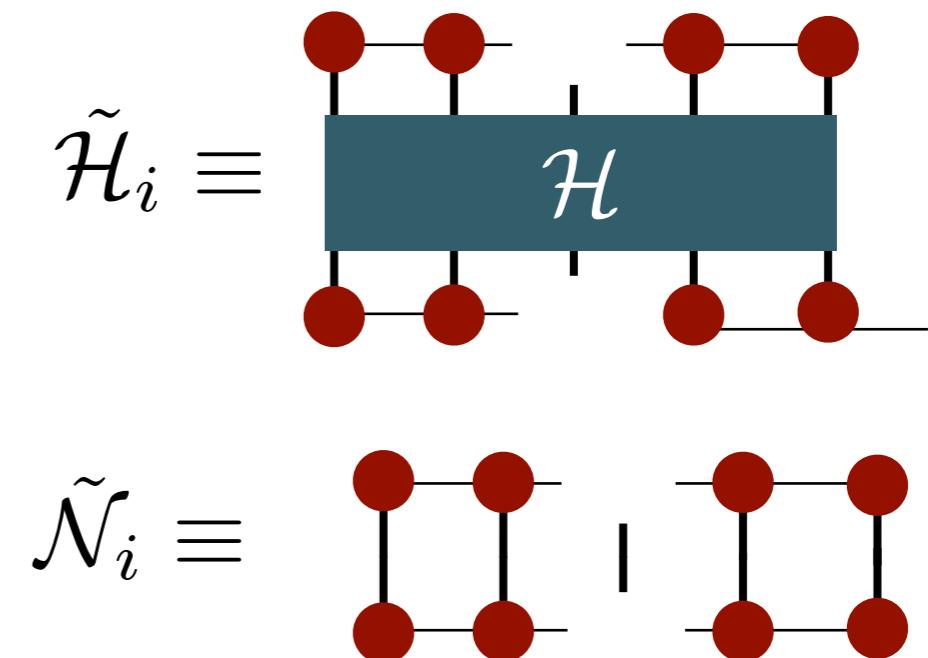
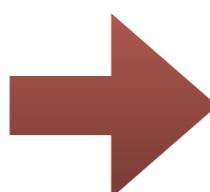
$$\tilde{\mathcal{H}}_i A_i = \epsilon \tilde{N}_i A_i$$

(Find the lowest eigenstate)

Notice: matrix size = $a\chi^2 \times a\chi^2$



Remove A_i

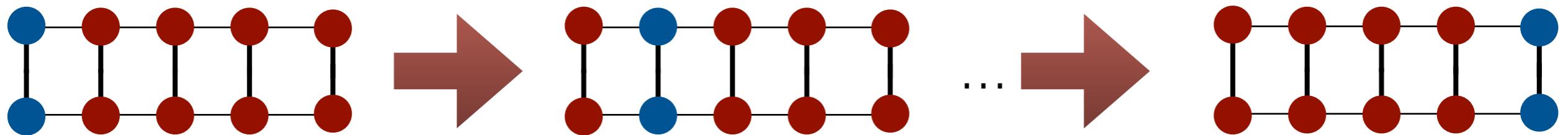


Notice: If we impose canonical form,
 \tilde{N} becomes a simple identity matrix.

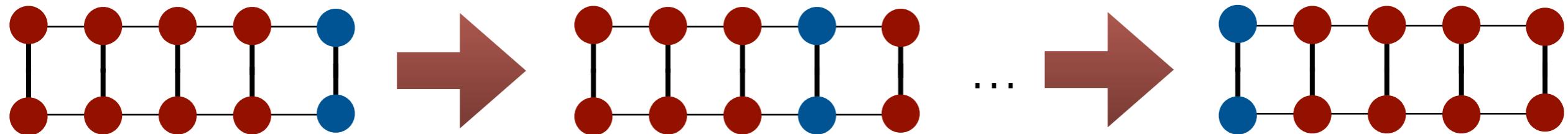
Iterative optimization

(F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004))

Update A_i s by "sweeping" sites $i = 1$ to N



Backward "sweeping" sites $i = N$ to 1



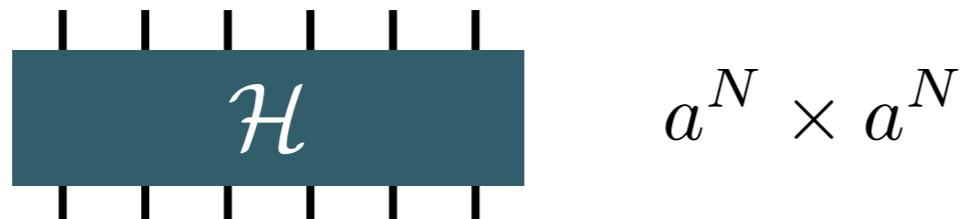
Repeat sweeping until convergence.

Compact representation of an operator

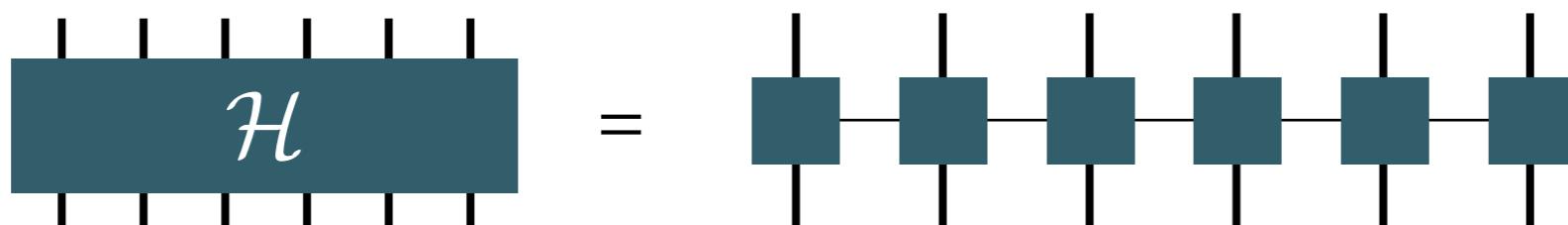
Notice!

We can conduct this algorithm when we can represent the matrix efficiently.

We consider the situation where we **cannot** store the matrix in the memory.



In practical applications, we usually represent the matrix in so called **Matrix Product Operator (MPO)** form.



E.g. The Hamiltonian of the Heisenberg model is represented by MPO with bond dimension $\chi = 5$.

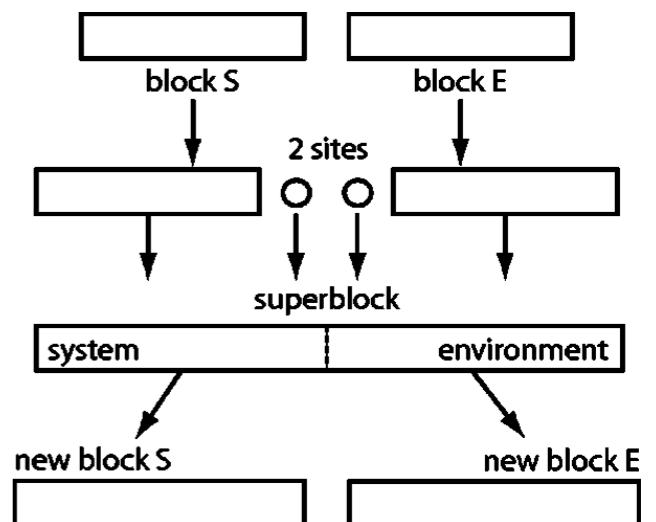
Relation to Density Matrix Renormalization Group

The variational MPS method is essentially same with Density Matrix Renormalization Group (DMRG) algorithm.

(密度行列繰り込み群)

DMRG selects compact basis based on entanglement between "System" and "Environment" blocks.

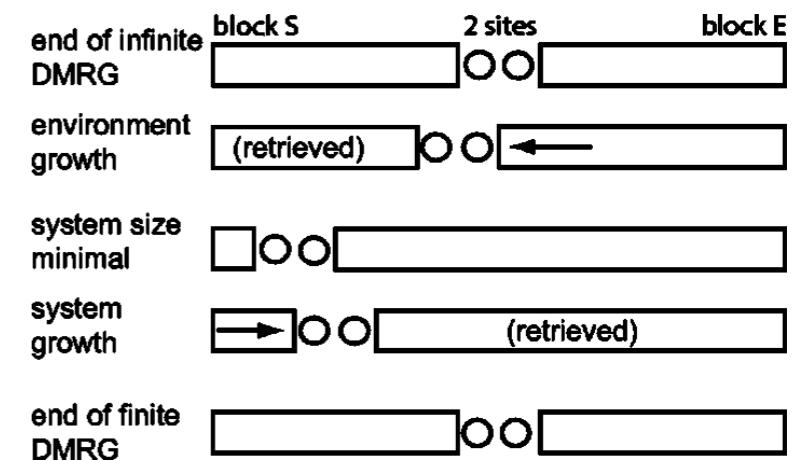
(S. R. White, Phys. Rev. Lett. **69**, 2863 (1992))
(U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005))
(U. Schollwöck, Annals. of Physics **326**, 96 (2011))



DMRG is a powerful tool in physics and chemistry

- One-dimensional spin systems
- One-dimensional electron systems
- Small molecules
- Small two-dimensional systems

The original DMRG did not use MPS explicitly.
But, MPS gives us a theoretical background
for why DMRG works well.

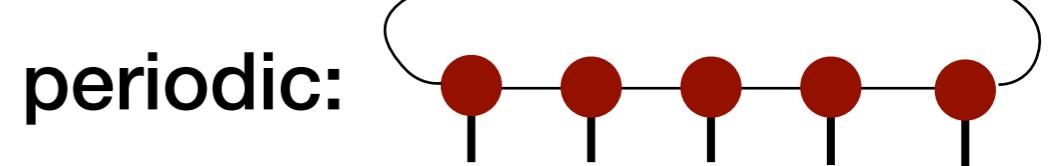
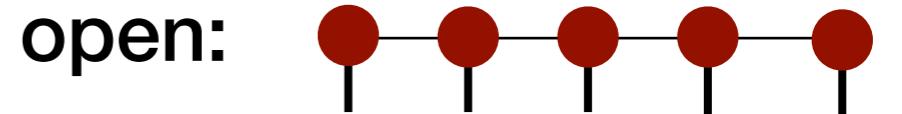


Relation to Density Matrix Renormalization Group

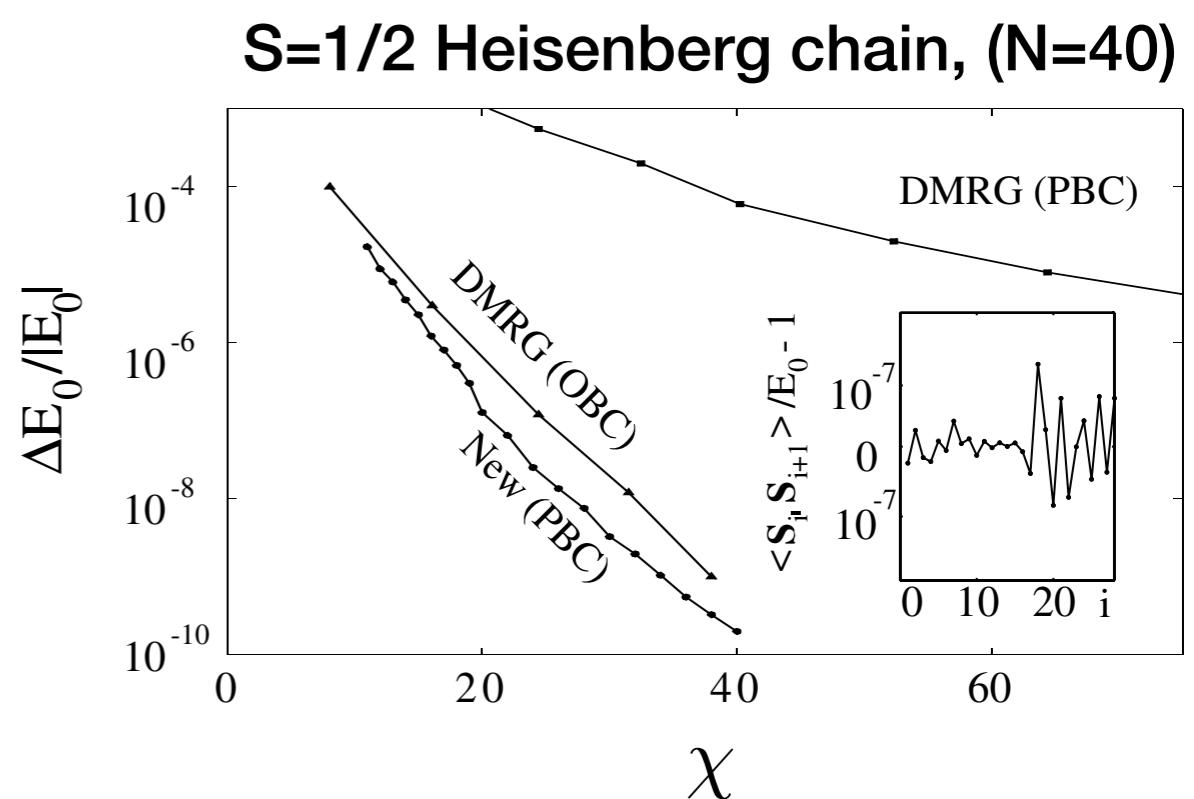
Conventional DMRG algorithm corresponds to variational calculation using **open boundary MPS**.

(F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004))

Accuracy becomes worse if we consider systems with periodic boundary condition.



If we use **periodic** MPS instead of **open** MPS, we can represent the ground state more efficiently.



Application to time evolutions of quantum system

*Similar algorithm can be used to **simulate quantum circuit**.

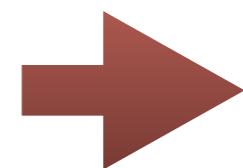
A. McCaskey et al, PLoS ONE **13**, e0206704 (2018)

Related reference:

C. Guo et al, Phys. Rev. Lett. **123**, 190501 (2019)

Time evolution of a quantum system

Schrödinger equation: $i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle$



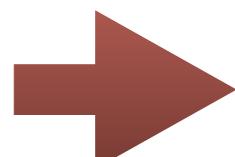
Formal solution:

$$|\psi(t)\rangle = \underbrace{e^{-it\mathcal{H}/\hbar}}_{\text{Time evolution operator}} |\psi(0)\rangle$$

Time evolution operator
(時間発展演算子)

Time evolution using MPS:

1. Multiply the time evolution operator to a MPS.
2. Find an approximate MPS representation for it.



When the time step (t) is small,
we can perform the above step efficiently.

Time evolution of a quantum system using MPS

Target: (Basically) one-dimensional quantum system
with short range interaction

Typical example: Chain of qubits or quantum spins

Transverse field Ising model

$$\mathcal{H} = - \sum_{i=1}^{N-1} S_i^z S_{i+1}^z - h \sum_{i=1}^N S_i^x$$

Heisenberg model

$$\mathcal{H} = \sum_{i=1}^{N-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) - h \sum_{i=1}^N S_i^z$$

Typical situation: Quantum quench

Initial state: Ground state of a Hamiltonian which well approximated by MPS

$t > 0$: Hamiltonian suddenly changes from the initial one.



For a "short" time interval, evolving state is
approximated by MPS efficiently.

Suzuki-Trotter decomposition

Suzuki-Trotter decomposition: (M. Suzuki, Commun. Math. Phys. **51**, 183 (1976))

Systematic approximation of exponential operator

$$\begin{aligned} e^{\tau(\mathcal{A}+\mathcal{B})} &= e^{\tau\mathcal{A}}e^{\tau\mathcal{B}} + O(\tau^2) \quad (\text{1st order}) \\ (\mathcal{A}\mathcal{B} \neq \mathcal{B}\mathcal{A}) \quad &= e^{\tau/2\mathcal{A}}e^{\tau\mathcal{B}}e^{\tau/2\mathcal{A}} + O(\tau^3) \quad (\text{2nd order}) \\ &= e^{\tau/2\mathcal{B}}e^{\tau\mathcal{A}}e^{\tau/2\mathcal{B}} + O(\tau^3) \quad (\text{2nd order}) \end{aligned}$$

→ If our Hamiltonian is represented as a sum of "local" operators,

$$\mathcal{H} = \sum_i H_i \quad \text{E.g. transverse field Ising model}$$

$$H_i = -S_i^z S_{i+1}^z - \frac{h}{2}(S_i^x + S_{i+1}^x)$$

Time evolution operator can be approximated as

$$e^{-it\mathcal{H}/\hbar} = (e^{-i\delta\mathcal{H}})^M = \left(\prod_j e^{-i\delta H_j} \right)^M + O(\delta) \quad \begin{matrix} (\text{1st order}) \\ \delta \equiv t/(M\hbar) \end{matrix}$$

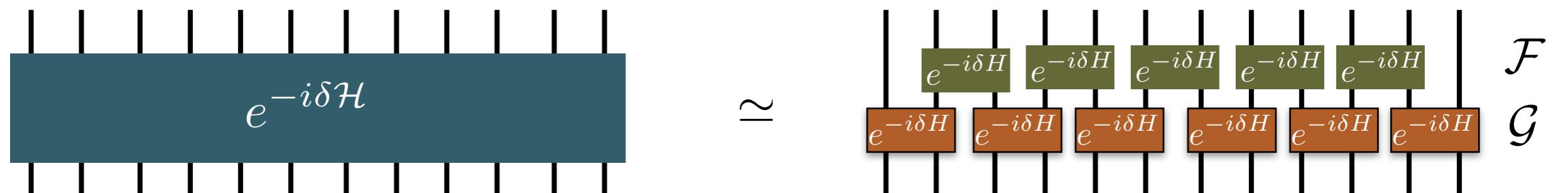
Graphical representation of Suzuki-Trotter decomposition

Suppose the Hamiltonian can be decomposed into the sum of two-body local terms

$$\begin{aligned}\mathcal{H} &= \sum_i H_i = \sum_{i \in \text{even}} H_i + \sum_{i \in \text{odd}} H_i \\ &= \mathcal{F} + \mathcal{G} \quad [\mathcal{F}, \mathcal{G}] \neq 0\end{aligned}$$

Suzuki-Trotter decomposition of time evolution operator

$$e^{-i\delta\mathcal{H}} = e^{-i\delta\mathcal{F}} e^{-i\delta\mathcal{G}} + O(\delta^2) \quad (\text{1st order})$$



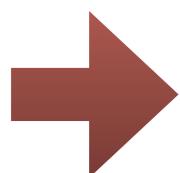
Multiplication of time evolution operator

If we have MPS representation of $|\psi\rangle$

$$|\psi\rangle = \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---}$$

Multiplying the time evolution operator is represented as

$$e^{-i\delta H} |\psi\rangle = \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \quad e^{-i\delta H} \quad \simeq \quad \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \quad e^{-i\delta H} \quad e^{-i\delta H} \quad e^{-i\delta H} \quad e^{-i\delta H}$$



If we can perform the transformation

$$\text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \quad e^{-i\delta H} \quad \simeq \quad \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---}$$

(Generally, all matrices change
for better approximation)

We continue the time evolution repeatedly.

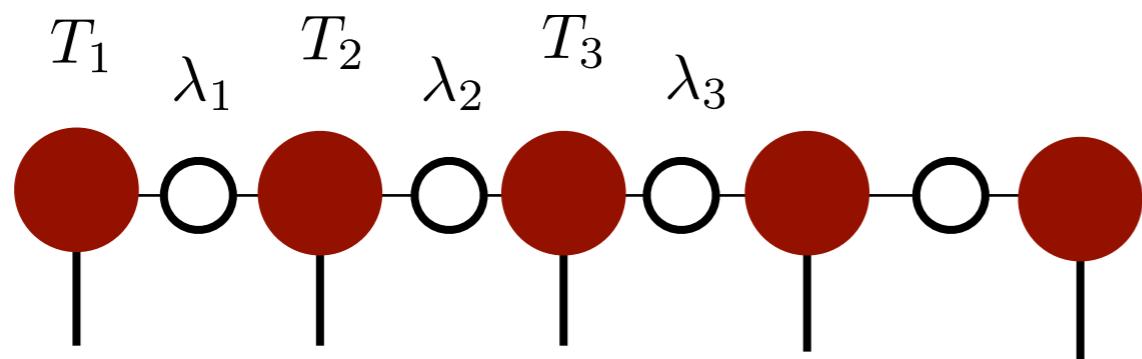
Notice: we want to keep the bond dimension χ constant along time evolution.

TEBD algorithm

Canonical form of MPS

Ref. U. Schollwöck, Annals. of Physics **326**, 96 (2011)

Vidal canonical form



(G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003))

:Diagonal matrix corresponding to Schmidt coefficient

:Virtual indices corresponding to Schmidt basis

Left canonical condition:

$$|\Psi\rangle, T = \begin{bmatrix} & \\ & \end{bmatrix}$$

A diagram showing a segment of an MPS. It consists of two red circles (tensors) connected by a horizontal line. This line connects to two white circles (virtual indices) below it, which are also connected by a horizontal line. This structure is followed by an equals sign and a large empty square bracket.

$\langle \Psi |, T^*$

Right canonical condition:

$$|\Psi\rangle, T = \begin{bmatrix} & \\ & \end{bmatrix} \langle \Psi |, T^*$$

A diagram showing a segment of an MPS. It consists of two white circles (virtual indices) connected by a horizontal line. This line connects to two red circles (tensors) below it, which are also connected by a horizontal line. This structure is followed by an equals sign and a large empty square bracket.

(Boundary)

$$\begin{bmatrix} & \\ & \end{bmatrix} = \begin{bmatrix} & \\ & \end{bmatrix}$$

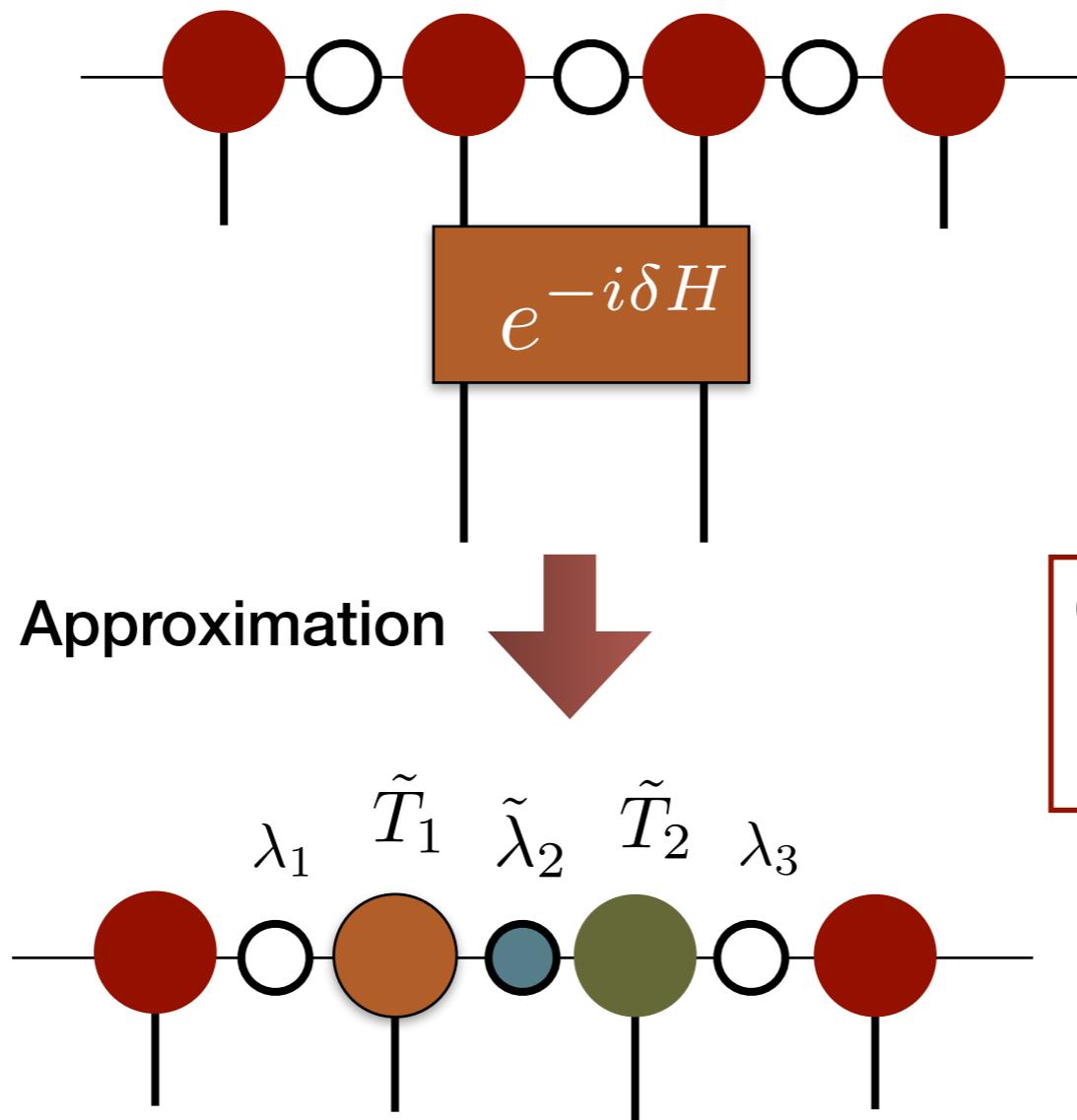
A diagram showing a single red circle (tensor) with two vertical lines extending downwards from its center, representing a boundary MPS segment.

TEBD algorithm:

(G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003))

Time Evolving Block Decimation (TEBD)

We can perform the accurate transformation **locally** by using canonical MPS.

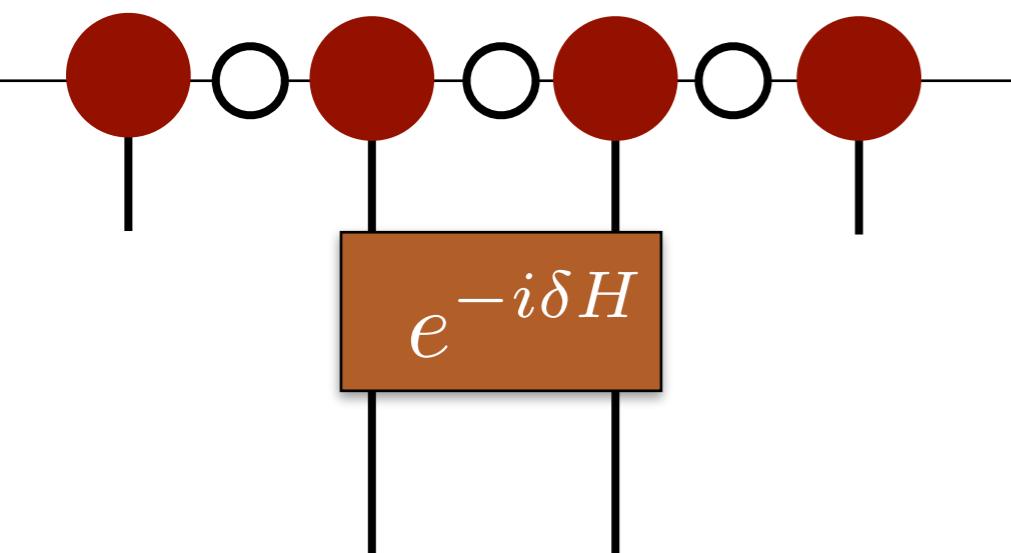


Only the two matrices which are directly applied TE operator changes in MPS.

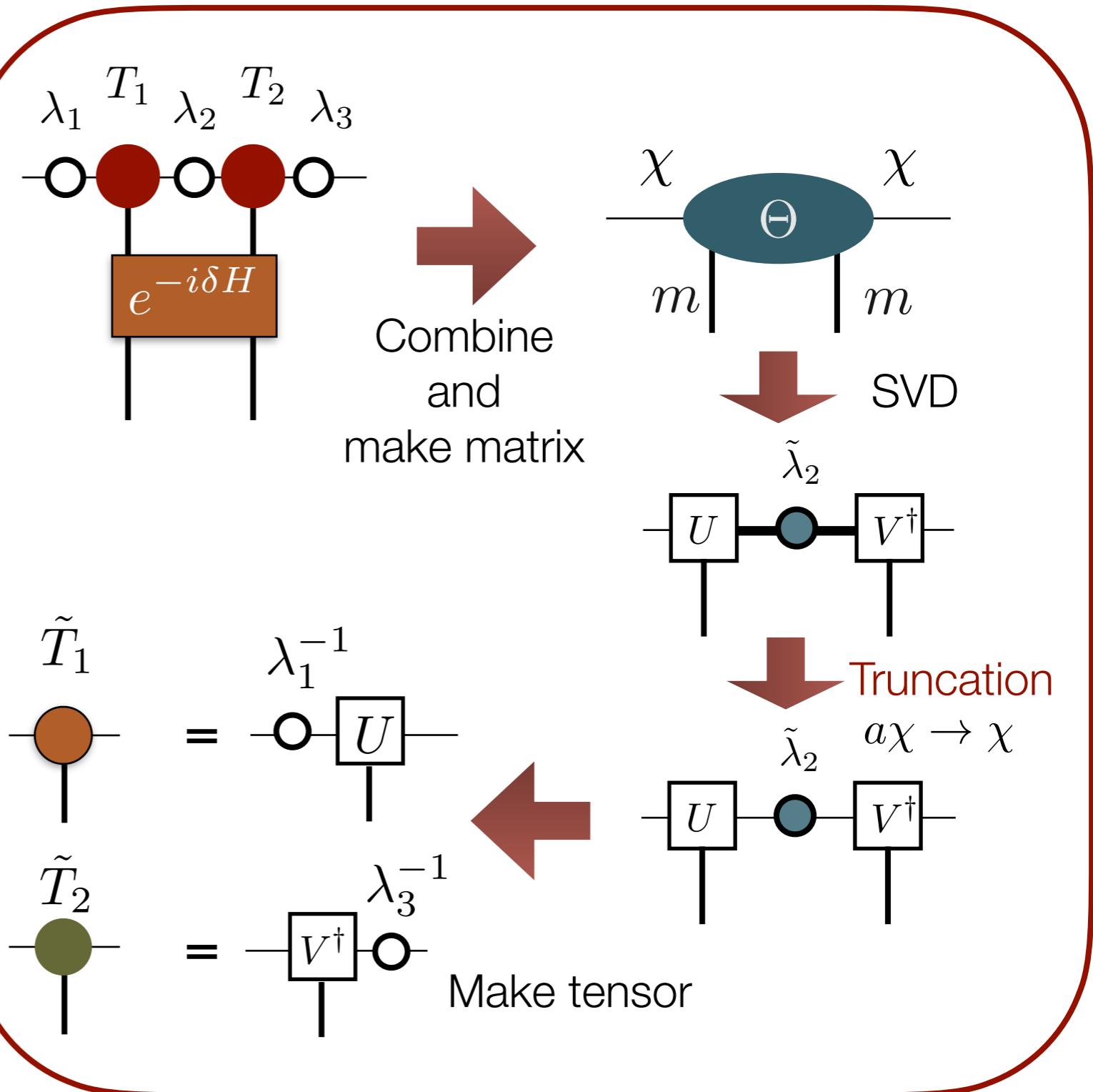
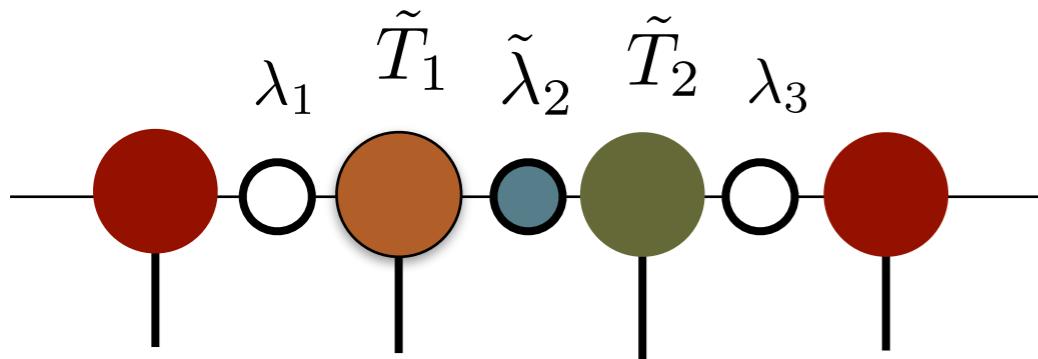
TEBD algorithm:

(G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003))

Apply TE operator



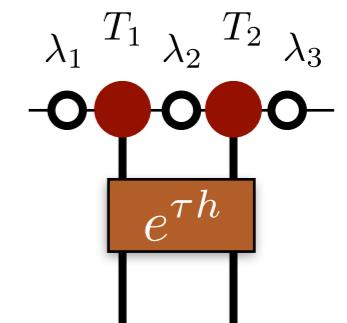
Approximation



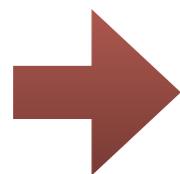
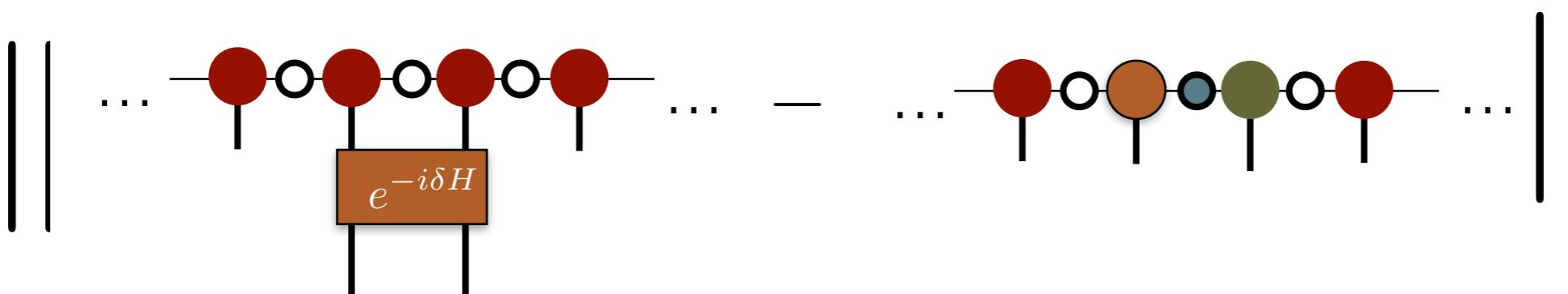
Why TEBD is accurate?

1. For accurate calculation, the canonical form is important.

If λ is equal to the Schmidt coefficient, it contains all information of the **remaining part** of the system.



Due to the canonical form, we can prove that TEBD algorithm minimize the distance of two quantum states:



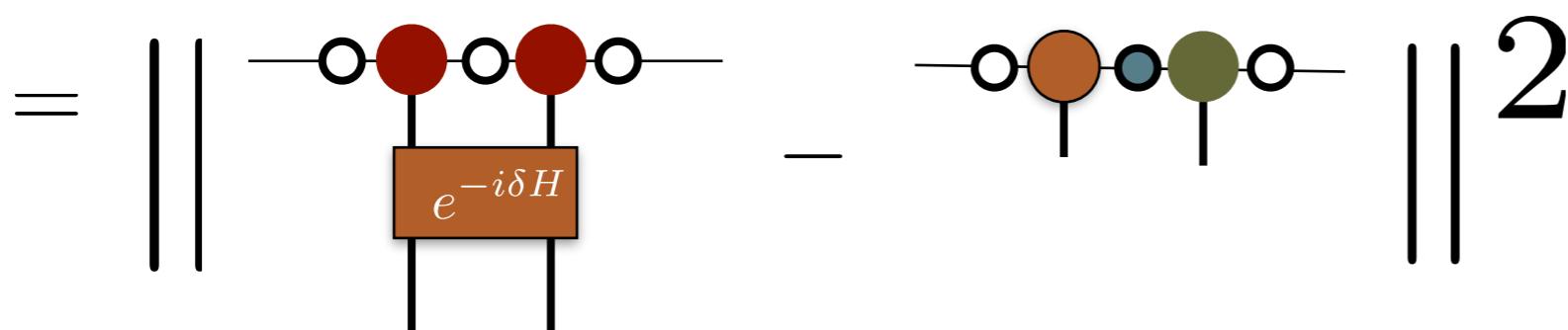
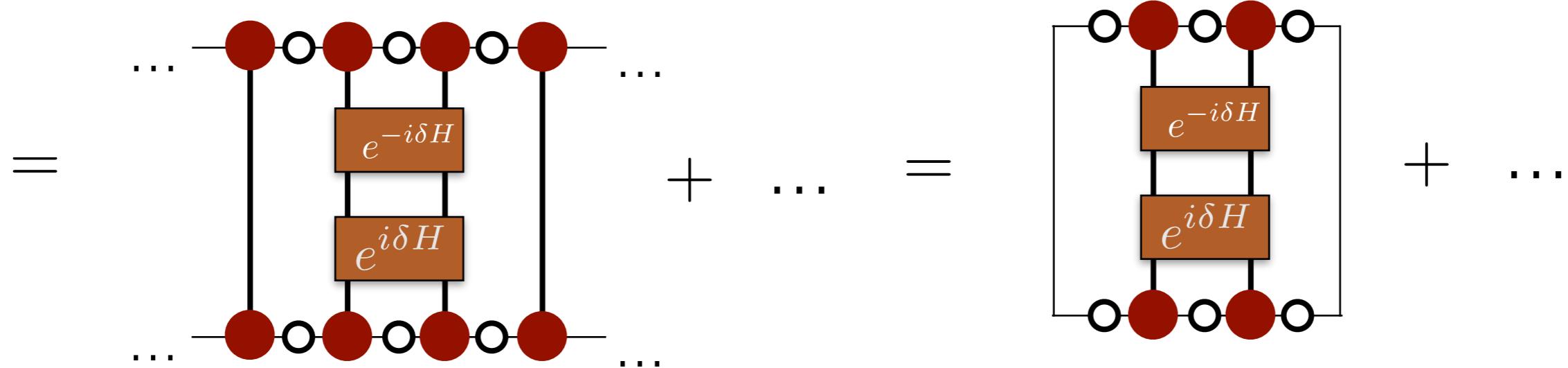
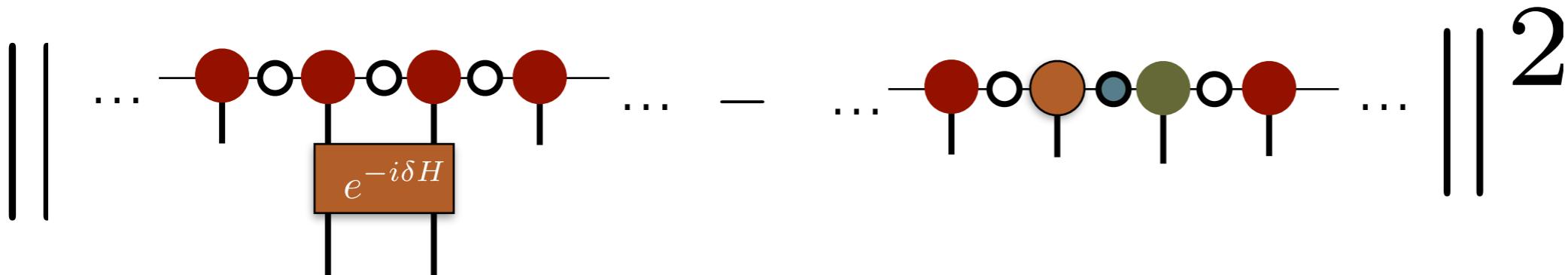
Truncation based on local SVD can be **globally optimal**, even if we look at a part of the MPS.

Calculation distance: remember the calculations

$$\langle \Psi | \Psi \rangle = T^\dagger \lambda = \begin{array}{c} \text{Diagram of } T^\dagger \lambda \\ \text{with red circles and black ovals} \end{array} = \boxed{\text{Diagram of Canonical form}} = \sum_i \lambda_i^2 = 1$$

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

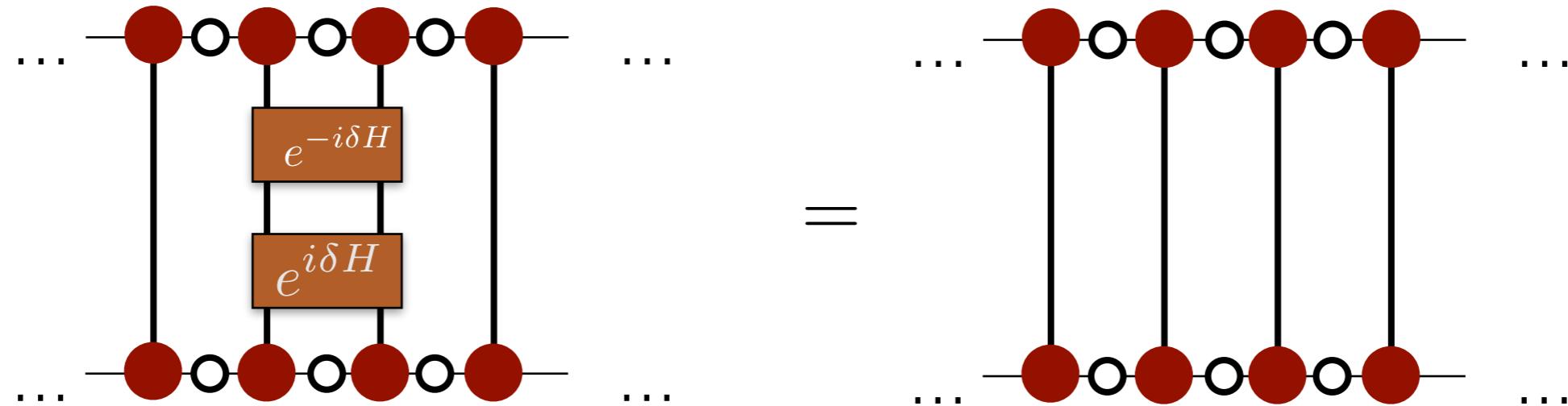
Calculation of the distance



*This is minimized by
the matrix Θ

Why TEBD is accurate?

2. If the operator is unitary, MPS keeps canonical form within truncation error



*Unitary operator does not affect to the other Schmidt coefficients

If we chose the initial MPS as the canonical form,
TEBD algorithm almost keep it.
(So, TEBD is almost "globally optimal")



iTEBD and (i)TEBD for eigenvalue problems

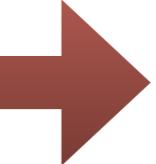
Extension to infinite system iTEBD:

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

Finite system: TEBD

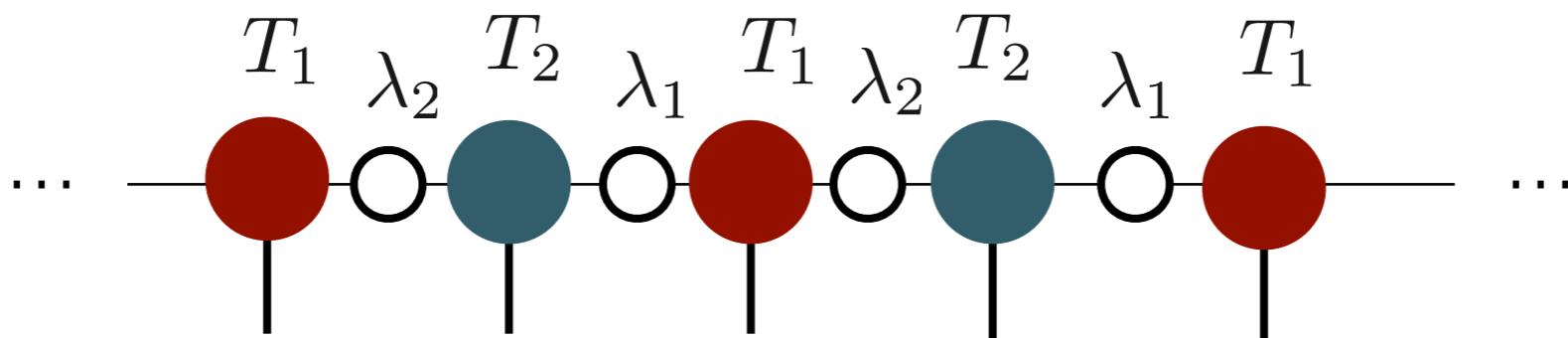
Sequentially apply ITE operators  $O(N)$ SVD for each step

Infinite system: iTEBD

Due to the translational invariance,
all SVD are equivalent.  $O(1)$ SVD for each step

*Note

Because of SVD in iTEBD algorithm, we need at least two independent tensors even in translationally invariant system



(i)TEBD can be used for eigenvalue problem

Method to optimize MPS for GS of a specific Hamiltonian

1. Variational optimization

Change matrix elements to reduce the energy: $\min_{T,\lambda} \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$

2. Imaginary time evolution

Simulate **imaginary time evolution**: $|\Psi_{\text{GS}}\rangle \propto \lim_{\beta \rightarrow \infty} e^{-\beta \mathcal{H}} |\Psi_0\rangle$
(虚時間発展)

For a initial state $\langle \Psi_{\text{GS}} | \Psi_0 \rangle \neq 0$



By replacing the time evolution operator to
the **imaginary time evolution operator**,

$$e^{-i\mathcal{H}t} \rightarrow e^{-\tau \mathcal{H}} \quad (t \rightarrow -i\tau)$$

We can use (**TEBD**) algorithm for eigenvalue problem.

Difference between TE and ITE

$e^{-i\mathcal{H}t}$: Time evolution operator is **unitary**

$e^{-\mathcal{H}\tau}$: Imaginary time evolution operator is **not unitary**

→ In general, by multiplying imaginary time evolution operator to MPS,
the canonical form is destroyed and TEBD becomes **less accurate**.

However, when τ is small the operator is **almost unitary**.

(Because it is almost identity matrix)

If we chose the initial MPS as the canonical form,
TEBD algorithm **almost keep it**.

(So, TEBD is almost "globally optimal" even in the
case of the imaginary time evolution.)

*Instead, we can transform the MPS into the canonical form
after multiplying ITE operator in every steps.

Details of CTMRG

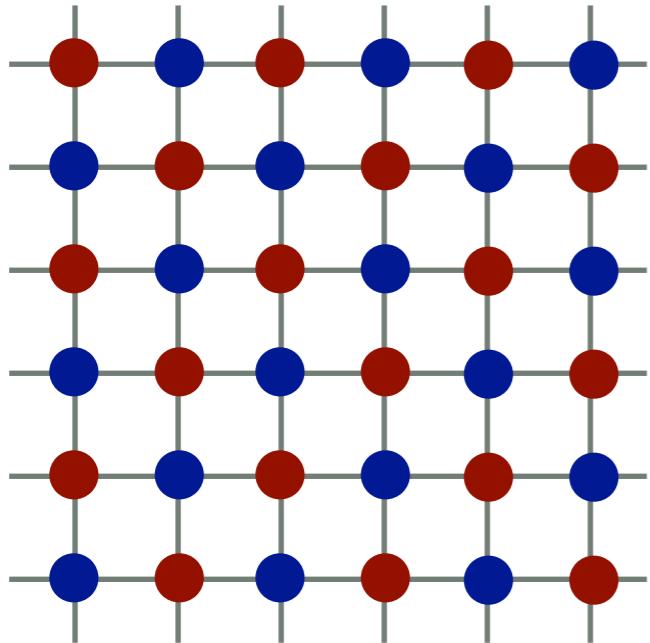
Corner transfer matrix method

For (infinite) open boundary system

(T. Nishino and K. Okunishi, JPSJ **65**, 891 (1996))
(R. Orus *et al*, Phys. Rev. B **80**, 094403 (2009))

Infinite PEPS

(with a translational invariance)



Double tensor

$$\begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array}$$



Mapping to a "classical" system

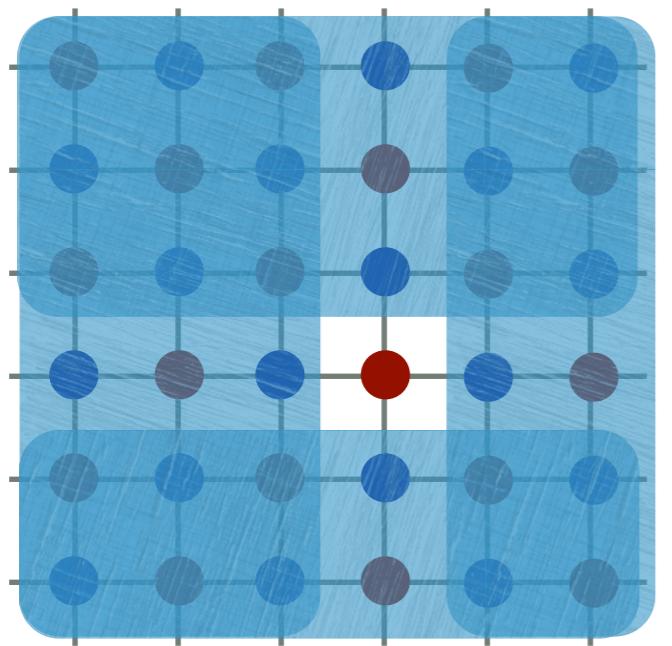
Corner transfer matrix method

For (infinite) open boundary system

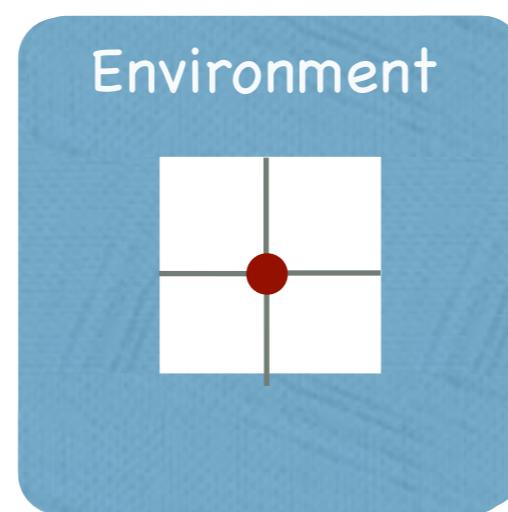
(T. Nishino and K. Okunishi, JPSJ **65**, 891 (1996))
(R. Orus *et al*, Phys. Rev. B **80**, 094403 (2009))

Infinite PEPS

(with a translational invariance)



Environment



Double tensor

$$\begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array}$$



Mapping to a "classical" system

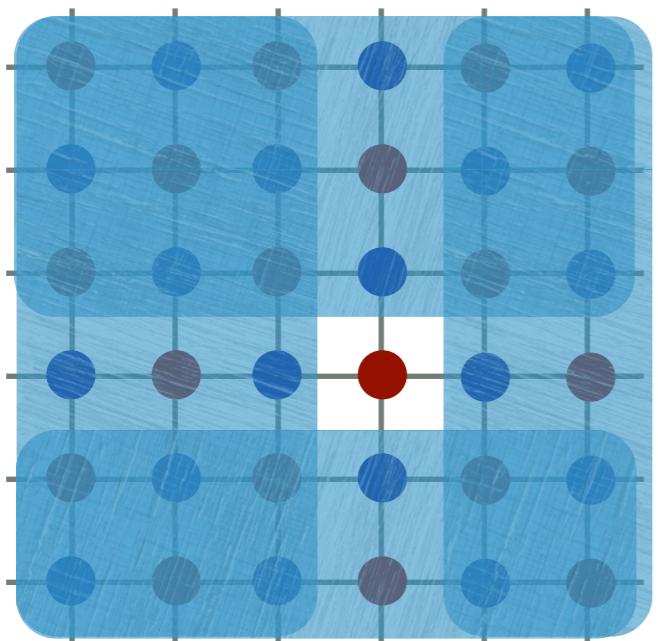
Corner transfer matrix method

For (infinite) open boundary system

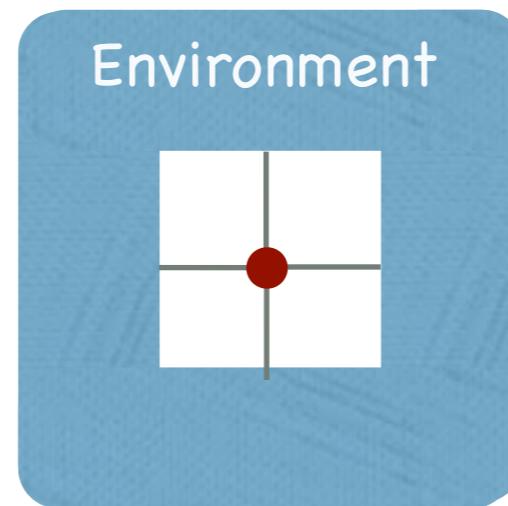
(T. Nishino and K. Okunishi, JPSJ **65**, 891 (1996))
(R. Orus *et al*, Phys. Rev. B **80**, 094403 (2009))

Infinite PEPS

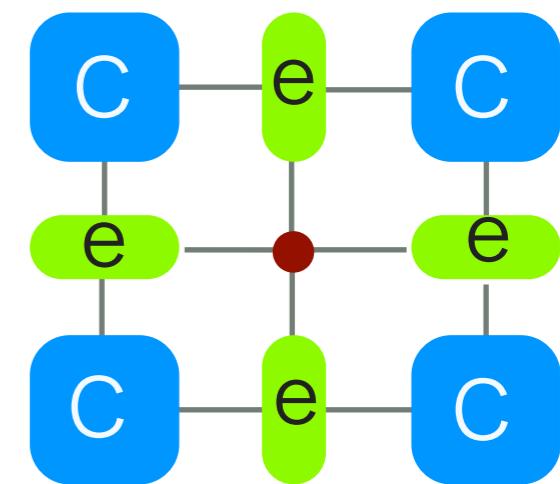
(with a translational invariance)



Environment



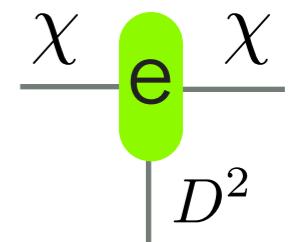
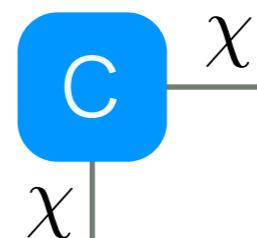
Corner transfer matrix Representation



Corner transfer matrix

Edge tensor

$$\text{Double tensor} = \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array}$$



→ **Mapping to a "classical" system**

χ = bond dimension $\chi \sim D^2$

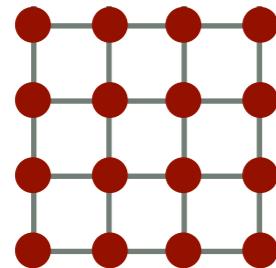
Original simple CTM renormalization group

- Successive "renormalization" method for contracting classical tensor network proposed by Nishino and Okunishi.
(J. Phys. Soc. Jpn. **65**, 81 (1996); **66**, 3040 (1997).)
 - Corner Transfer Matrix Renormalization Group (CTMRG)
- Contract classical tensor network by changing the system size as $L \rightarrow L+2$, sequentially
- Recently, it is also used for environment calculation in two-dimensional quantum many body system represented by iPEPS (iTPS)

**First, I explain the simplest CTMRG for
2d classical Ising model**

Outline of CTMRG

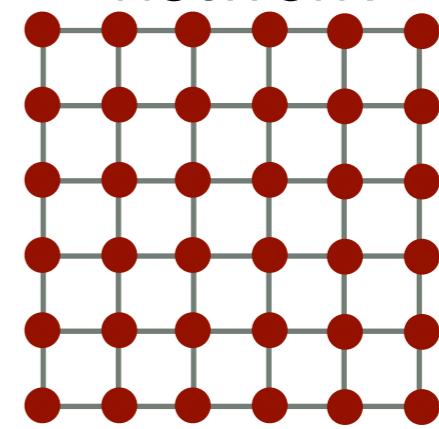
Suppose we have
(approximately) calculated
contraction of $L \times L$ network.



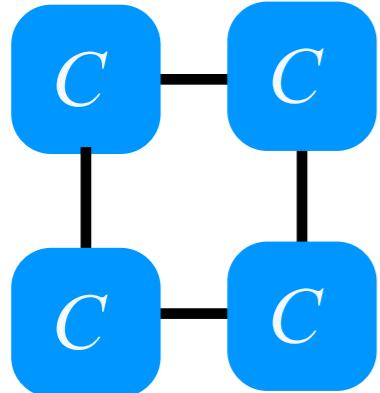
$A: m \times m \times m \times m$

Increase system size slightly

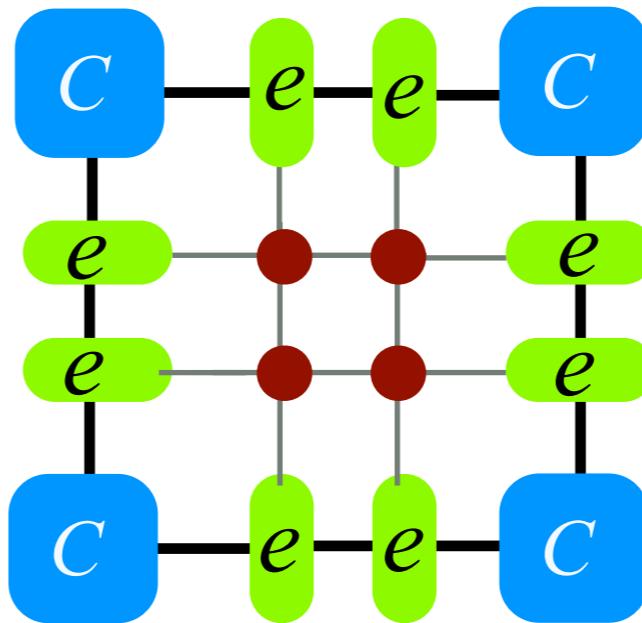
Contraction of $(L+2) \times (L+2)$
network



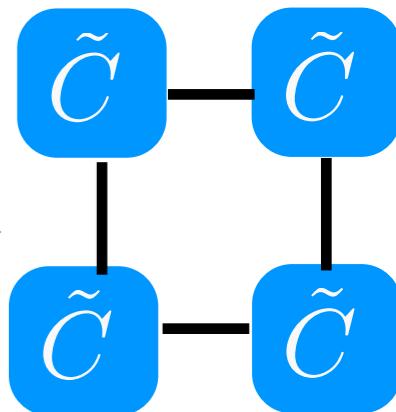
CTM representation



Increase system size slightly



approximation

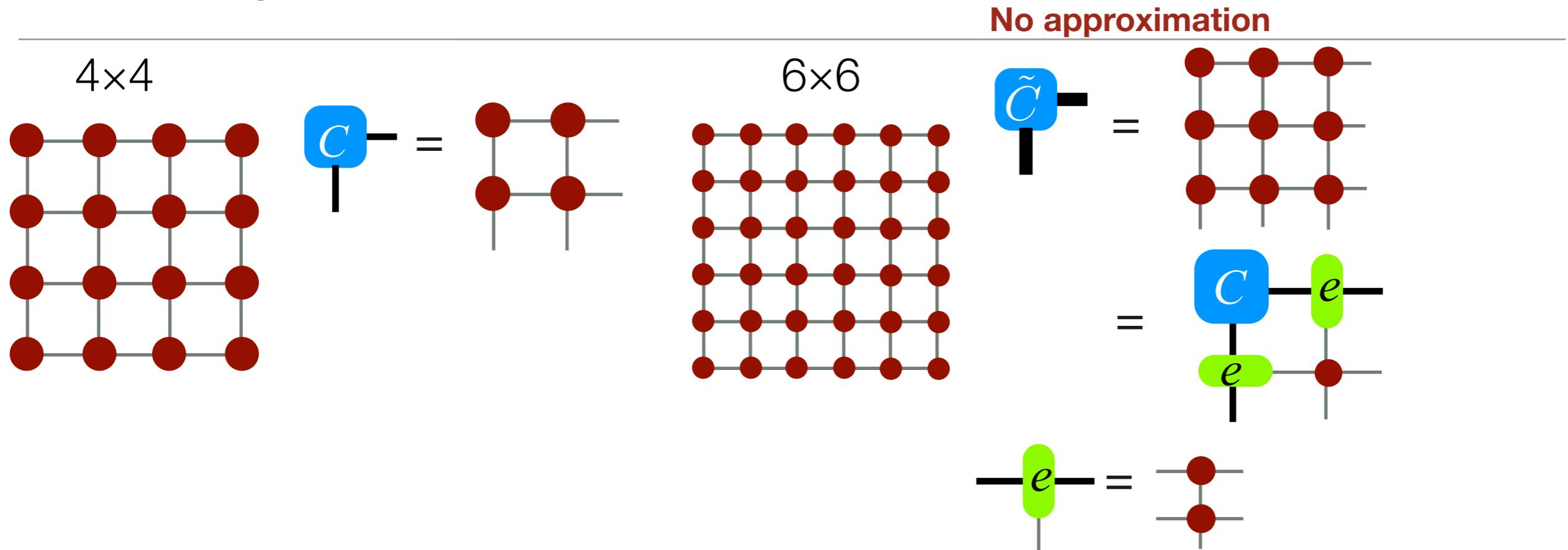


$C: D \times D$

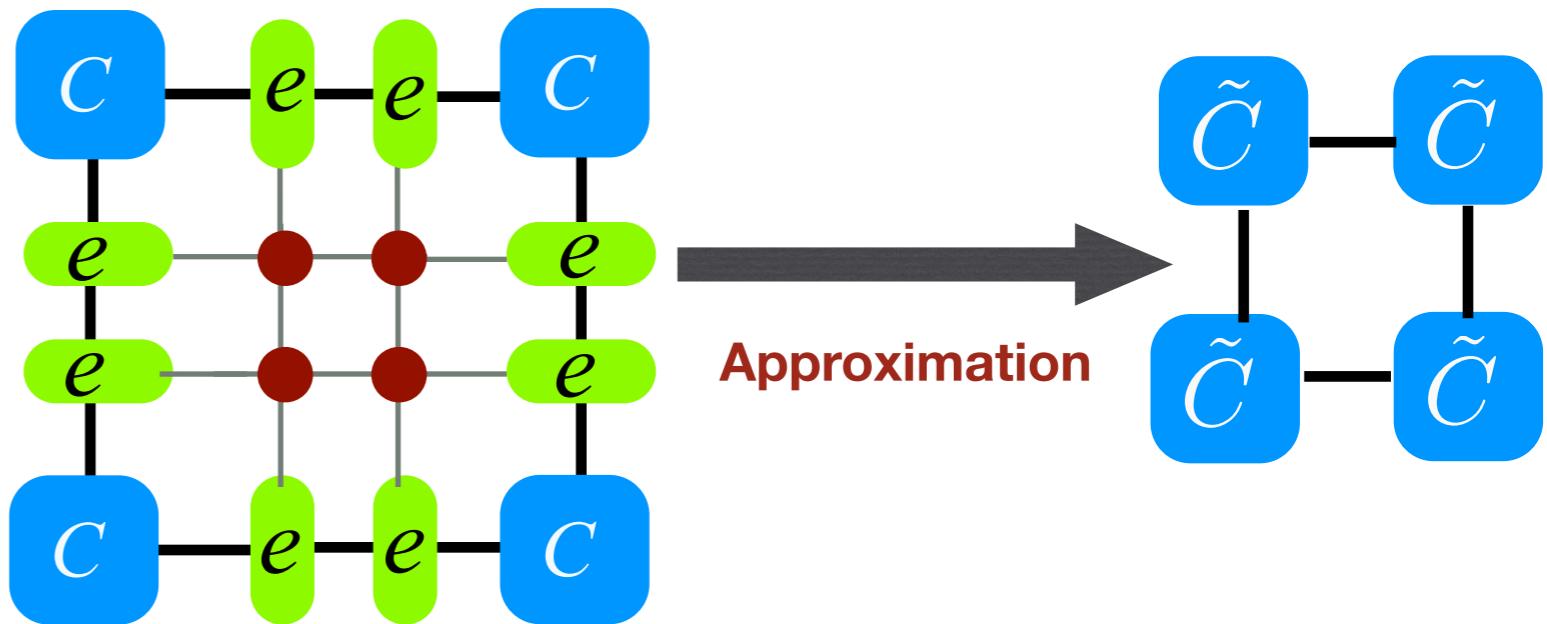
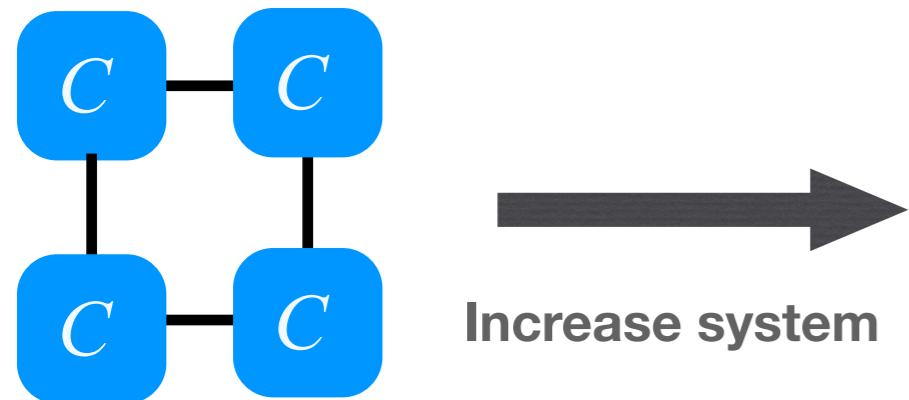
$\tilde{C}: D \times D$

Increase system size
by keeping the size of C

Meaning of Corner Transfer Matrix



CTM representation

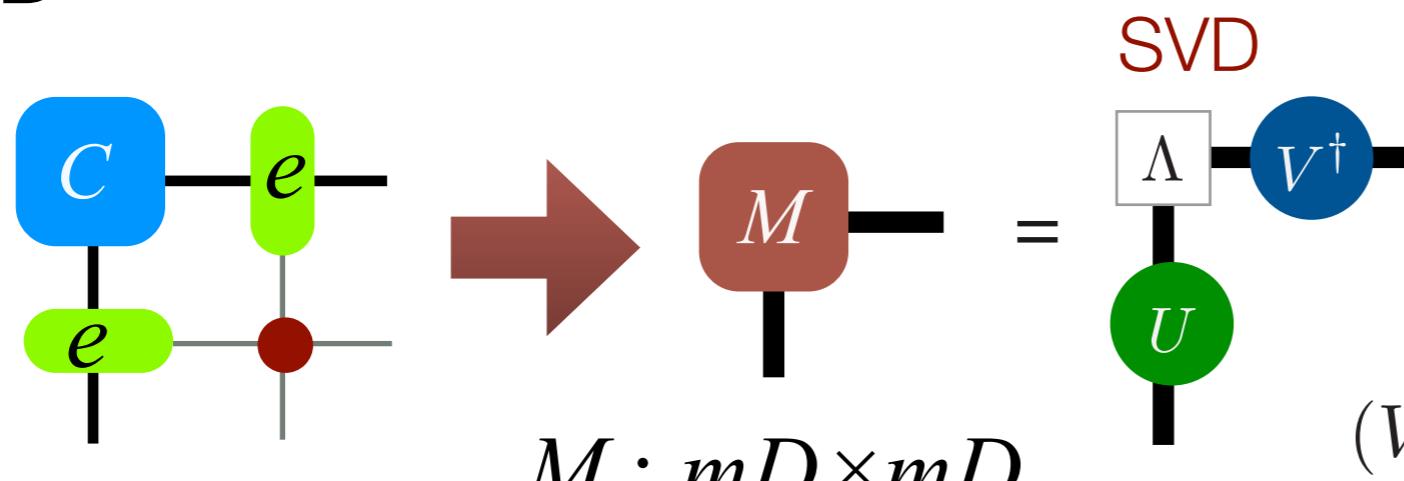


Recipe of CTMRG

Cost

contraction: $O(D^3m^2), O(D^2m^4)$
 svd: $O(D^3m^3), O(D^3m^2)$

1. SVD

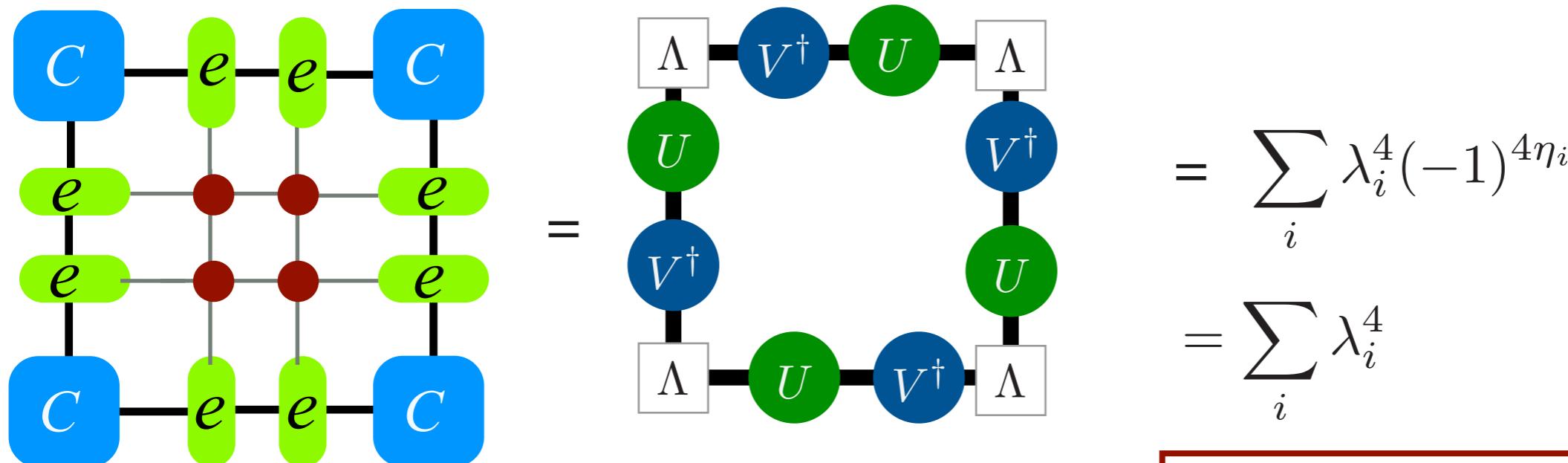


SVD

In the case of Ising mode,
 M is a real symmetric matrix

$$(V^\dagger U)_{i,j} = (U^\dagger V)_{i,j} = (-1)^{\eta_i} \delta_{i,j}$$

$$\eta_i = 0, 1$$

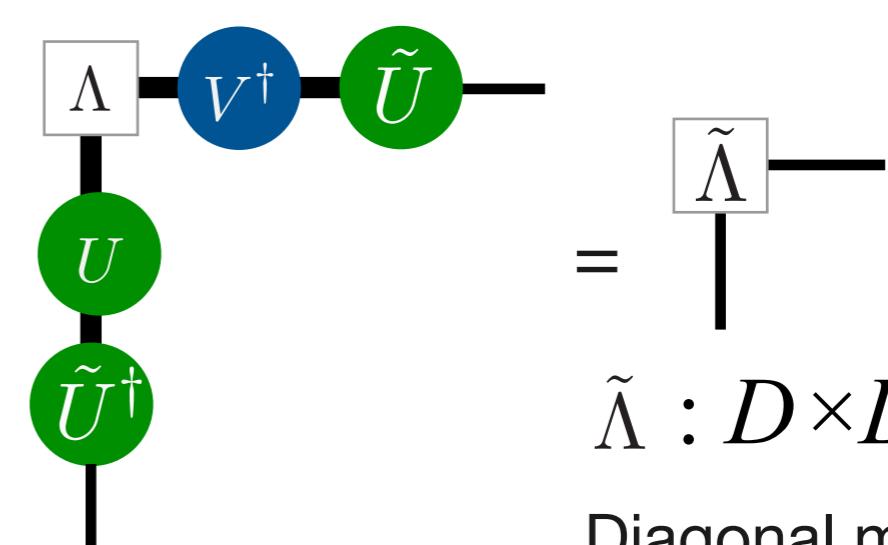
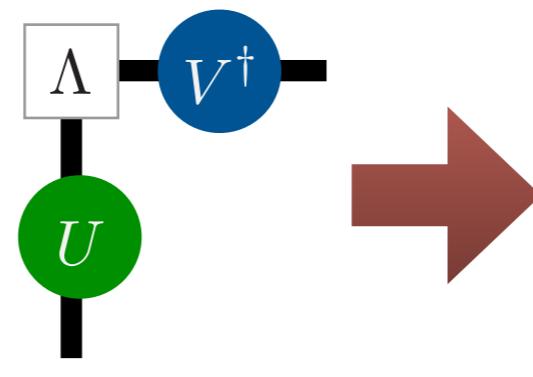
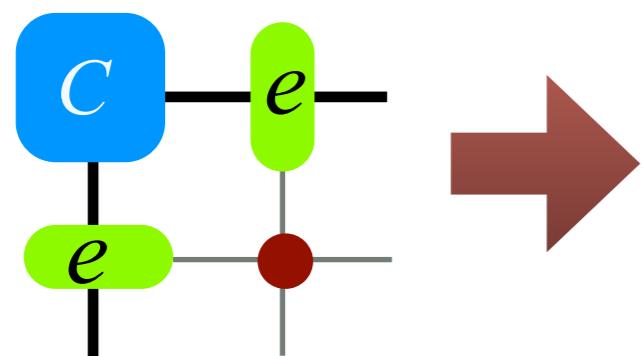


Using symmetry

Good approximation when we
 keep largest singular values!

Recipe of CTMRG

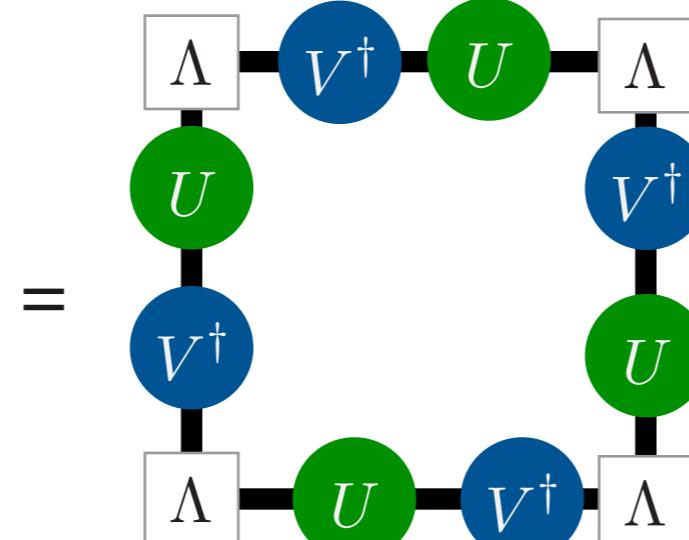
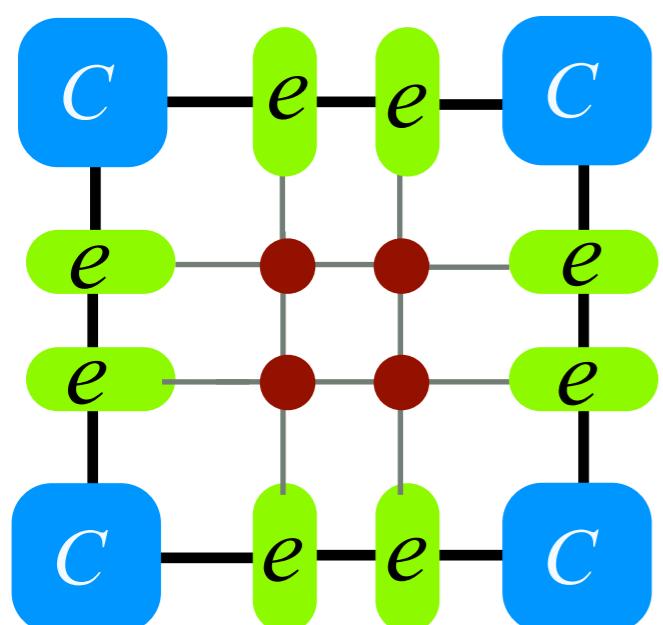
2. Approximation



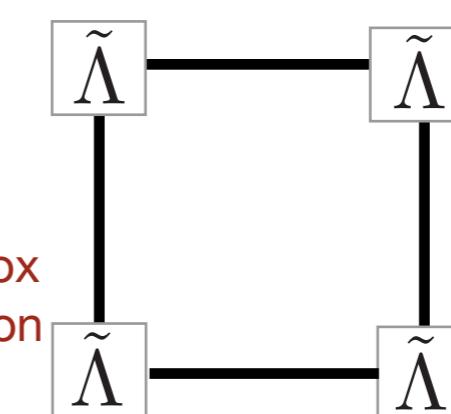
$$\tilde{U} : mD \times D$$

$$= \tilde{\Lambda} : D \times D$$

Diagonal matrix
with $(-1)^{\eta_i} \lambda_i$



\approx
approximation



$$Z = \sum_i^{2D} \lambda_i^4$$

$$Z \simeq \sum_i^D \lambda_i^4$$

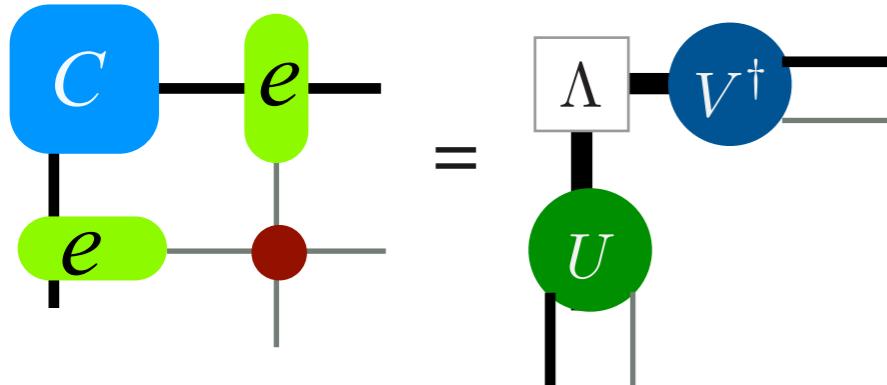
Cost

Recipe of CTMRG

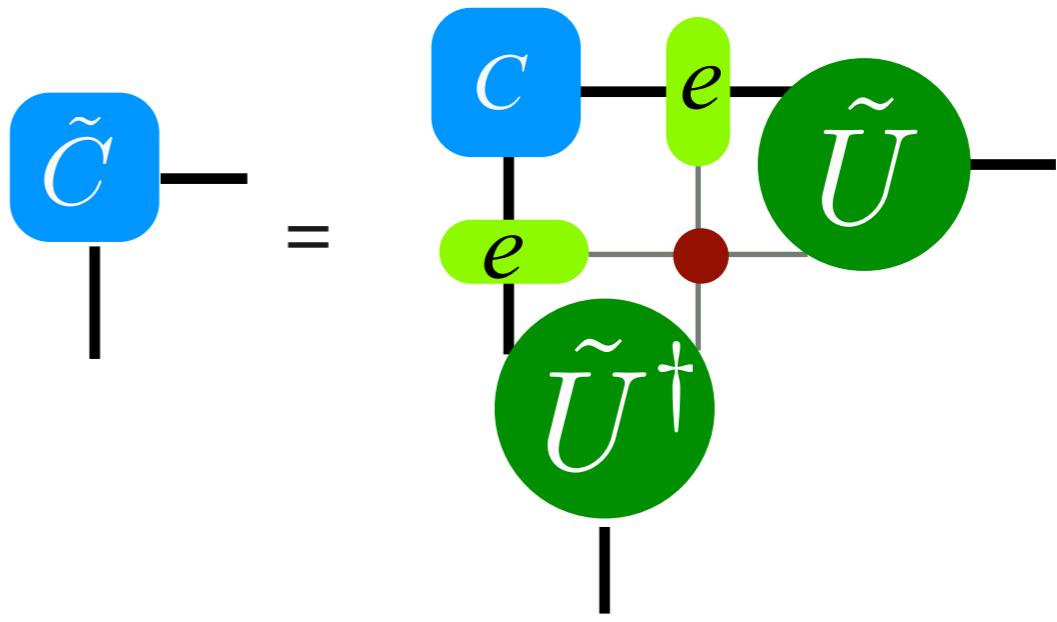
C,e contraction: $O(D^3m^2), O(D^2m^4)$

Summary of renormalization

1. SVD of the corner matrix for $(L+2) \times (L+2)$ system

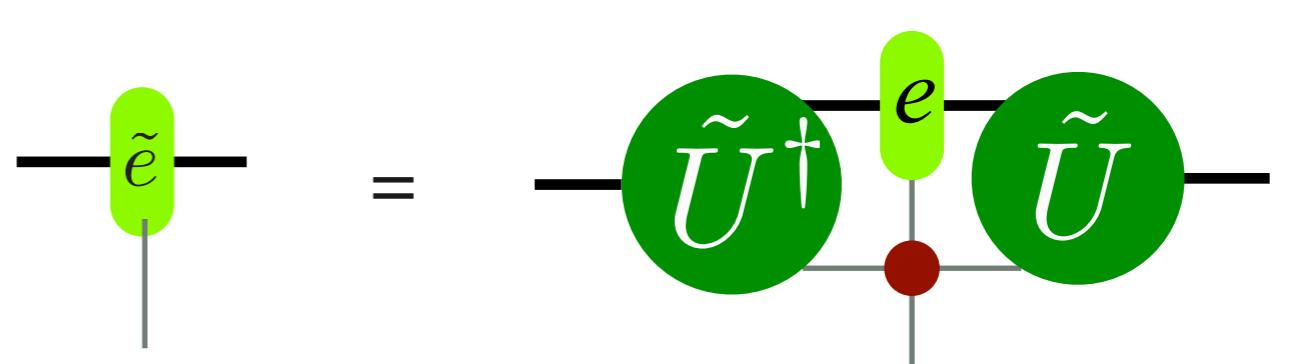
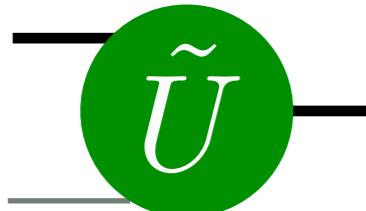


3. Make new corner and edge matrices



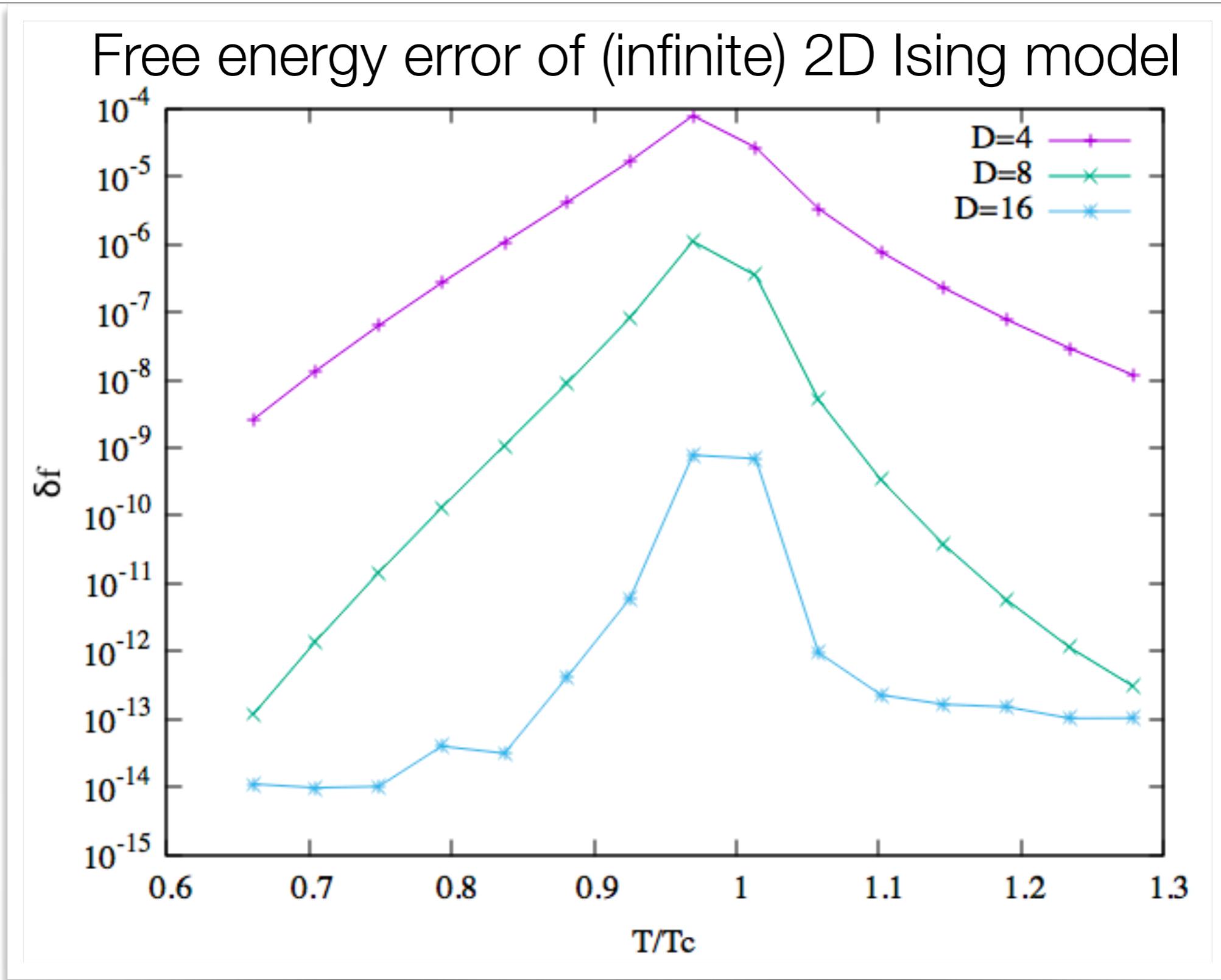
2. Make projector

Keep the largest D singular values



We can calculate tensor network contraction successively

Accuracy of CTMRG



Application to quantum system

Difference from the Ising model

"Classical" tensor is represented by product of two "quantum" tensors

Double tensor

-
- Typically, bond dimension "m" becomes much larger than that of classical models
 - We can **reduce computational cost** by using this structure explicitly

The tensor network has larger periodicity than Ising model.

In addition, the local tensor does not necessarily have rotational symmetry

-
- We use more complicated renormalization steps
 - left, right, top, bottom moves
 - We use different **definition of the projector**

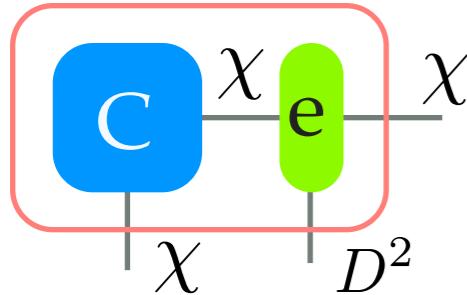
Update for quantum model

(R. Orus *et al*, Phys. Rev. B **80**, 094403 (2009))

Iterative update of environment tensors

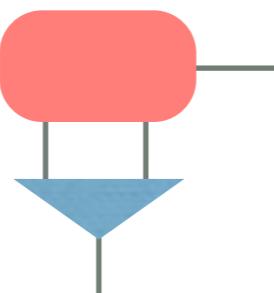
Absorption

(ex. left move)

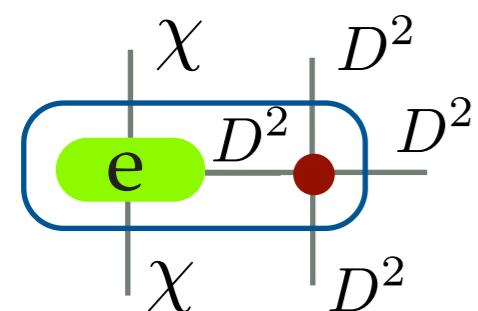
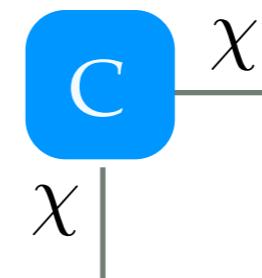


$\star O(\chi^3 D^2)$

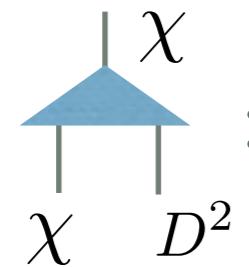
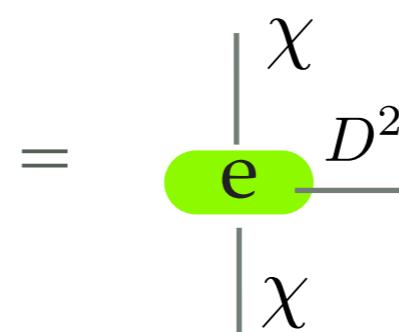
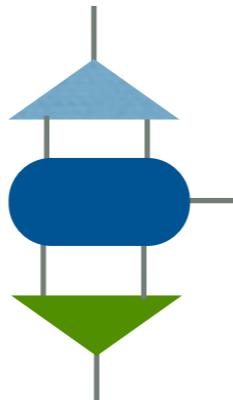
Truncation



New

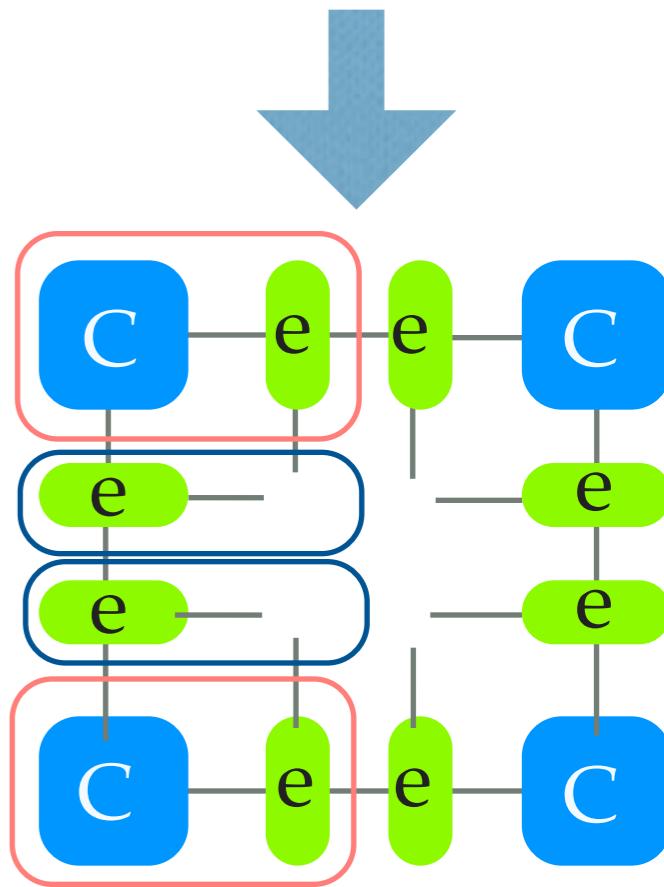
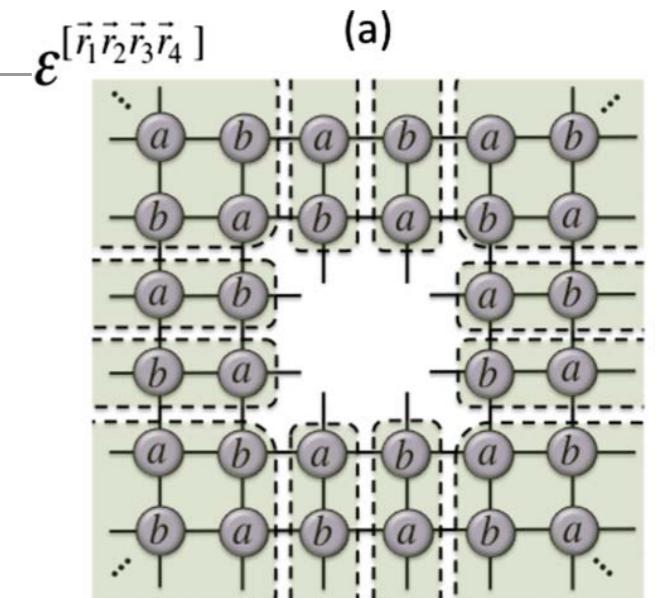


$\star O(\chi^2 D^8)$



:Projector

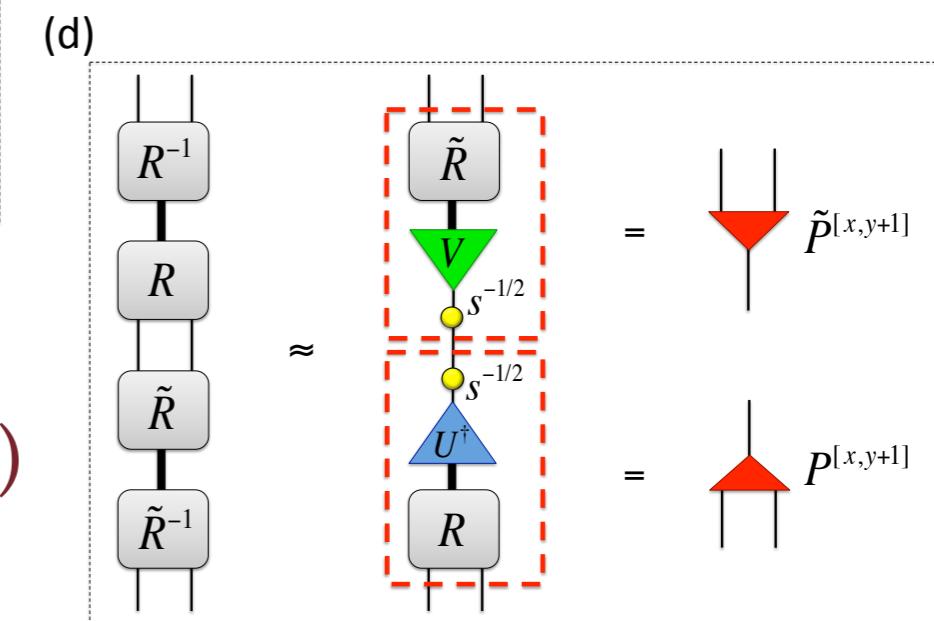
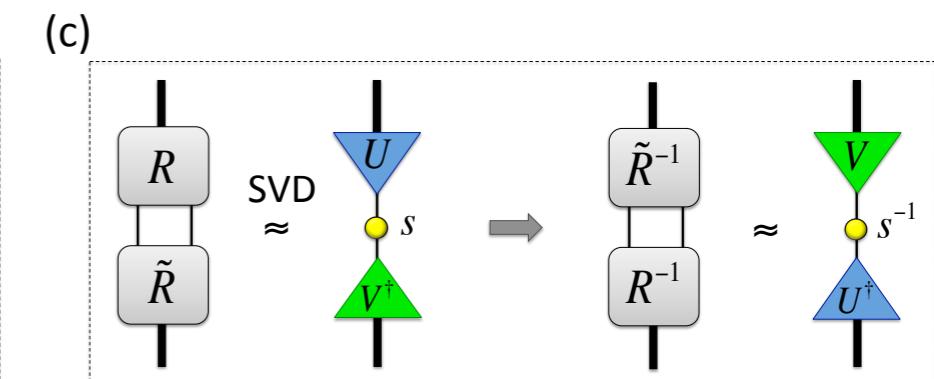
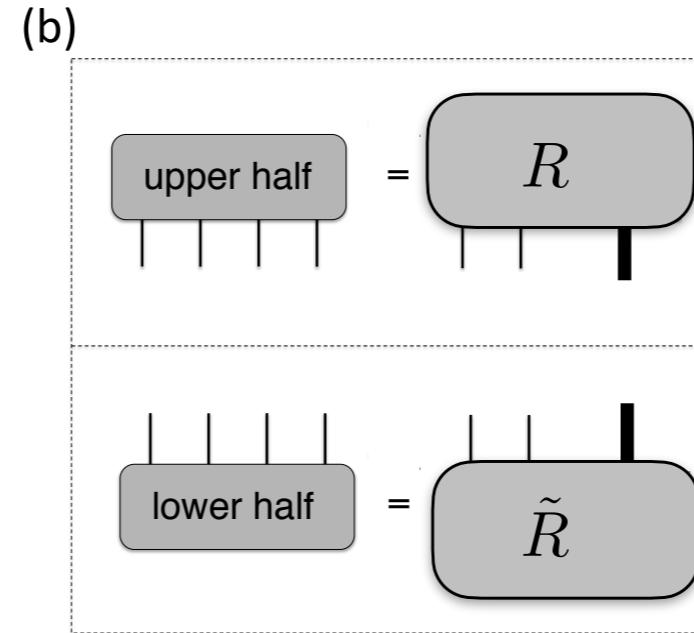
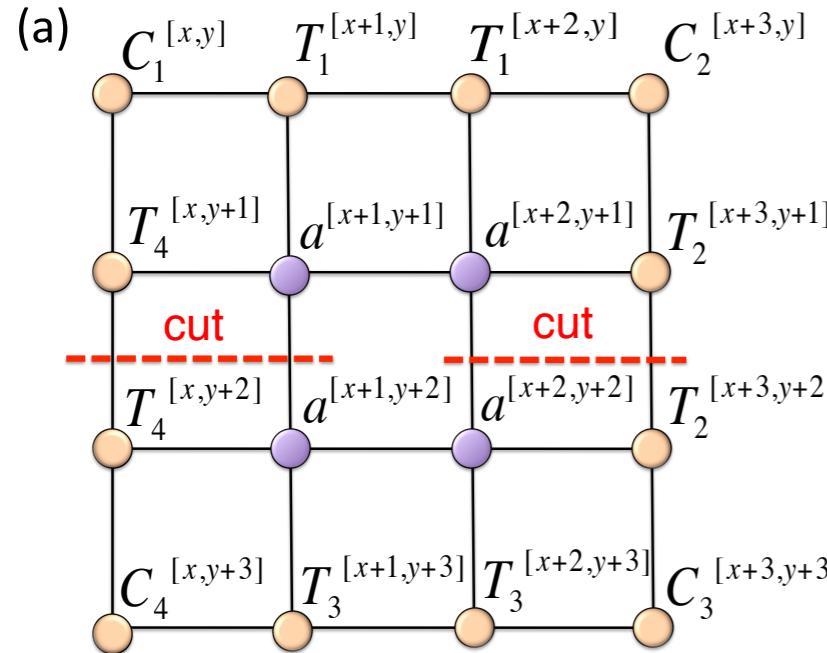
Same ways for right, top, bottom moves.



Repeat until convergence. (Typically several tens steps)

Calculation of projectors

(P. Corboz *et al*, Phys. Rev. Lett. **113**, 046402 (2014))



The heaviest part of the iPEPS + CTM
(with naive ways)

- (1) Update of the edge tensors: $O(\chi^2 D^8)$
- (2) Half-environment contraction: $O(\chi^3 D^6), O(\chi^2 D^8)$
- (3) SVD of RR matrix: $O(\chi^3 D^6)$

*Typically,

$$\chi \geq D^2 \quad \text{or} \quad \chi \simeq D^2$$



Naive implementation:
 $O(D^{12})$ calculation cost!

Useful techniques to reduce the cost

i) Use **internal tensor structure** explicitly

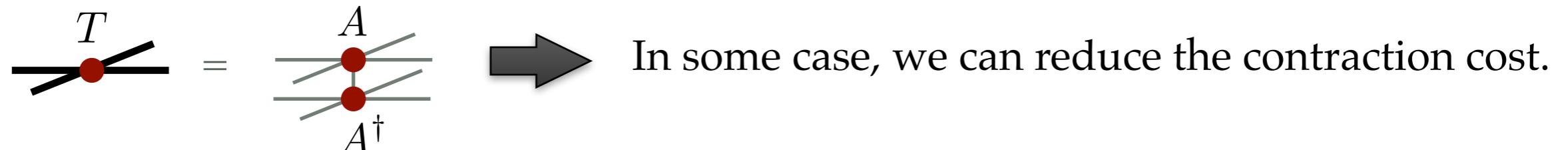
In the case of PEPS, the tensor "T" is **the product of smaller tensors**.

$$\begin{array}{c} T \\ \text{---} \\ \text{---} \end{array} = \begin{array}{c} A \\ \text{---} \\ \text{---} \\ \text{---} \\ A^\dagger \end{array} \quad \rightarrow \quad \text{In some case, we can reduce the contraction cost.}$$

Useful techniques to reduce the cost

i) Use internal tensor structure explicitly

In the case of PEPS, the tensor "T" is the product of smaller tensors.



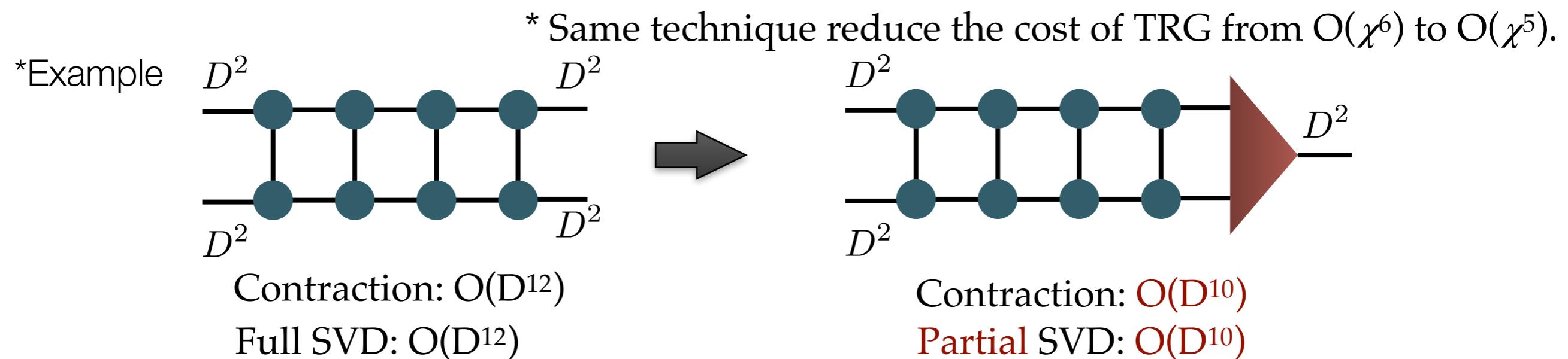
ii-1) Use partial SVD instead of full SVD

Typically, we need only higher $O(D^2)$ mode among $O(D^4)$ full SV spectrum.

Full SVD: $O(D^{12})$ Partial SVD: $O(D^{10})$

ii-2) Do not create the full matrix at SVD

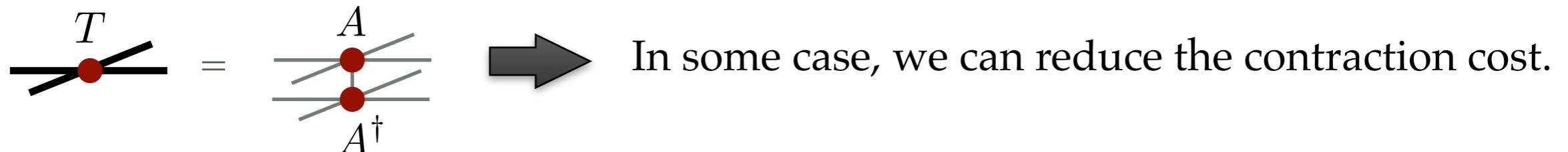
By using partial SVD algorithms consist of matrix-matrix or matrix-vector products, we do not need the half environment contraction.



Useful techniques to reduce the cost

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In the case of PEPS, the tensor "T" is the product of smaller tensors.



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$$\text{Full SVD: } O(D^{12}) \rightarrow \text{Partial SVD: } O(D^{10})$$

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By using partial SVD algorithms consist of matrix-matrix or matrix-vector products, we do not need the half environment contraction.

The heaviest part of the iPEPS + CTM

$$(1) \text{Update of the edge tensors: } O(\chi^2 D^8) \rightarrow O(\chi^2 D^6), O(\chi^3 D^4)$$

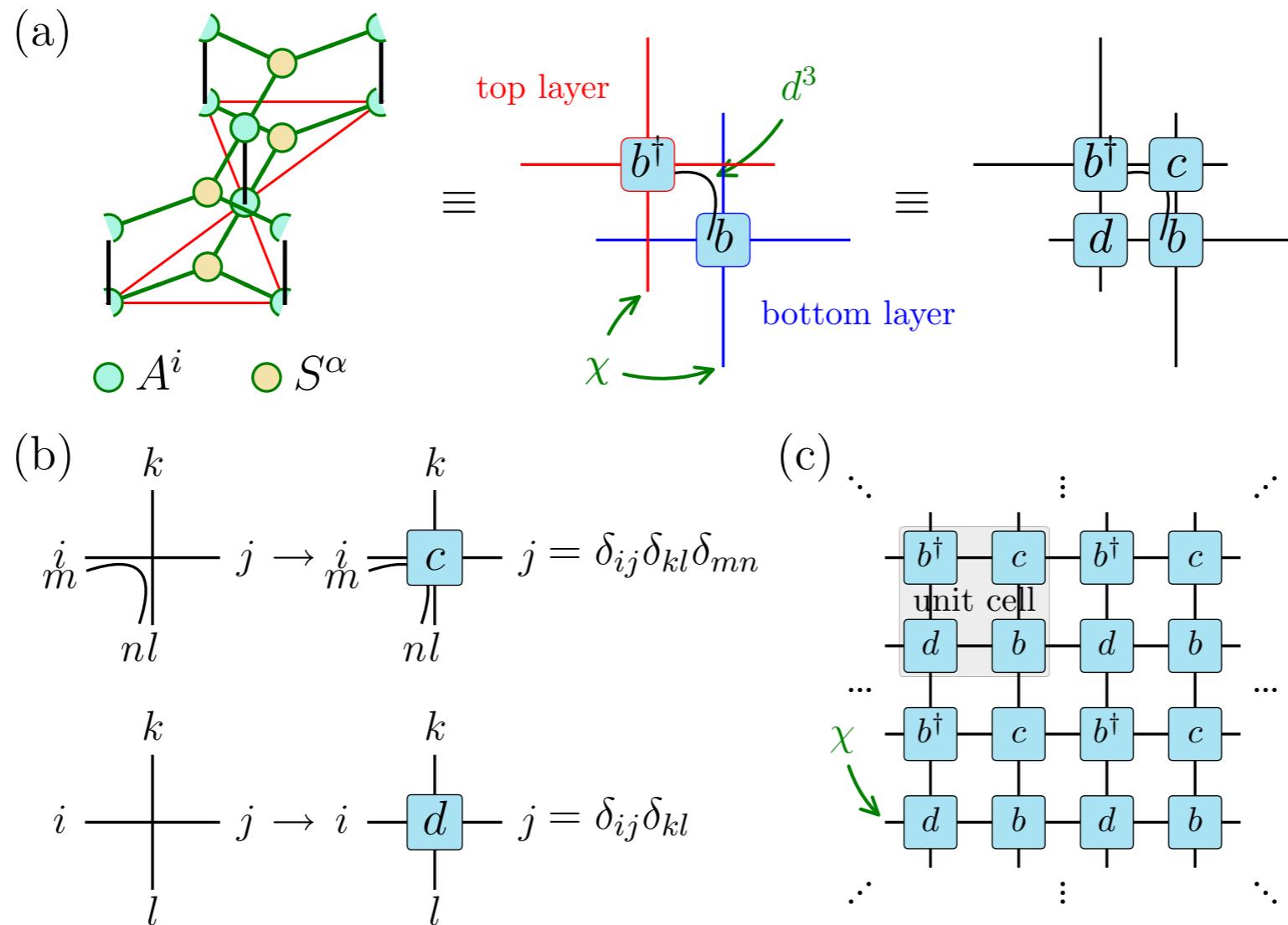
$$(2) \text{Half-environment contraction: } O(\chi^3 D^6), O(\chi^2 D^8) \rightarrow \text{not need}$$

$O(D^{10})$

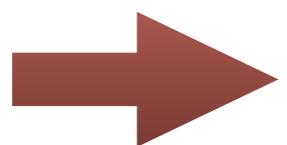
$$(3) \text{SVD of RR matrix: } O(\chi^3 D^6) \rightarrow O(\chi^2 D^6)$$

Single layer approach for CTMRG

(Chih-Yuan Lee *et al*, PRB **98**, 224414 (2018))



We can map double layer TN to a single layer.



Computation cost is reduced to $O(D^8)$.

$(\chi \sim D^2)$

Details of simple and full update for iTPS

Simple update

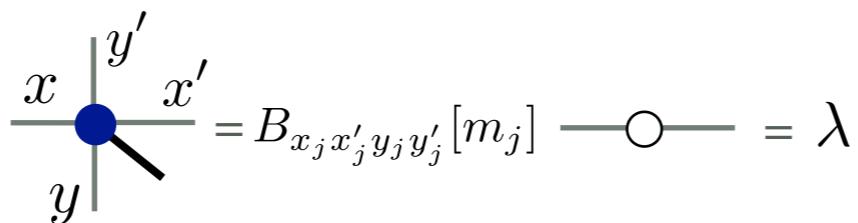
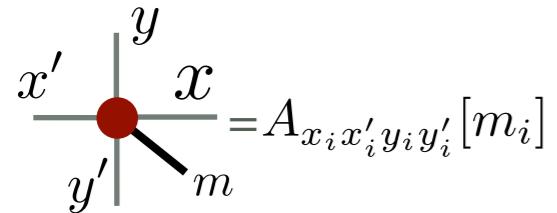
(H. G. Jiang *et al*, Phys. Rev. Lett. **101**, 090603 (2008))

Extended iTPS:

Insert (positive) diagonal matrix representing "weight" of bonds.

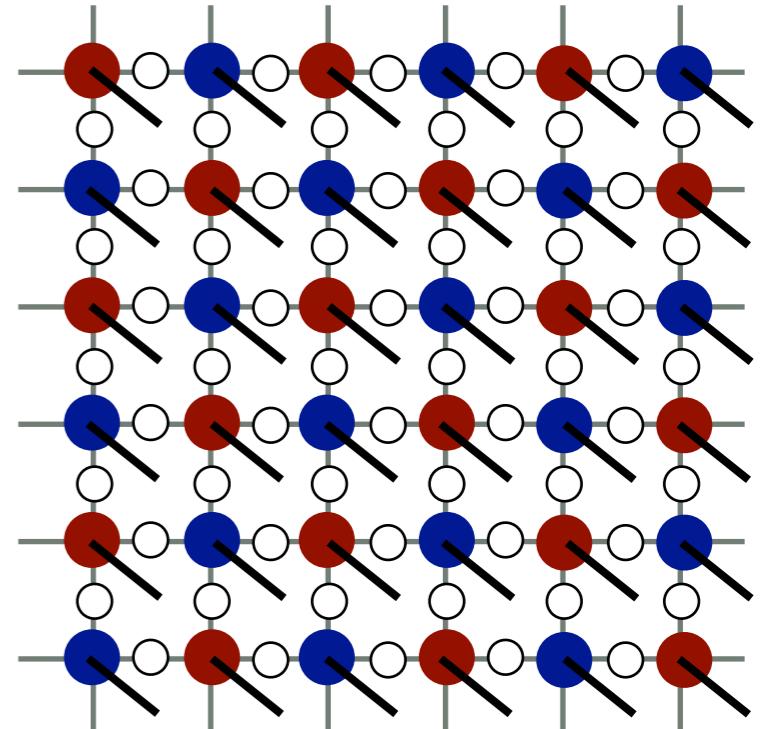
(cf. iTEBD)

$$|\Psi\rangle = \text{Tr} \prod_{i \in A, j \in B} \lambda_{x_i} \lambda_{x'_i} \lambda_{y_i} \lambda_{y'_i} A_{x_i x'_i y_i y'_i} [m_i] B_{x_j x'_j y_j y'_j} [m_j] |m_i m_j\rangle$$



$$x, y, x', y' = 1, 2, \dots D$$

Extended PEPS



Simple update with naive SVD

$$e^{-\tau H_x} |\Psi\rangle = \text{Tr} \prod_{i \in A, j \in i+x} \sum_{m_i, m_j} \langle m'_i m'_j | e^{-\tau H_{ij}} | m_i m_j \rangle \lambda_{x_i} \lambda_{x'_i} \lambda_{y_i} \lambda_{y'_i} A_{x_i x'_i y_i y'_i} [m_i] B_{x_j x'_j y_j y'_j} [m_j] | m'_i m'_j \rangle$$

Truncation by SVD

1. Define a matrix “S”

$$S_{y_i x'_i y'_i m_i, y_j x'_j y'_j m_j} = \sum_{m_i, m_j} \sum_x \langle m'_i m'_j | e^{-\tau H_{ij}} | m_i m_j \rangle \lambda_{y_i} \lambda_{x'_i} \lambda_{y'_i} A_{x_i x'_i y_i y'_i} [m_i] \lambda_x B_{x_j x'_j y_j y'_j} [m_j] \lambda_{y_j} \lambda_{x'_j} \lambda_{y'_j}$$

2. Do SVD ★

$$S_{y_i x'_i y'_i m_i, y_j x'_j y'_j m_j} = \sum_x U_{y_i x'_i y'_i m_i, x} \tilde{\lambda}_x V_{x, y_j x'_j y'_j m_j}^T$$

3. Truncate the matrix leaving upper D singular values

$$\tilde{A}_{x_i x'_i y'_i} [m_i] = \lambda_{y_i}^{-1} \lambda_{x'_i}^{-1} \lambda_{y'_i}^{-1} U_{y_i x'_i y'_i m_i, x}$$

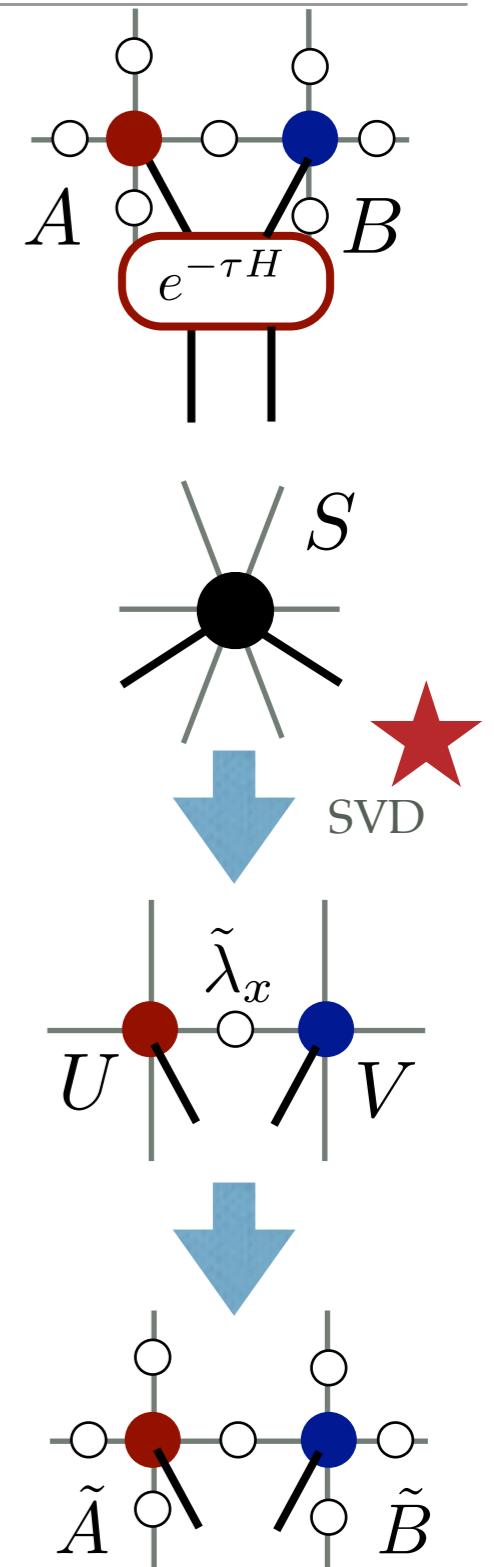
$$\tilde{B}_{x_j x'_j y'_j} [m_j] = \lambda_{y_j}^{-1} \lambda_{x'_j}^{-1} \lambda_{y'_j}^{-1} V_{x, y_j x'_j y'_j m_j, x}$$

* Meaning of λ

At SVD, λ provides information of **local environment**.

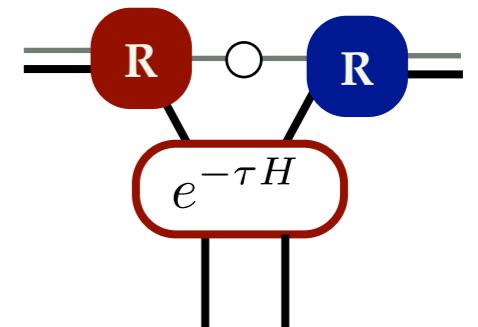
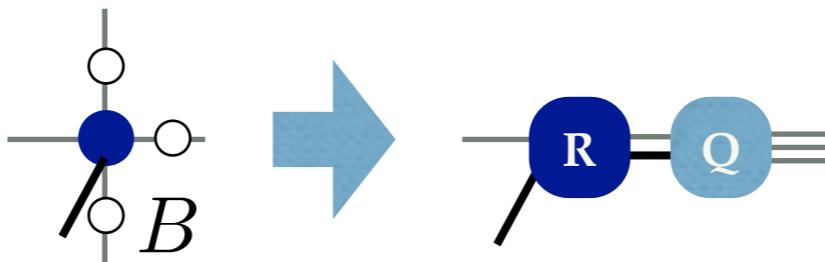
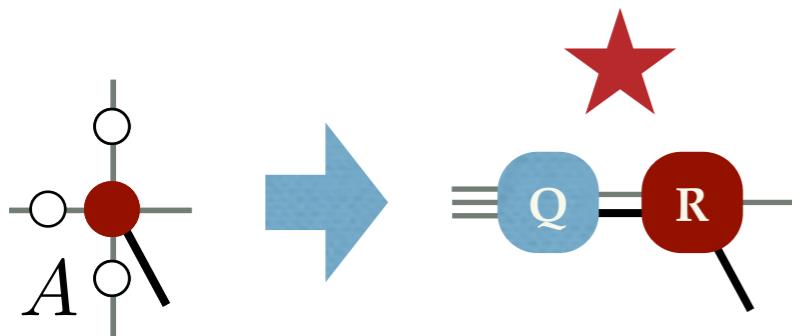


In the case of iMPS, λ give us **global information**, thanks to the canonical form.



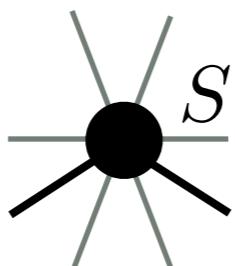
Simple update with QR decompositions

QR decomposition before SVD



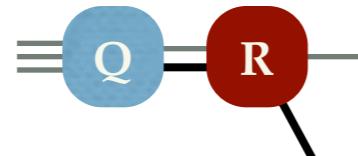
Calculation cost

Direct SVD:

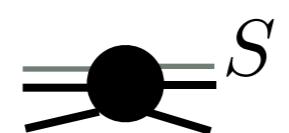


$O(D^9 m_d^3)$

QR decomposition:

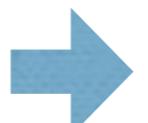


$O(D^5 m_d^2)$

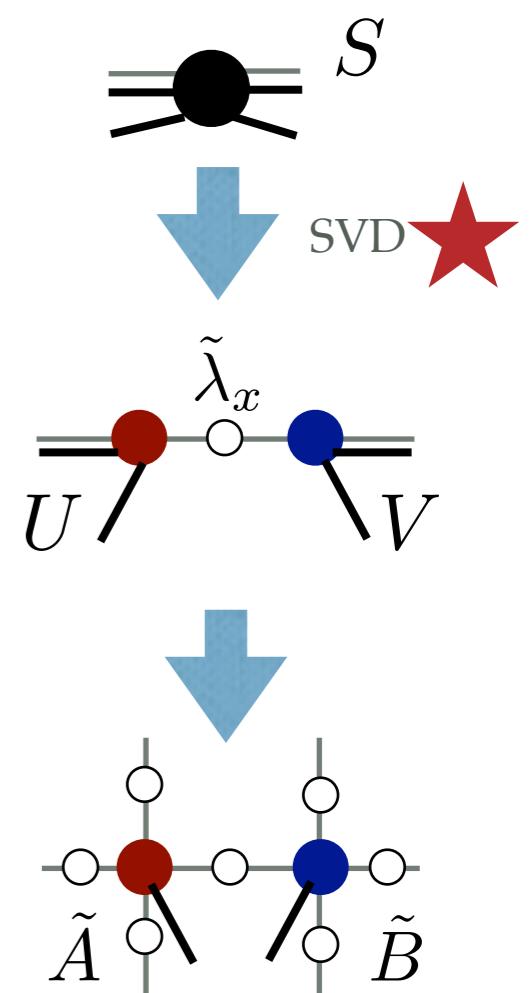


$O(D^3 m_d^6)$

Usually $D > m_d$



QR method is cheaper.



Full update

Minimize the difference between wave functions

$$||\Psi\rangle - |\tilde{\Psi}\rangle||^2 = \langle\Psi|\Psi\rangle + \langle\tilde{\Psi}|\tilde{\Psi}\rangle - 2\text{Re}\langle\Psi|\tilde{\Psi}\rangle = f$$

$|\Psi\rangle$: wave function just operated an ITE operator

$|\tilde{\Psi}\rangle$: wave function after **truncation**

Necessary conditions for minimization

$$\frac{\partial f}{\partial \tilde{A}^*} = 0, \frac{\partial f}{\partial \tilde{B}^*} = 0$$

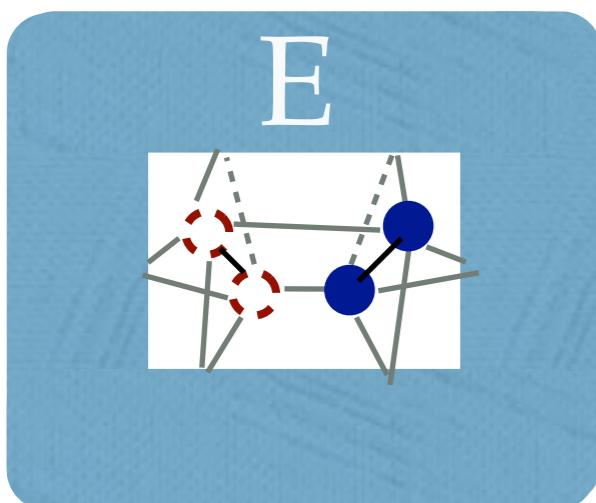
Iterative calculation by solving linear equation

$$\frac{\partial f}{\partial \tilde{A}^*} = 0 \rightarrow N_A(\tilde{B})\tilde{A} = W_A$$

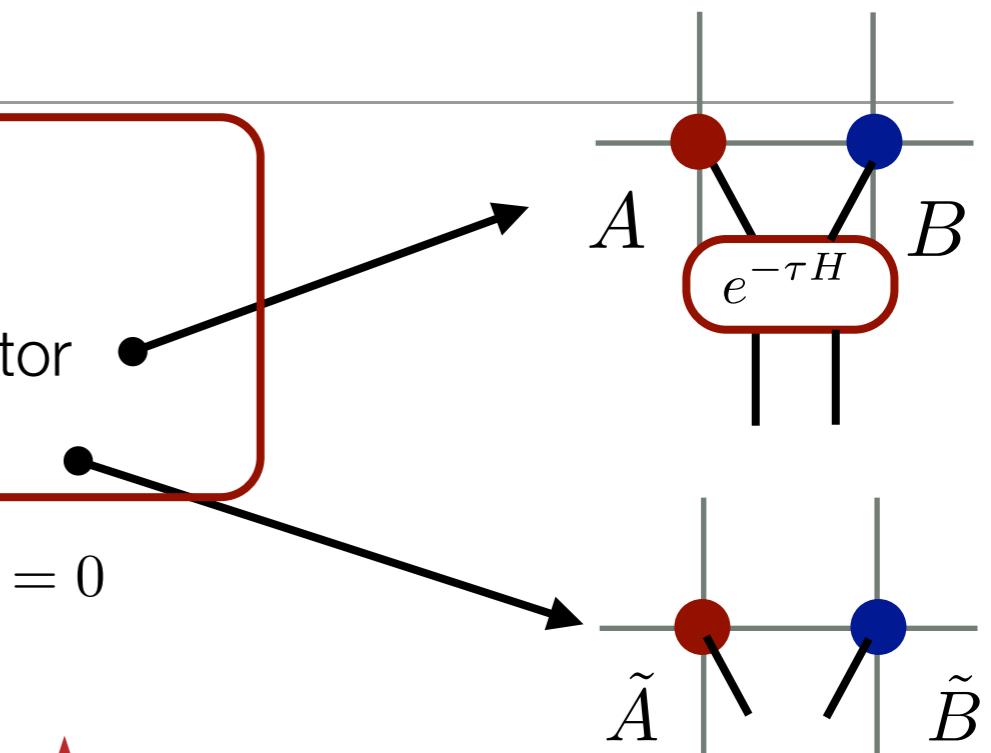
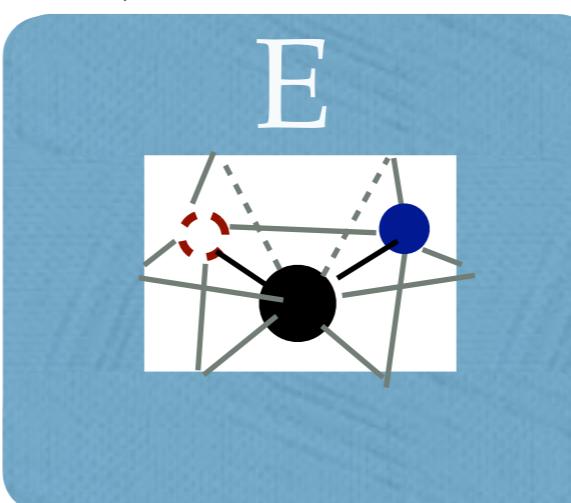
$$\frac{\partial f}{\partial \tilde{B}^*} = 0 \rightarrow N_B(\tilde{A})\tilde{B} = W_B$$

*Environment is **fixed** during the iteration

N_A, N_B : "Matrices"



W_A, W_B : "Vectors"



★ $O(D^{12}m_d^3)$

*Environment: $O(D^8) \sim O(D^{10})$

*Alternatively, we can also use the CG.

* QR decomposition method:

Dimensions of vectors and matrices are reduced into $D^2m_d^2$



★ **linear equation**
 $O(D^6m_d^6)$