Tensor network approach to two-dimensional frustrated spin systems

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Frustration in spin systems

Frustration：Competition among several optimization conditions

Optimization：minimization of the total energy

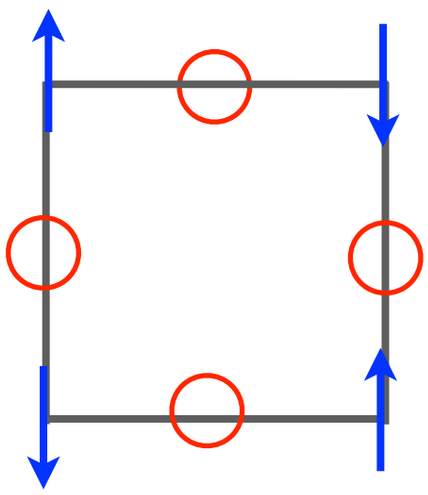
$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \qquad J > 0$$

Antiferromagnetic

local energy minimization ： anti-parallel spin pair

Ising spins

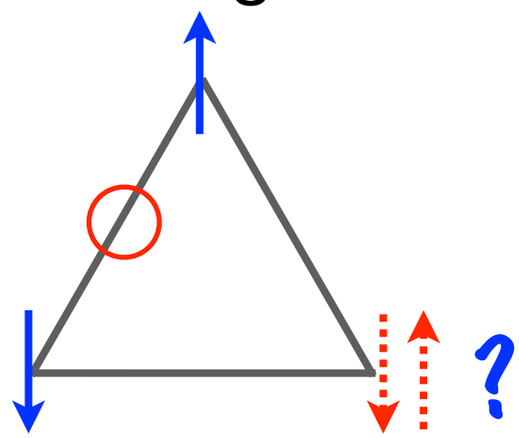
Square



All pairs can be anti-parallel

No frustration

Triangle



One of three pairs is necessarily parallel

Frustration!

Frustration in spin systems

Frustration：Competition among several optimization conditions

Optimization：minimization of the total energy

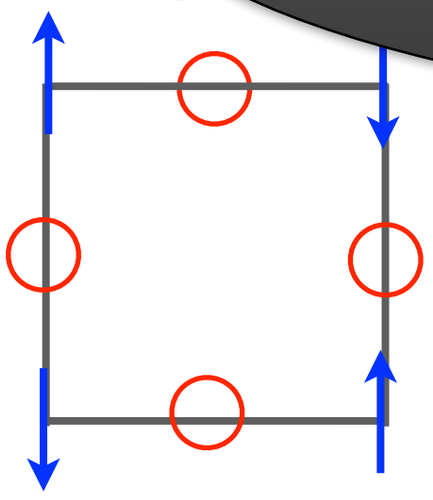
$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \qquad J > 0$$

Antiferromagnetic

local

Ising spins

Sq

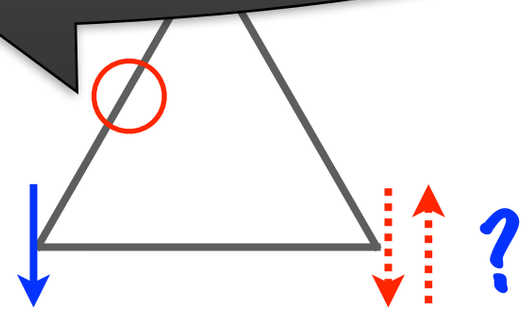


All pairs can be anti-parallel

No frustration

Huge degeneracy in the ground state.

Large fluctuations!



One of three pairs is necessarily parallel

Frustration!

Targets of the study in frustrated spin systems

Frustrated spin system

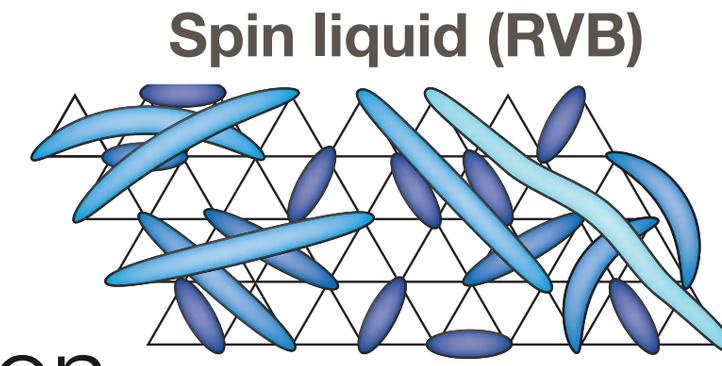
$$\mathcal{H} = \sum_{i,j} J_{ij} S_i S_j$$

S_i : Spin operator, typically S=1/2

*Spins located on a lattice:
square, triangular, cubic, …

- We want to find novel states of the matter
  - Quantum spin liquids
  - Topological phases
  - Valence Bond Solids
  - …
- We want to investigate phase transition
  - (Quantum) critical phenomena
  - Topological phase transition
  - …

(L. Balents, Nature (2010))



Targets of the study in frustrated spin systems

A lot of interesting things occur
in the Avogadro scale ~ 10^{23}
→We need large scale calculations!

- We want to find novel states of the matter
  - Quantum spin liquids
  - Topological phases
  - Valence Bond Solids
  - …
- We want to investigate phase transition
  - (Quantum) critical phenomena
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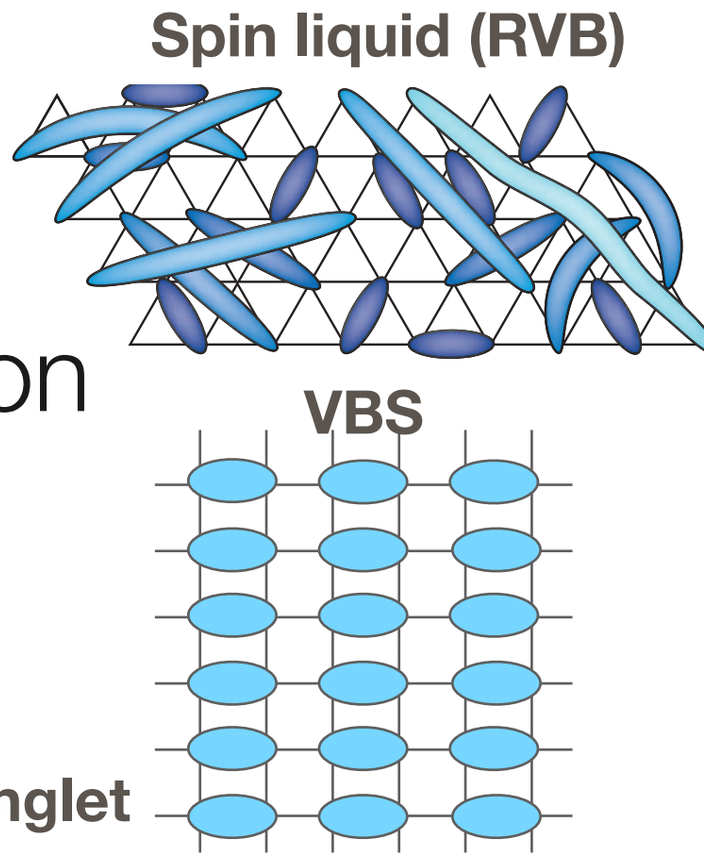
(L. Balents, Nature (2010))



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)

Information compression by tensor networks

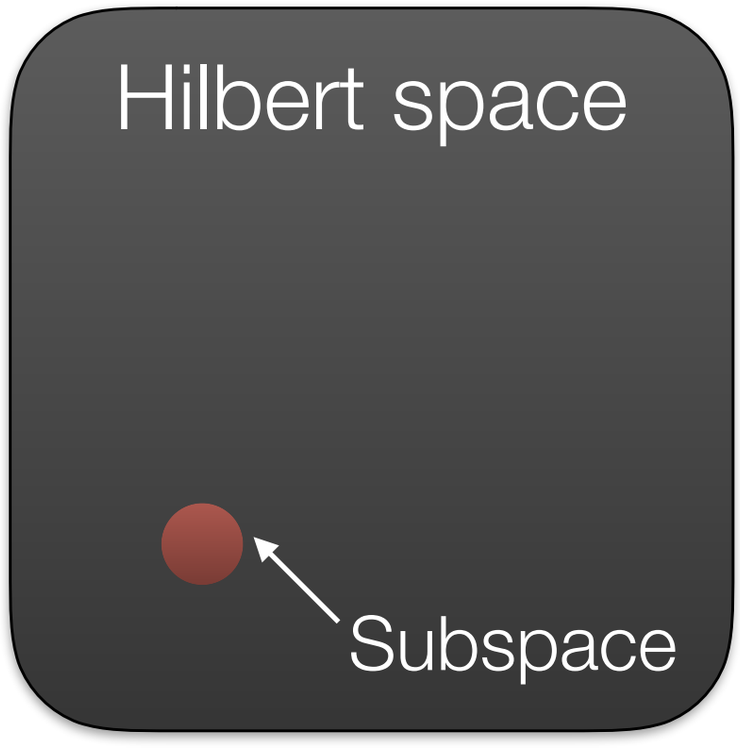
We can not treat entire data in the present computers.

→ Try to reduce the "effective" dimension of (Hilbert) space

By considering proper subspace of the Hilbert space, we can represent a quantum state efficiently.

↓

Tensor network quantum states!



When we efficiently compress a vector?

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

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

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

+

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

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

eg. array of quantum bits

Tensor network decomposition

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

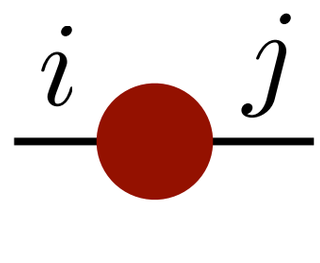
$i_n = 0, 1, \ldots, a-1$: index of local Hilbert space

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

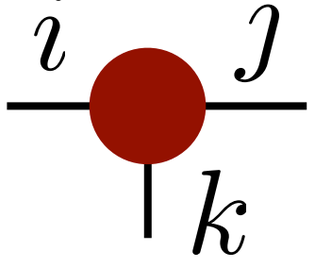
Graphical representations for tensor network

- Vector $\vec{v} : v_i$

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

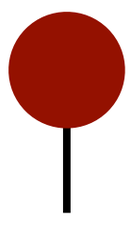


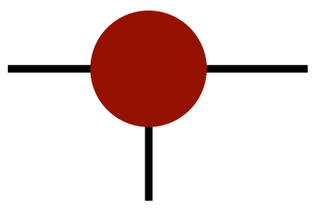
- Tensor $T : T_{i,j,k}$



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

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

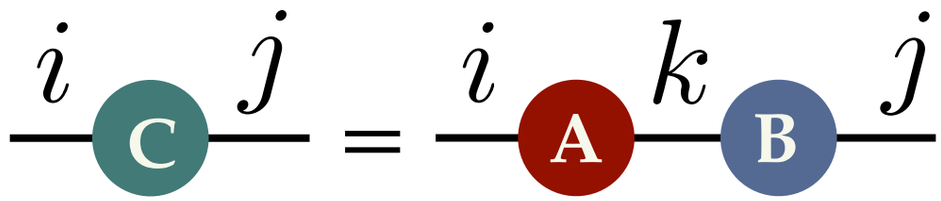
$\vec{v} =$ 

$T =$ 

Graphical representations for tensor network

Matrix product

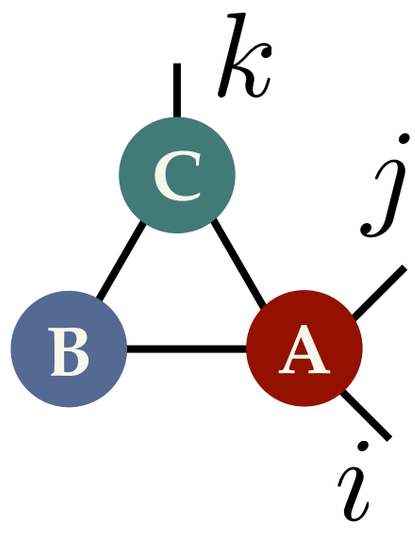
$$C_{i,j} = (AB)_{i,j} = \sum_k A_{i,k} B_{k,j}$$



$$C = AB$$

Generalization to tensors

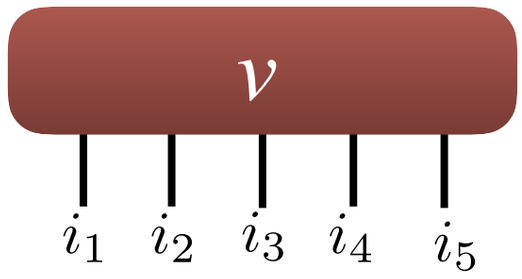
$$\sum_{\alpha,\beta,\gamma} A_{i,j,\alpha,\beta} B_{\beta,\gamma} C_{\gamma,k,\alpha}$$



Contraction of a network = Calculation of a lot of multiplications

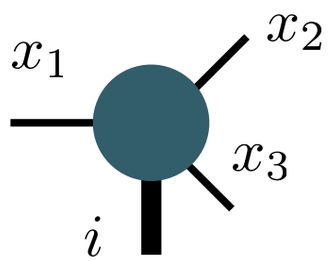
Graph for a tensor network decomposition

- Vector v_{i_1,i_2,i_3,i_4,i_5}



*Vector looks like a tensor

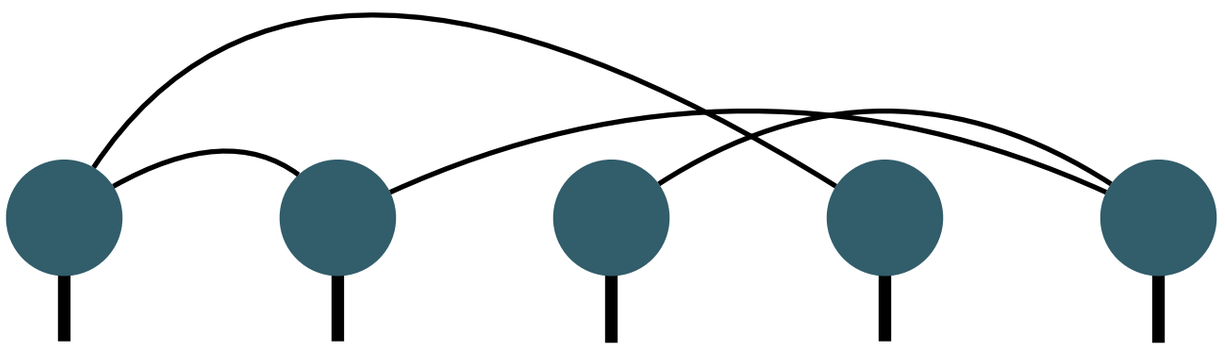
- Tensor $T[i]_{x_1,x_2,x_3}$



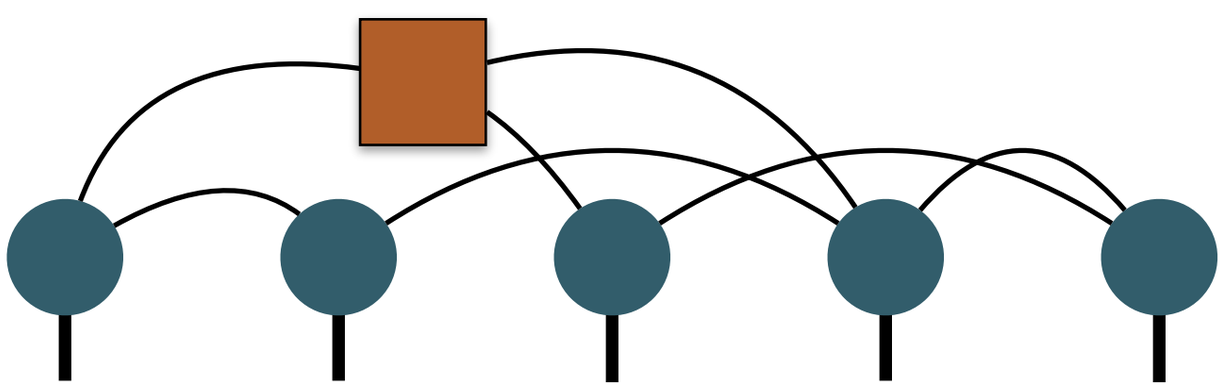
*We treat i as an index of the tensor.

Tensor network decomposition

$\vec{v} =$



$\vec{w} =$



*We can consider tensors independent of i.

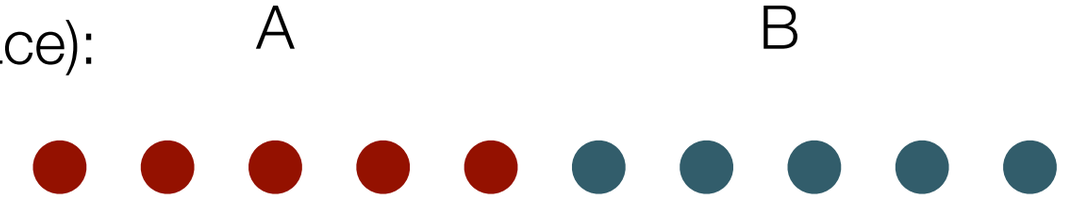
Area law of entanglement and tensor network state

Entanglement entropy

Entanglement entropy:

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

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



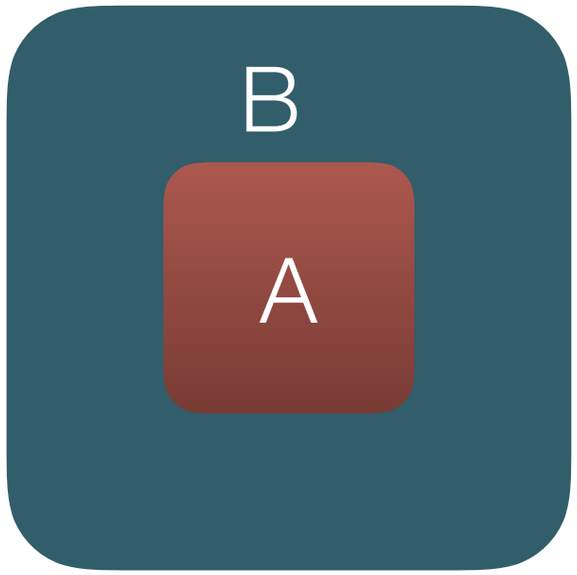
Entanglement entropy = von Neumann entropy of ρ_A

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right)$$

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

$$\rho_A = \sum_i \lambda_i^2 |\alpha_i\rangle\langle\alpha_i|$$

$$S = -\sum_i \lambda_i^2 \log \lambda_i^2$$



Entanglement entropy is calculated through
the spectrum of Schmidt coefficients

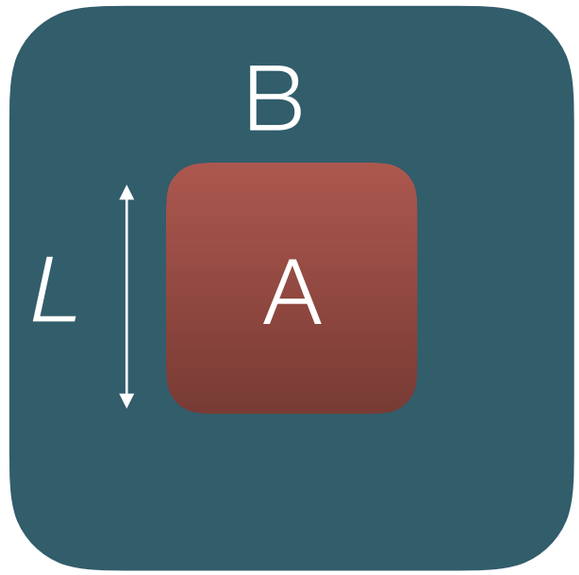
Area law of the entanglement entropy in physics

General wave functions:

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

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right) \propto L^d$$

(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)

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

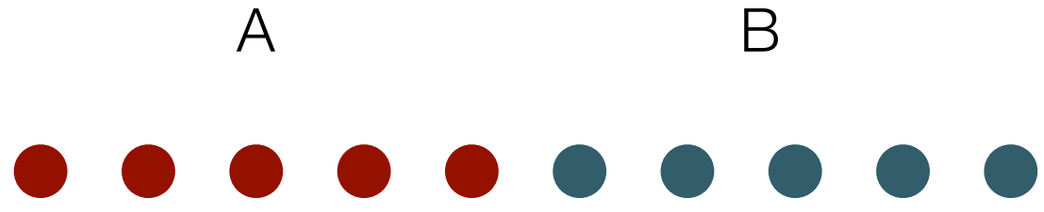
In the case of one-dimensional system:

Gapped ground state for local Hamiltonian

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

$$S = O(1)$$

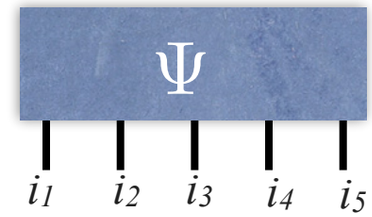
Ground state are in a small part of the huge Hilbert space



Tensor network state

G.S. wave function: $|\Psi\rangle = \sum_{\{i_1, i_2, \ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$

Vector (or N-rank tensor): $\Psi_{i_1 i_2 \ldots i_N}$ =

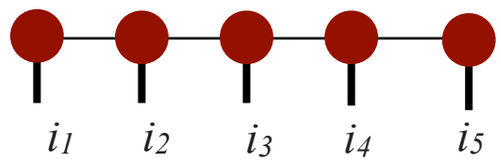


# of Elements = a^N

``Tensor network" decomposition

* Matrix Product State (MPS)

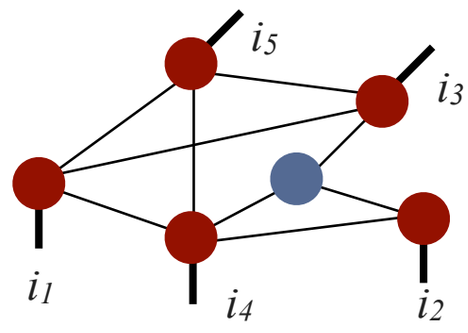
$A_1[i_1] A_2[i_2] \cdots A_N[i_N]$ =



$A[m]$: Matrix for state m

* General network

$\mathrm{Tr} X_1[i_1] X_2[i_2] X_3[i_3] X_4[i_4] X_5[i_5] Y$



X,Y : Tensors

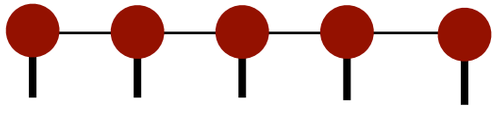
Tr : Tensor network contraction

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

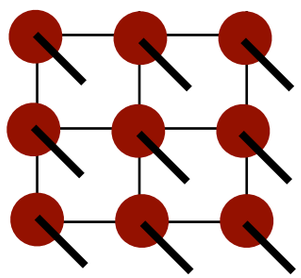
ex. MPS: # of elements $= 2ND^2$ D: dimension of the matrix A

Exponential → Linear *If D does not depend on N…

Examples of TNS

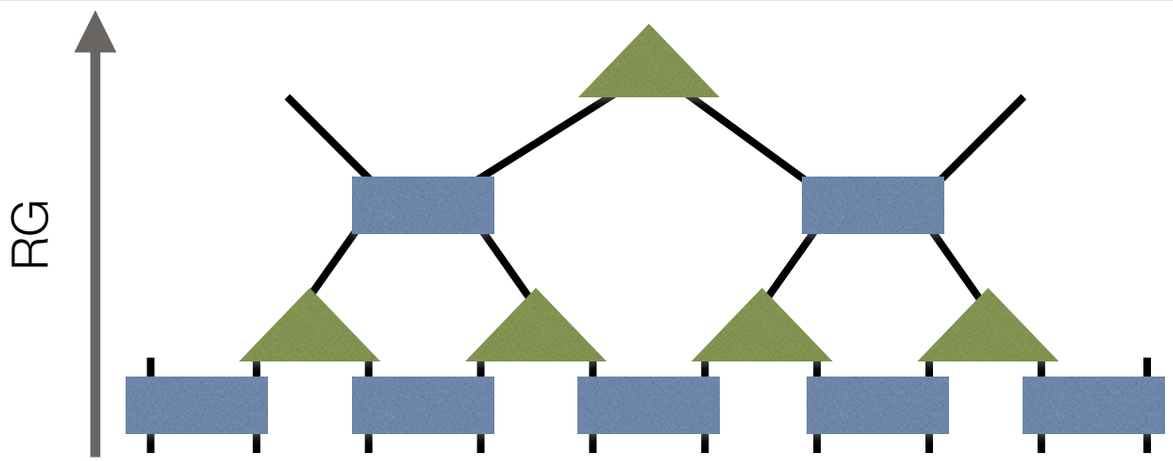
MPS: 

Good for 1-d gapped systems

PEPS, TPS: 

For higher dimensional systems

Extension of MPS

MERA: 

Scale invariant systems

Matrix product state (MPS)

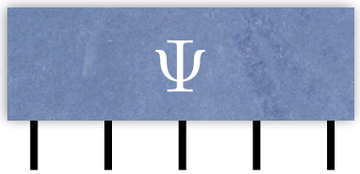
Good reviews:

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

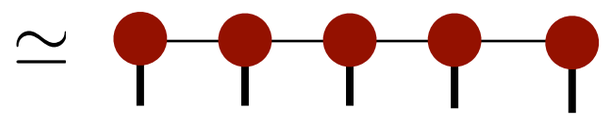
$$|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

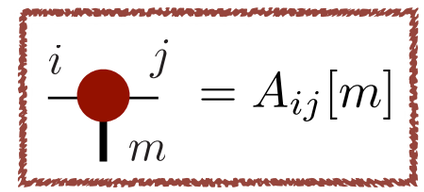
$$\Psi_{i_1 i_2 \ldots i_N} \simeq A_1[i_1] A_2[i_2] \cdots A_N[i_N]$$

$A[i]$: Matrix for state i



MPS





Note:

- MPS is called as "tensor train decomposition" in applied mathematics

(I. V. Oseledets, SIAM J. Sci. Comput. **33**, 2295 (2011))

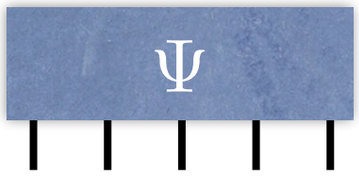
- A product state is represented by MPS with 1×1 "Matrix" (scalar)

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

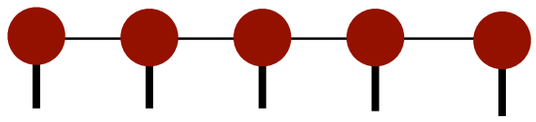
$$\Psi_{i_1 i_2 \ldots i_N} = \phi_1[i_1] \phi_2[i_2] \cdots \phi_N[i_N]$$

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

Upper bound of Entanglement entropy

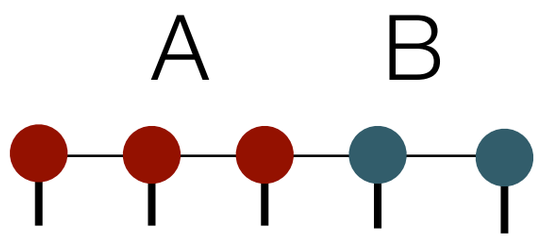


$\simeq$

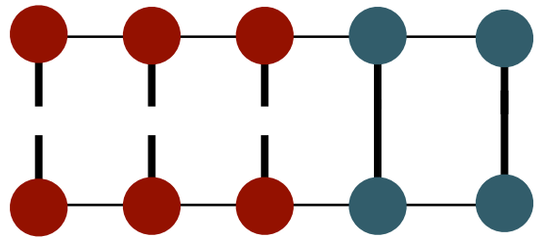


$\equiv |\tilde{\Psi}\rangle$:MPS with χ

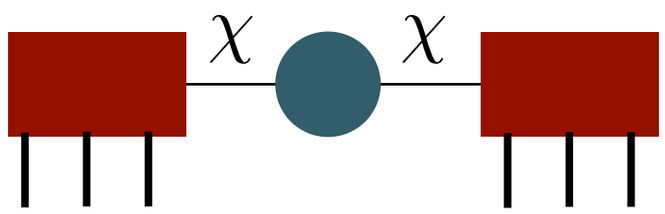
Reduced density matrix of region A:



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



★ Structure of ρ_A:

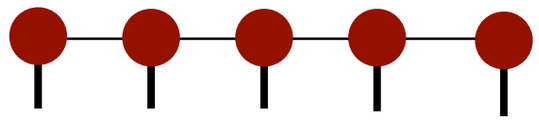


$$\mathrm{rank}\ \rho_A \leq \chi$$

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

Required bond dimension in MPS representation

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



The upper bound is independent of the "length".

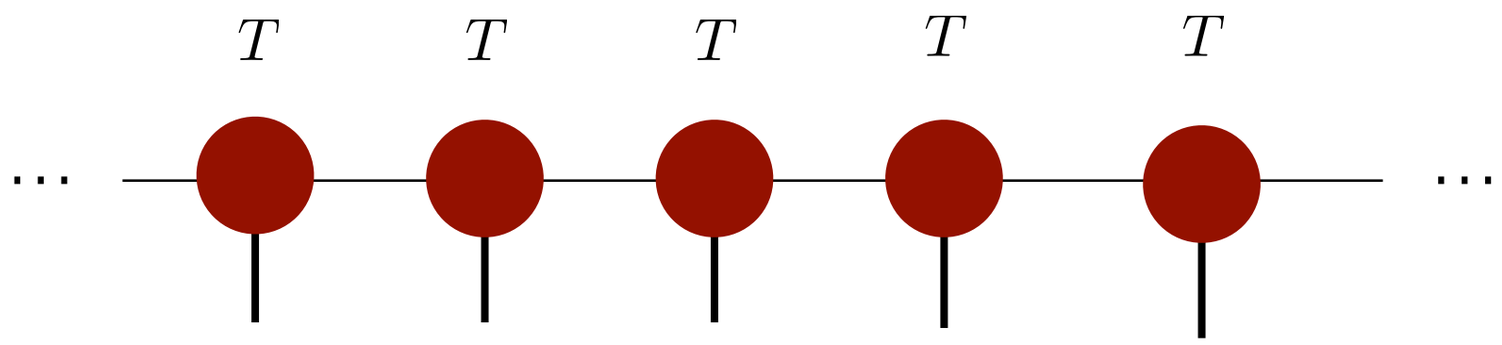
length of MPS ⇔ size of the problem

N $\qquad\qquad$ a^N

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

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 low, we efficiently approximate infinite system with a finite size matrix (tensor) T.

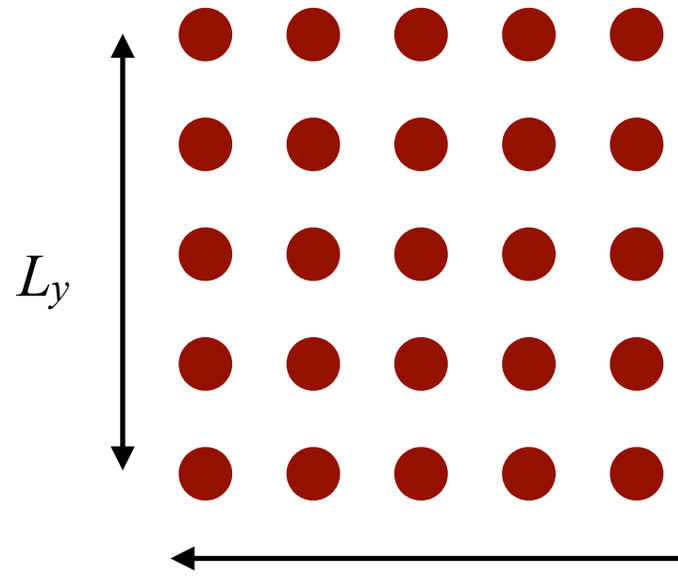
Higer dimensional system

Transverse field Ising model on square lattice:

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

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

Two-dimensional array



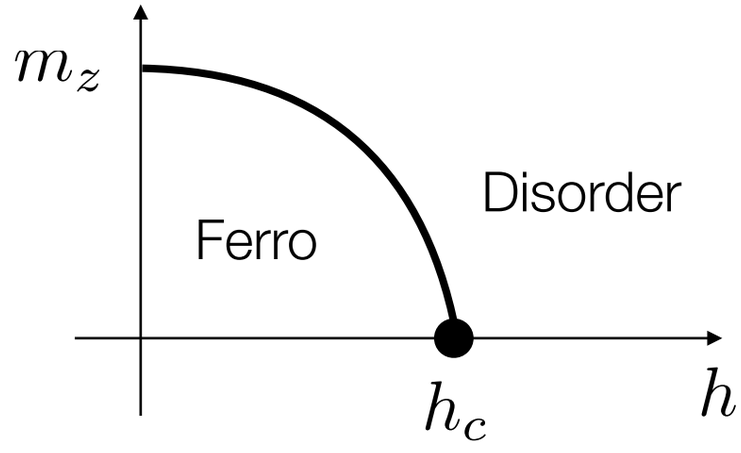
$$N = L_x \times L_y$$

Area law

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

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

Phase diagram



MPS for two-dimensional system

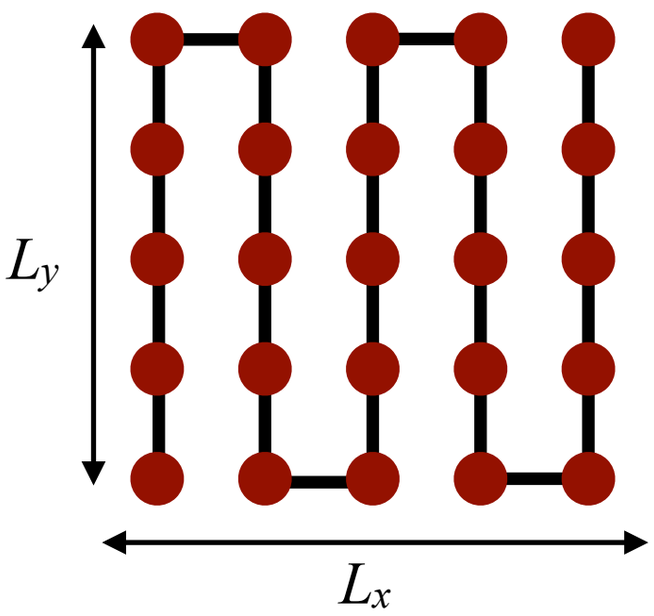
When we apply MPS representation for a square lattice system:

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!

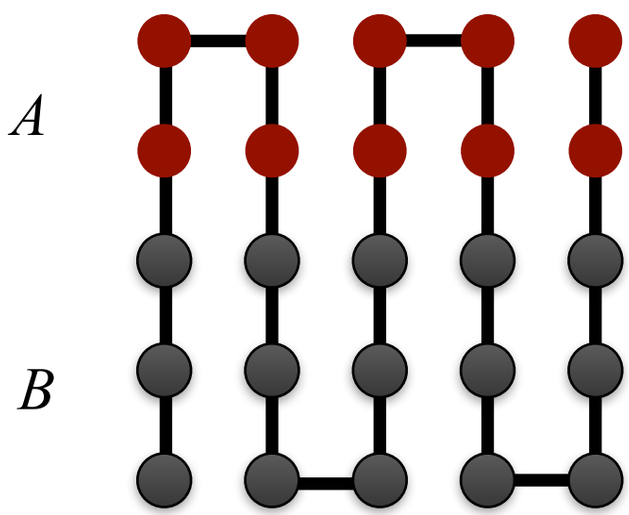
MPS cannot cover the area law of the entanglement entropy in higher (d =2,3, ...) dimensions.

Possible MPS (Snake form)

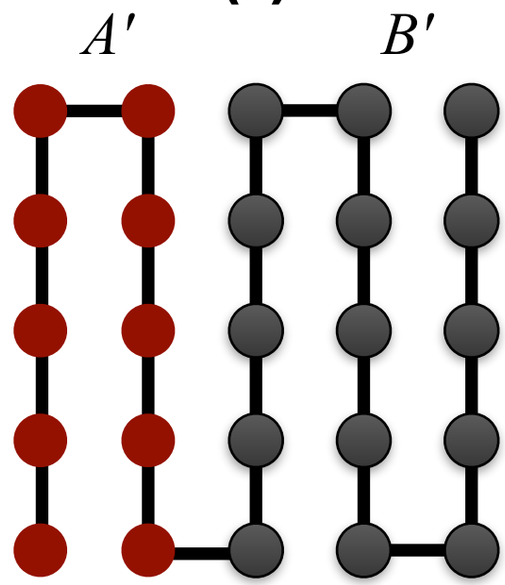


Two settings of system and environment

(1)



(2)



MPS for two-dimensional system: comment

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

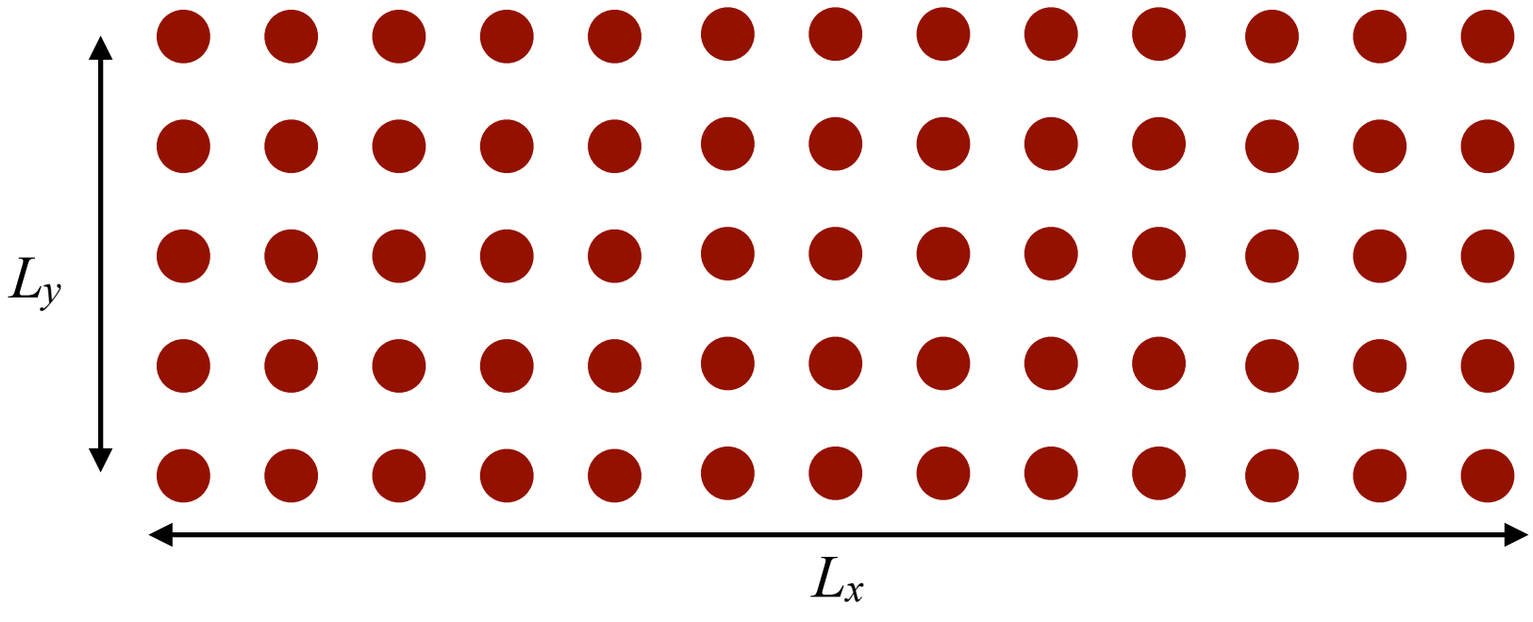
In setting (1), MPS can satisfy the area low partially.

➡ We can increase L_x easily with keeping L_y constant.

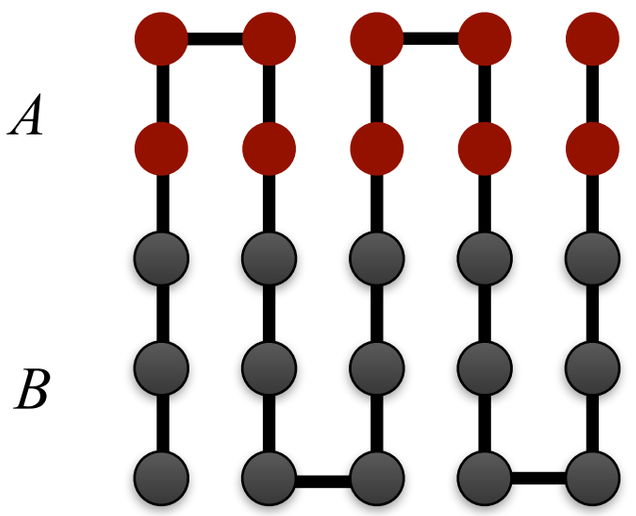
$$\chi = O(e^{L_y})$$

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

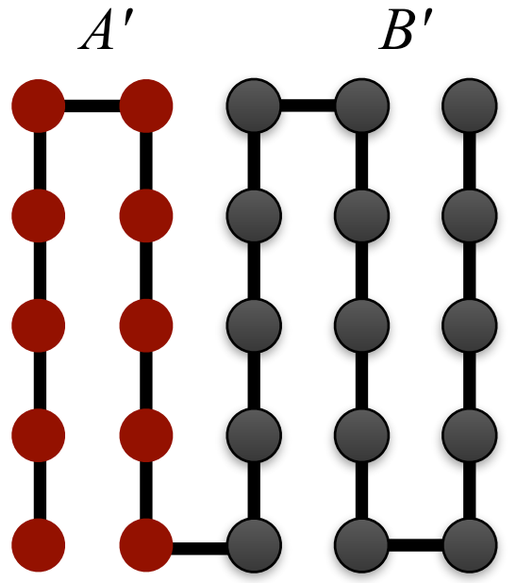
Quasi one dimensional system ("strip" or "cylinder")



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



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



Tensor product states

Entanglement entropy in higher dimensions

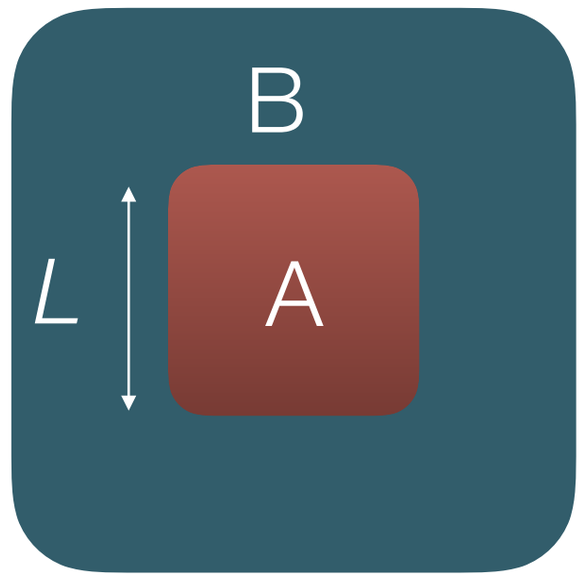
Ground state wave functions:

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 low:

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



In d=1, MPS satisfies the area low.

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

A. It is Tensor Product State (TPS)!

Tensor Product State (TPS)

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

PEPS (Projected Entangled-Pair State)

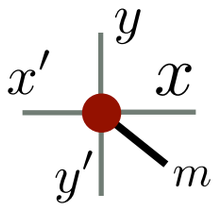
(F. Verstraete and J. Cirac, arXiv:cond-mat/0407066)

d-dimensional tensor network representation
for the wave function of a d-dimensional quantum system

$$|\Psi\rangle = \sum_{\{m_i=1,2,\cdots,m\}} \mathrm{Tr}\ A_1[m_1]A_2[m_2]\cdots A_N[m_N]|m_1 m_2 \cdots m_N\rangle$$

Tr: tensor network "contraction"

$A_{x_i x_i' y_i y_i'}[m_i]$: Rank 4+1 tensor

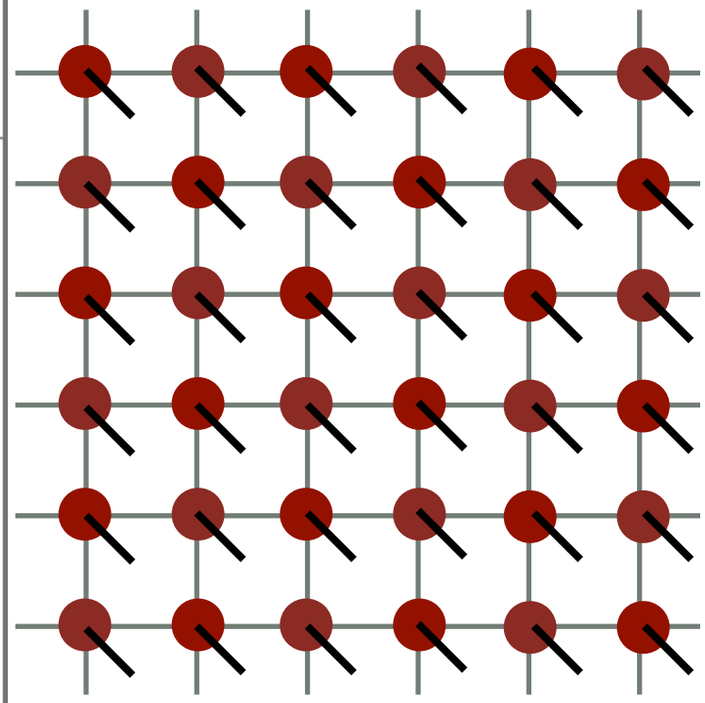


$x,y,x',y' = 1,2, \ldots D$ $\quad D =$ "bond dimension"

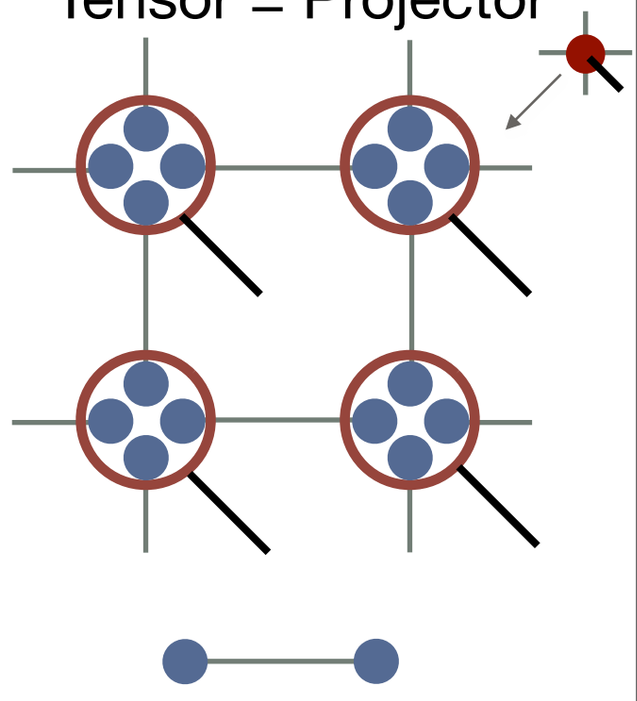
$m_i = 1,2, \ldots m$ $\quad m =$ dimension of the local Hilbert space

*D can be larger than m. "Virtual state "

TPS on square lattice

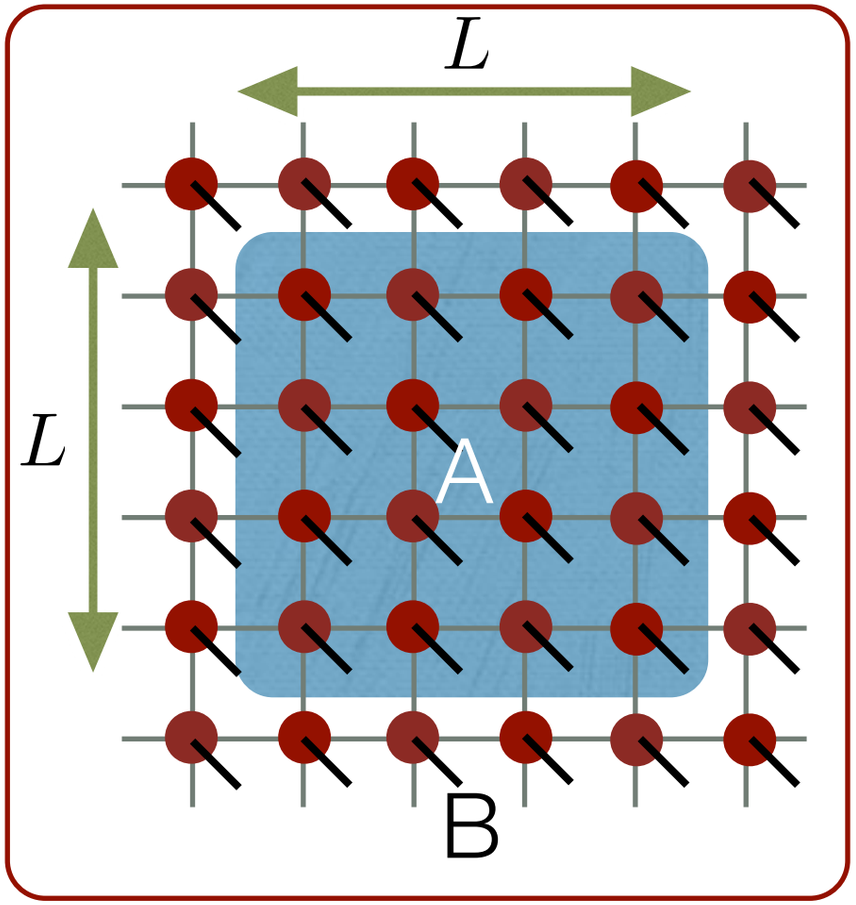


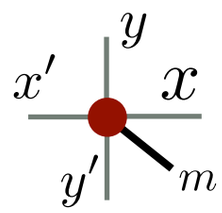
Tensor = Projector



Maximally entangled state
between D-state spins

Entanglement entropy of TPS (PEPS)





Bond dimension = D

# of bonds connecting regions A and B

$N_c(L) = 4L$ (square lattice)

$N_c(L) = 2dL^{d-1}$ (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!

Difference between MPS and TPS

Cost of tensor network contraction:

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

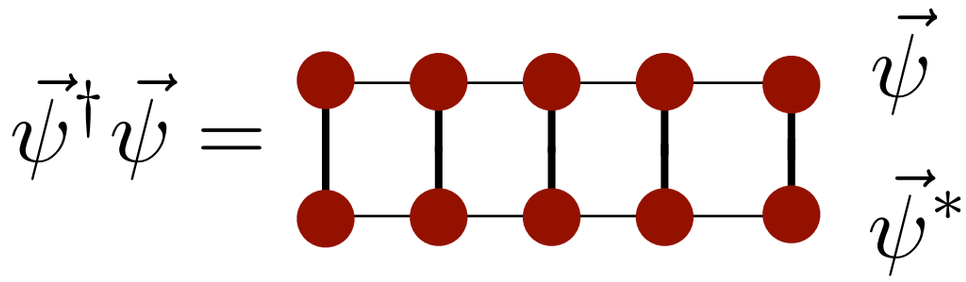
MPS: $O(N)$

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

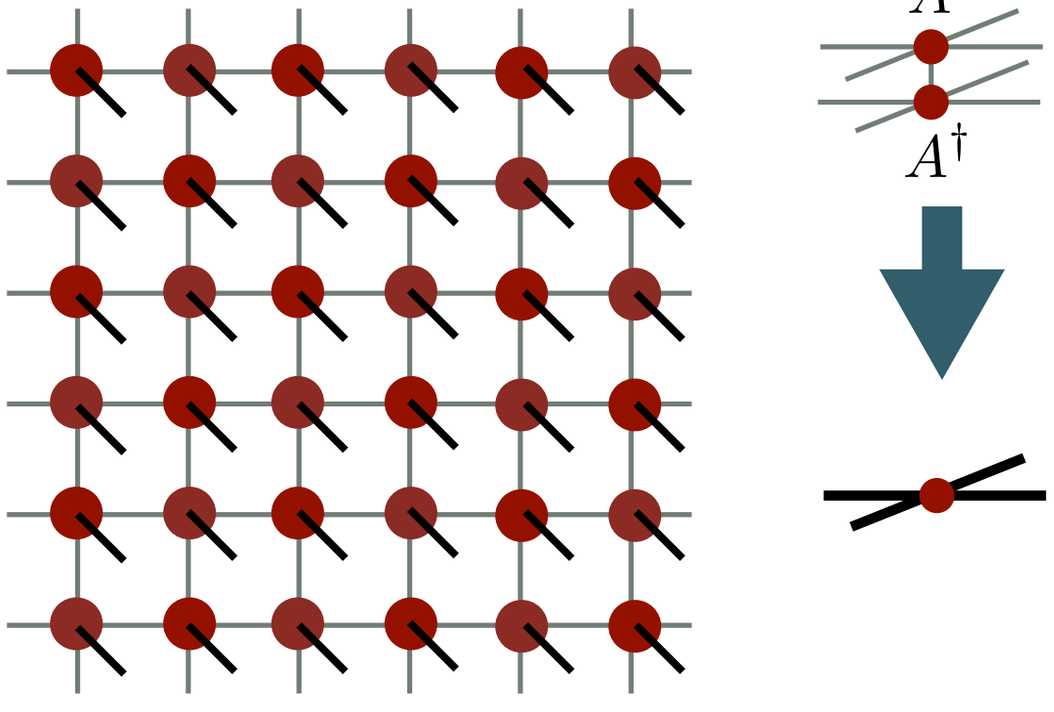
It is impossible to perform exact contraction even if we know local tensors in the case of TPS.

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

MPS



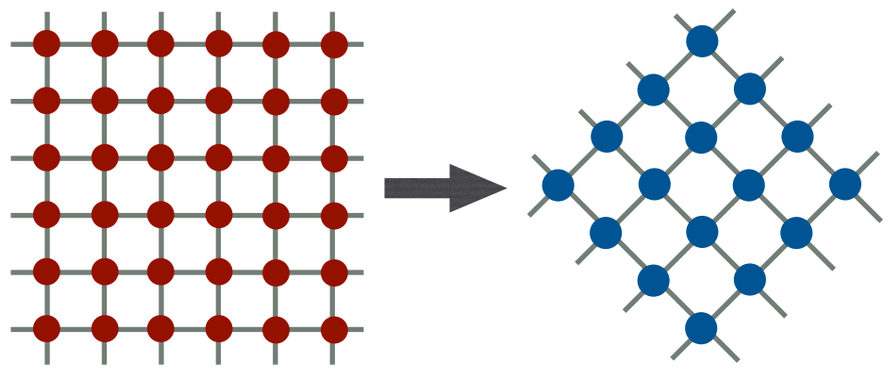
TPS (PEPS)



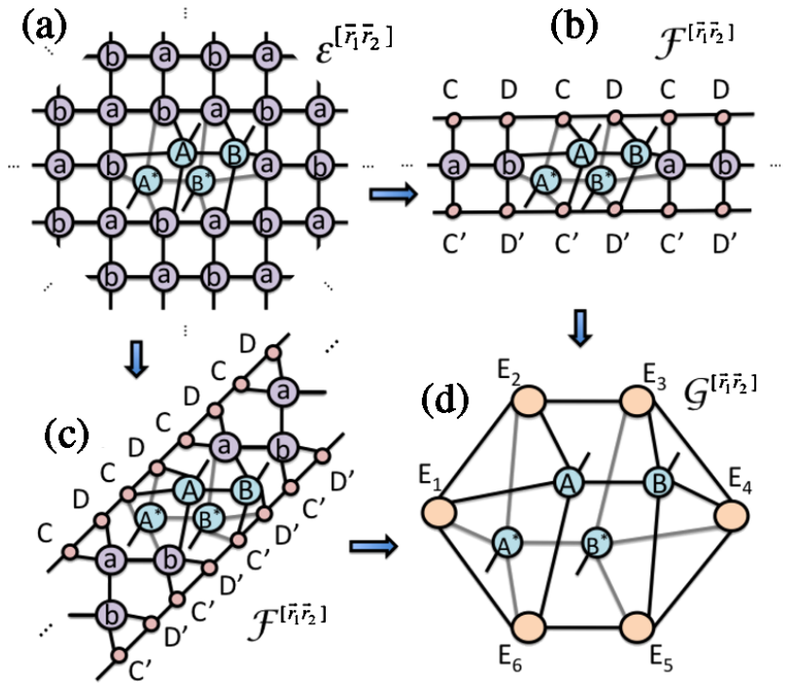
Contraction of iTPS

Methods for approximate contraction of iTPS:

- Tensor network renormalizations
  - TRG, HOTRG, SRG, TNR, loop-TNR, ...
    (cf. lecture of T. Xiang)
- 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. Orus *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) .



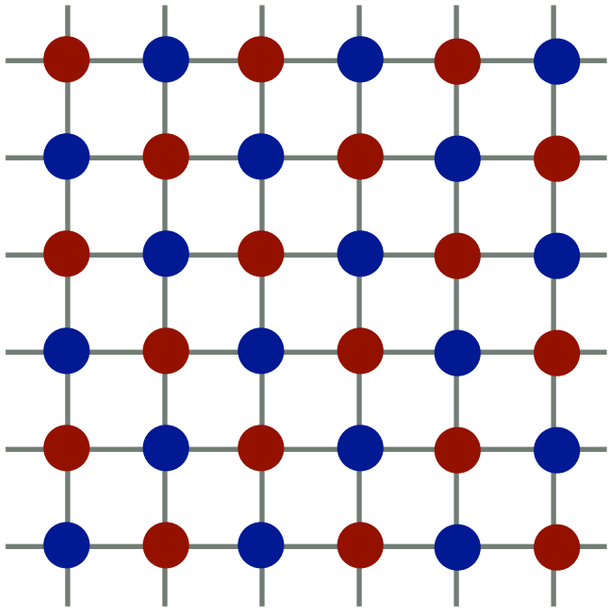
Corner transfer matrix method

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

Mapping to a "classical" system

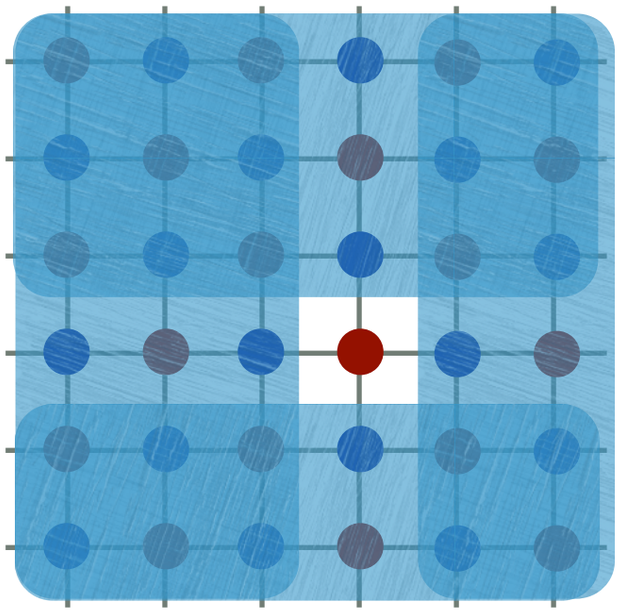
Corner transfer matrix method

For (infinite) open boundary system

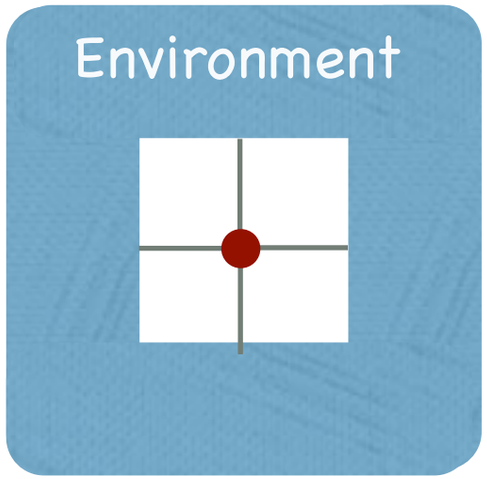
(T. Nishino and K. Okunishi, JPSJ **65**, 891 (1996))
(R. Orus *et al*, Phys. Rev. B **80**, 094403 (2009))

Infinite PEPS

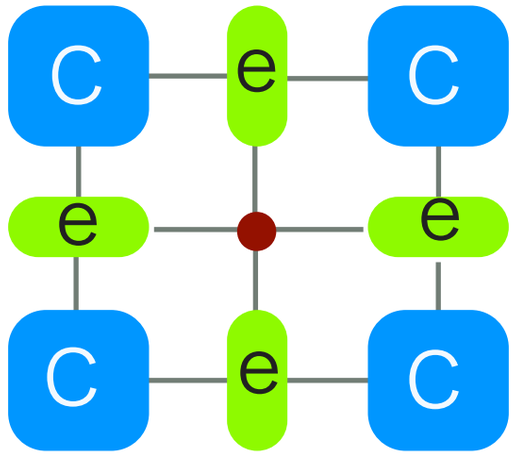
(with a translational invariance)



Environment

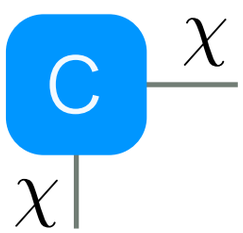


Corner transfer matrix Representation

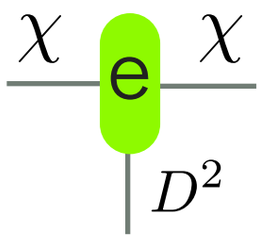


Double tensor

Corner transfer matrix



Edge tensor



Mapping to a "classical" system

χ =bond dimension $\chi \sim D^2$

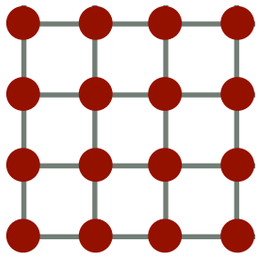
Original simple CTM renormalization group

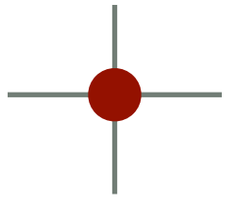
- Successive "renormalization" method for contracting classicl tensor network proposed by Nishino and Okunishi.
(J. Phys. Soc. Jpn. **65**, 81 (1996); **66**, 3040 (1997).)
  - Corner Transfer Matrix Renormalization Group（CTMRG）
- Contract classical tensor network by changing the system size as L→L+2, sequentially
- Recently, it is also use 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×L network.

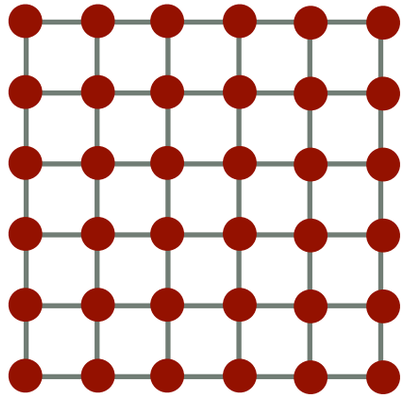




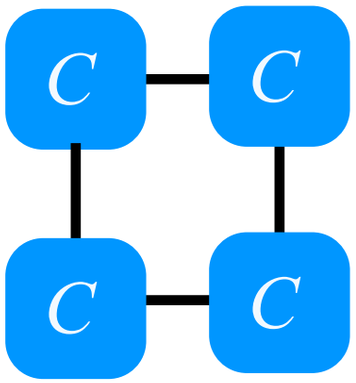
A: $m \times m \times m \times m$

Increase system size slightly

Contraction of (L+2)×(L+2) network

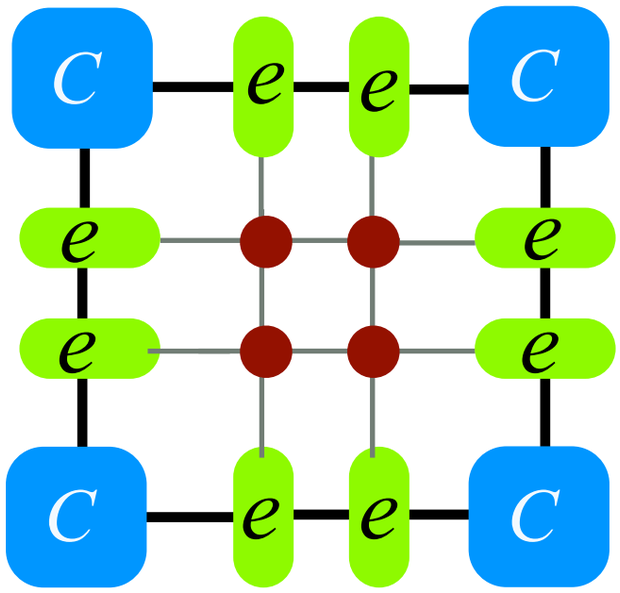


CTM representation

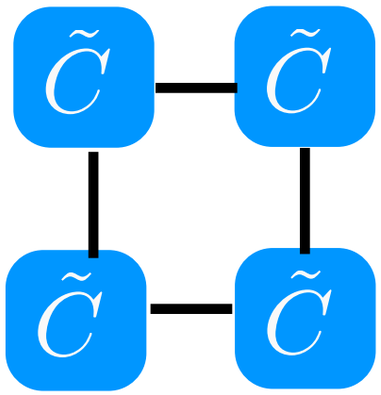


C: $D \times D$

Increase system size slightly



approximation



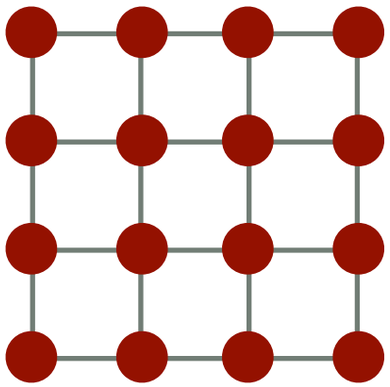
$\tilde{C}$: $D \times D$

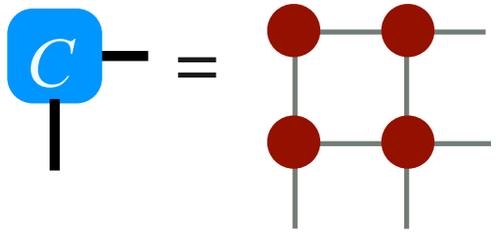
Increase system size
by keeping the size of C

Meaning of Corner Transfer Matrix

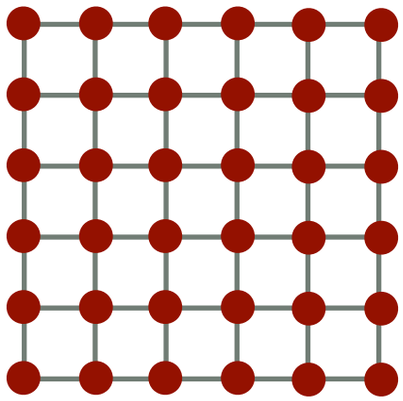
No approximation

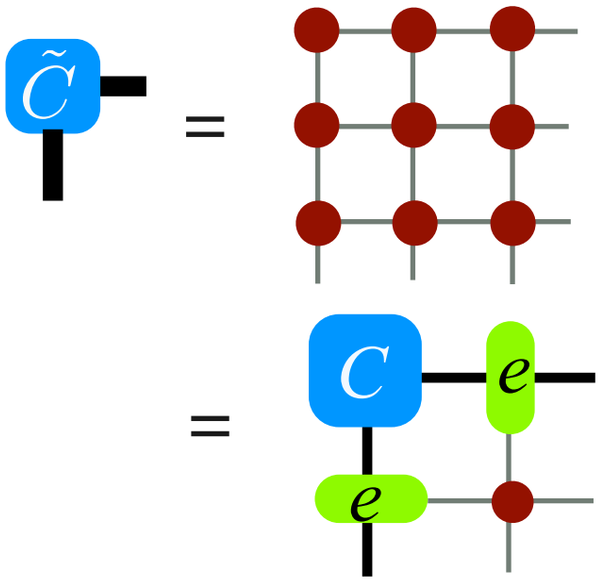
4×4

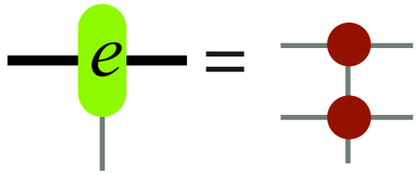




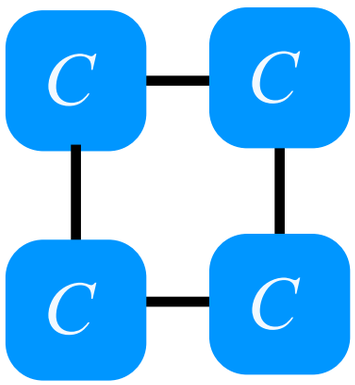
6×6



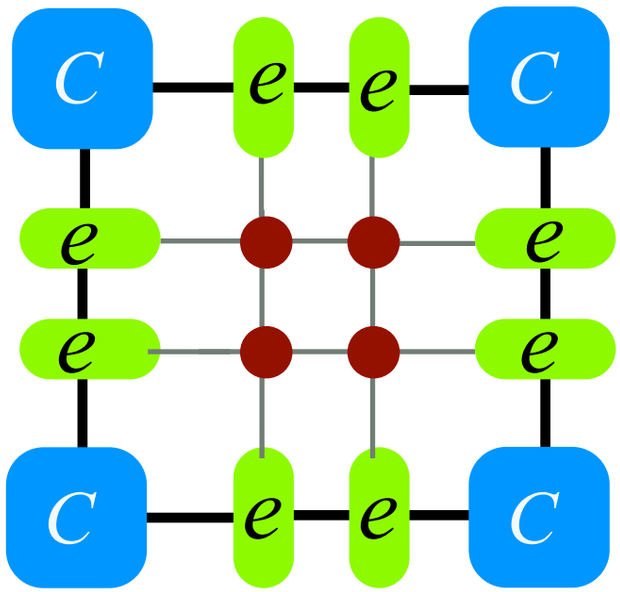




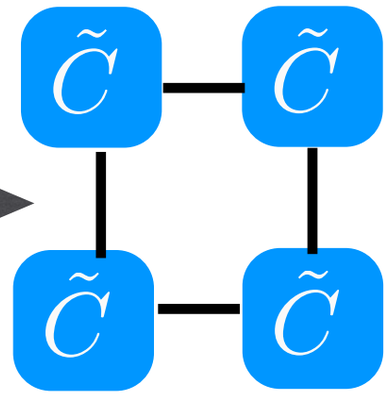
CTM representation



Increase system



Approximation



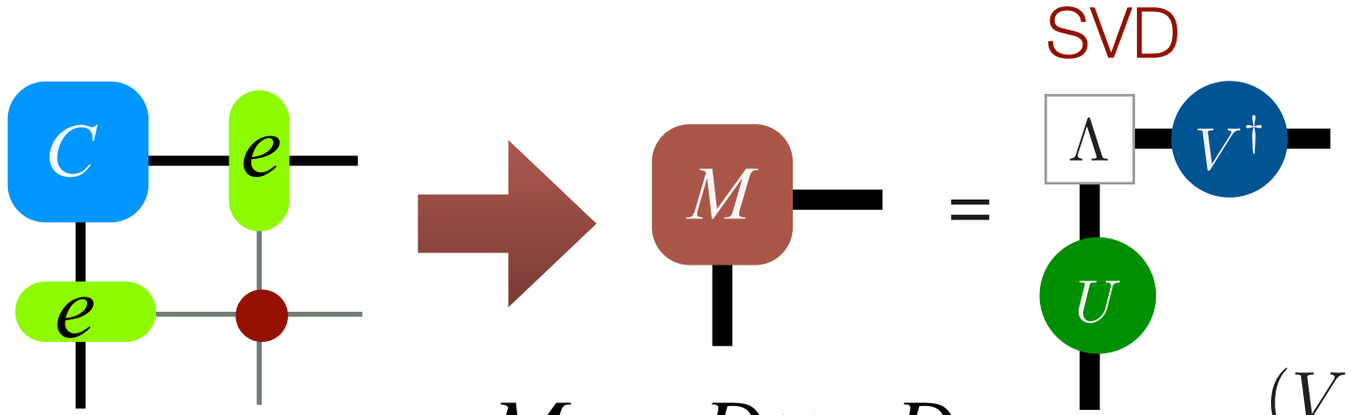
Cost

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

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

Recipe of CTMRG

1. SVD

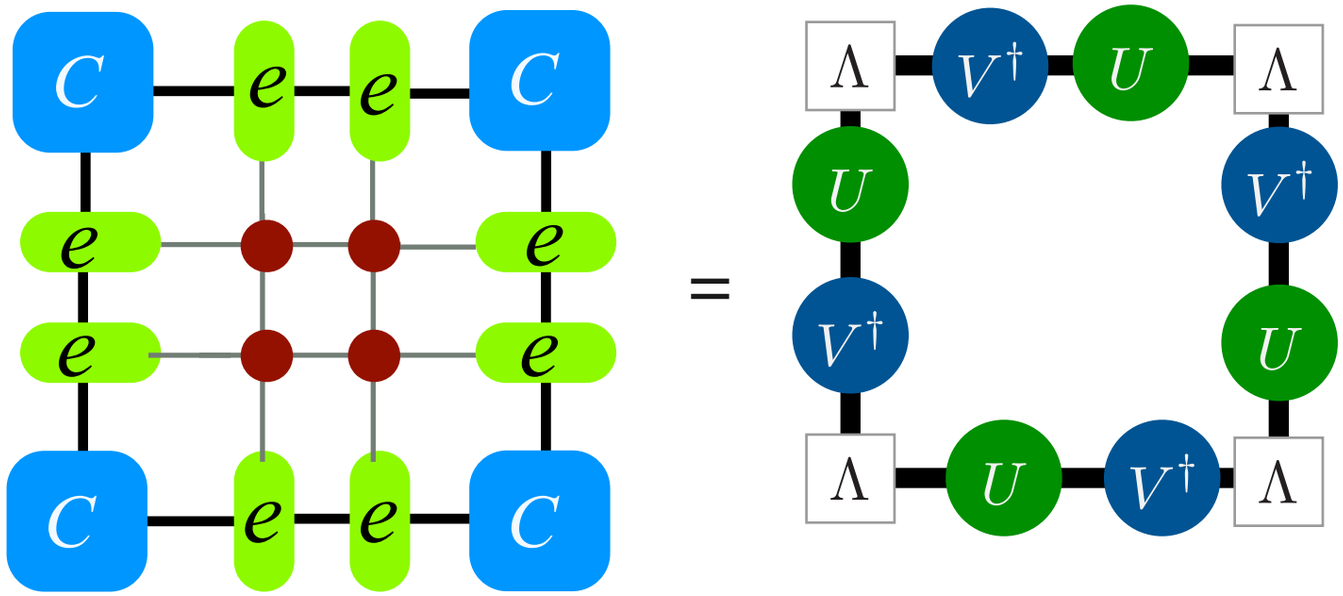


$M : mD \times mD$

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

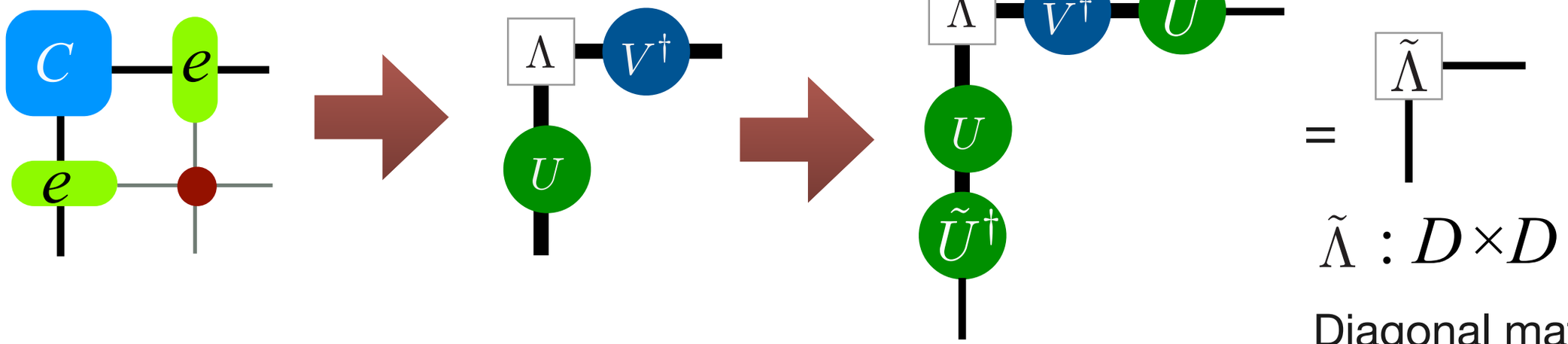
$$= \sum_i \lambda_i^4 (-1)^{4\eta_i}$$

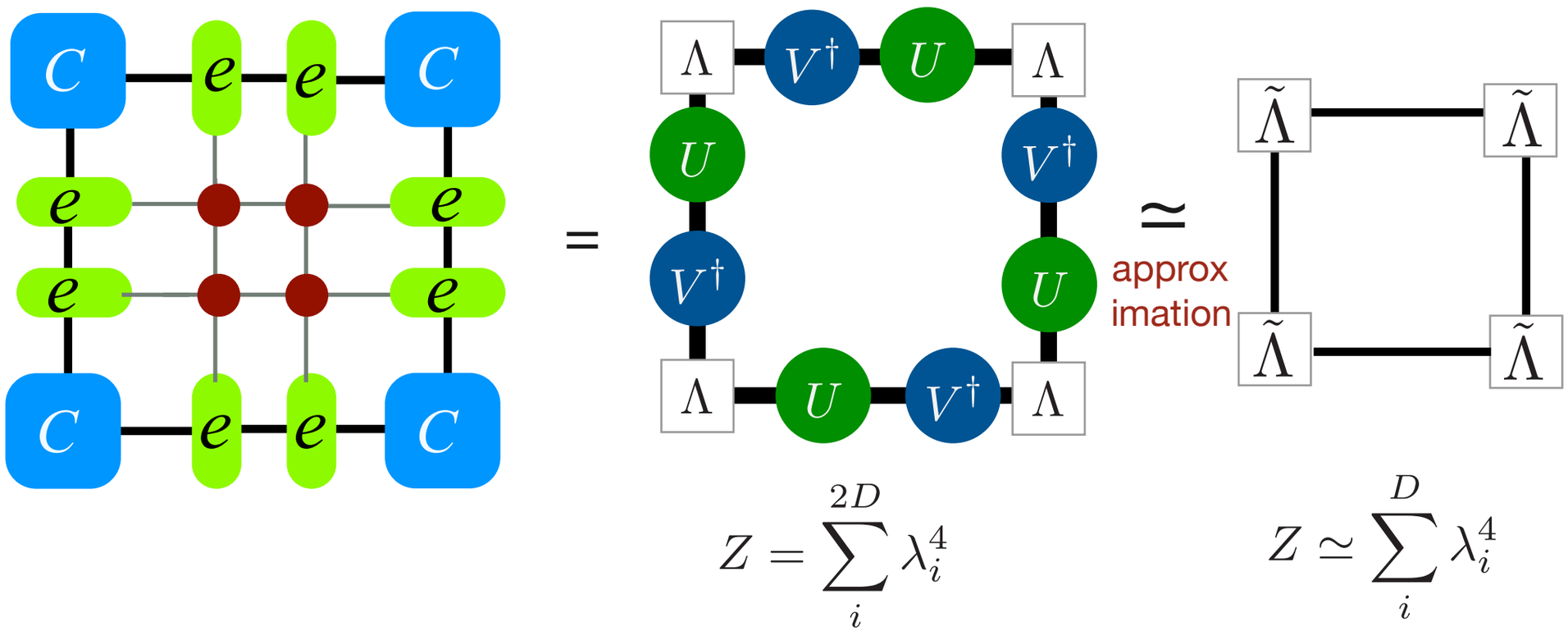
$$= \sum_i \lambda_i^4$$

Good approximation when we keep largest singular values!

Recipe of CTMRG

2. Approximation





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

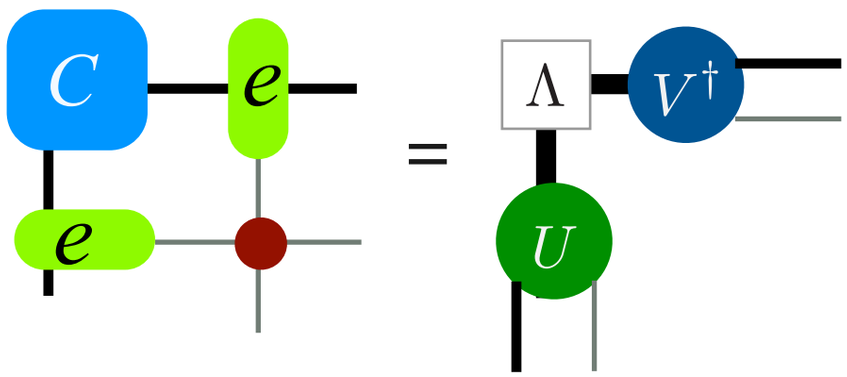
Cost

Recipe of CTMRG

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

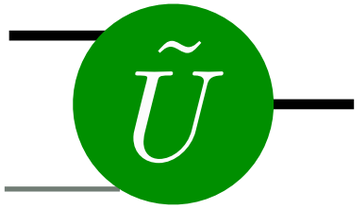
Summary of renormalization

1. SVD of the corner matrix for (L+2)×(L+2) system

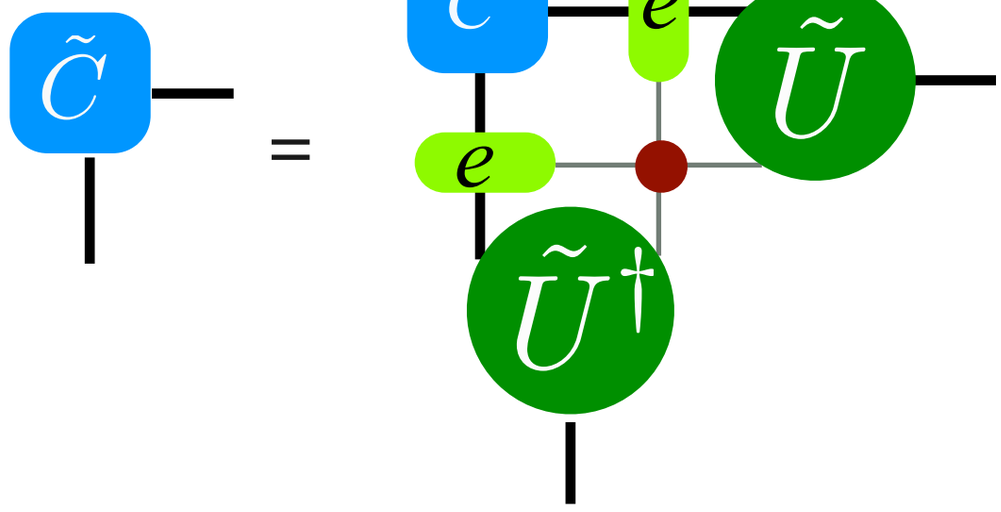


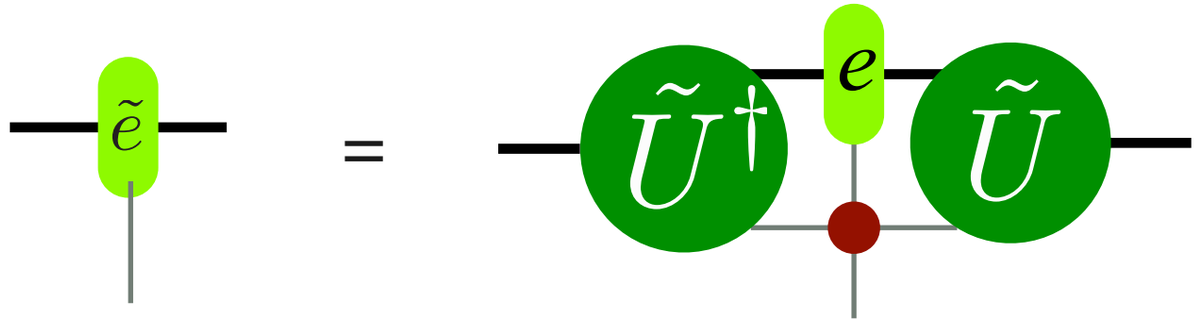
2. Make projector

Keep the largest
D singular values



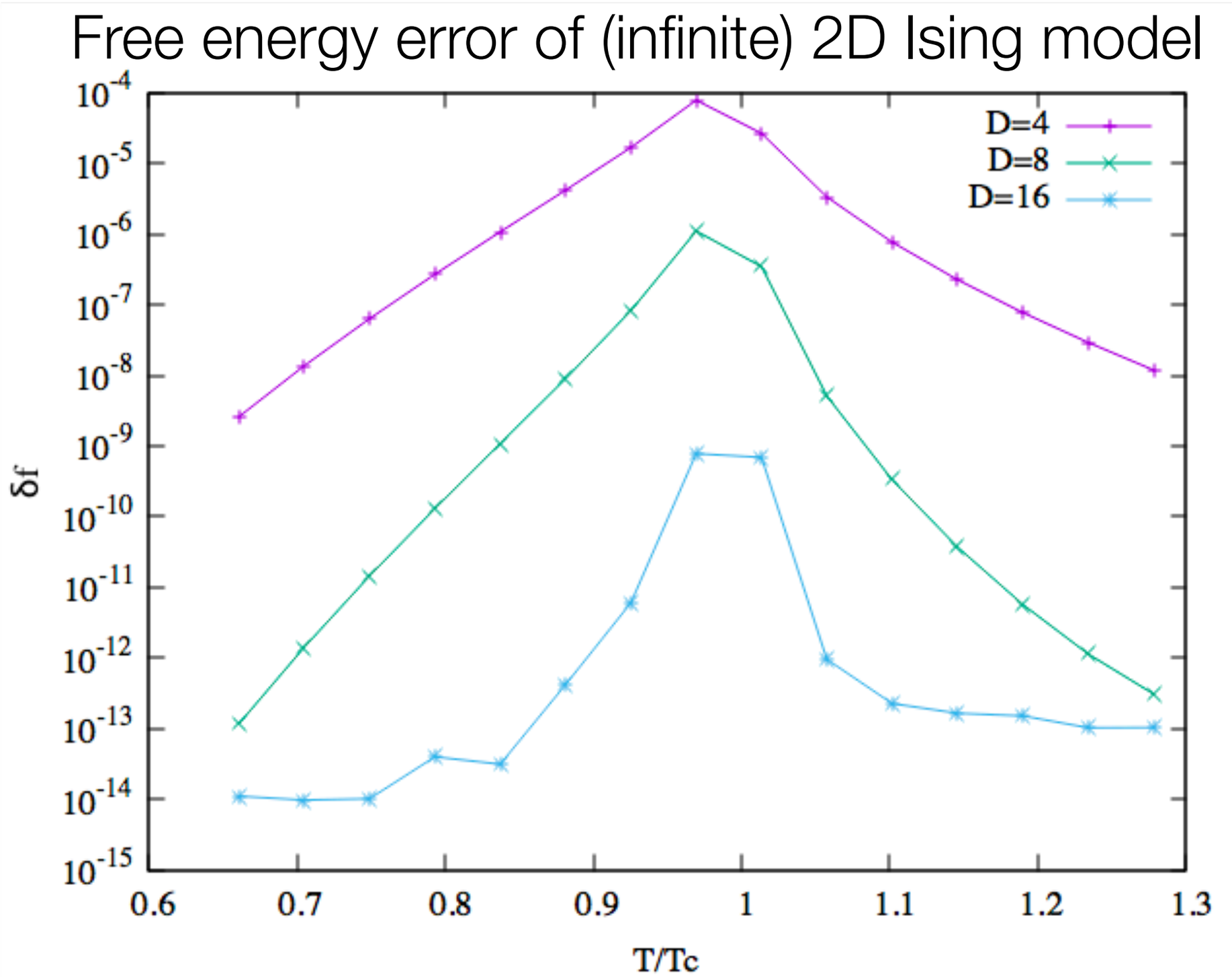
3. Make new conner and edge matrices





We can calculate tensor network contraction successively

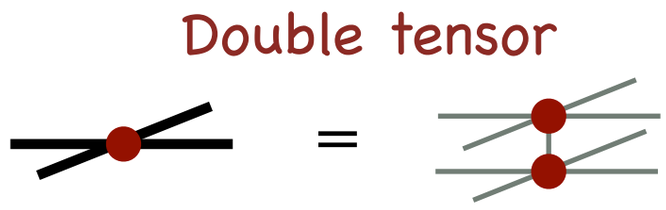
Accuracy of CTMRG



Application to quantum system

Difference from the Ising model

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



- 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

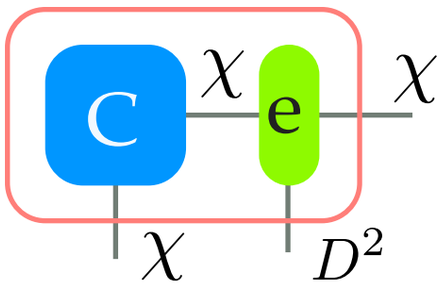
Update for quantum model

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

Iterative update of environment tensors

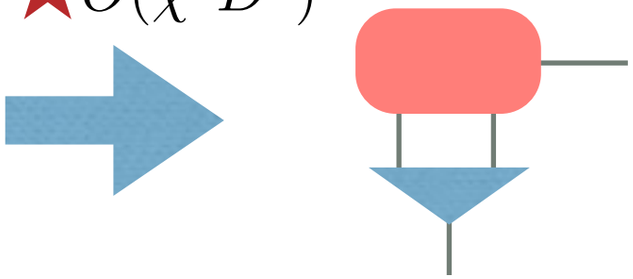
Absorption

(ex. left move)

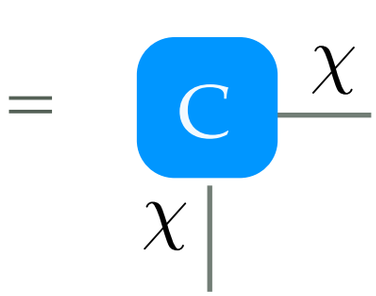


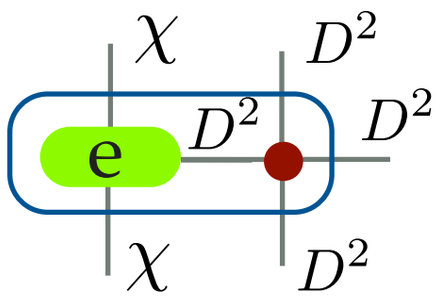
★$O(\chi^3 D^2)$

Truncation

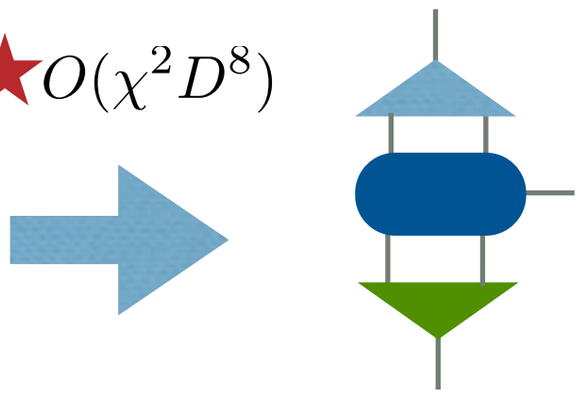


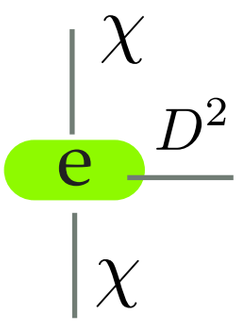
New

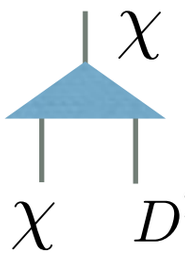




★$O(\chi^2 D^8)$



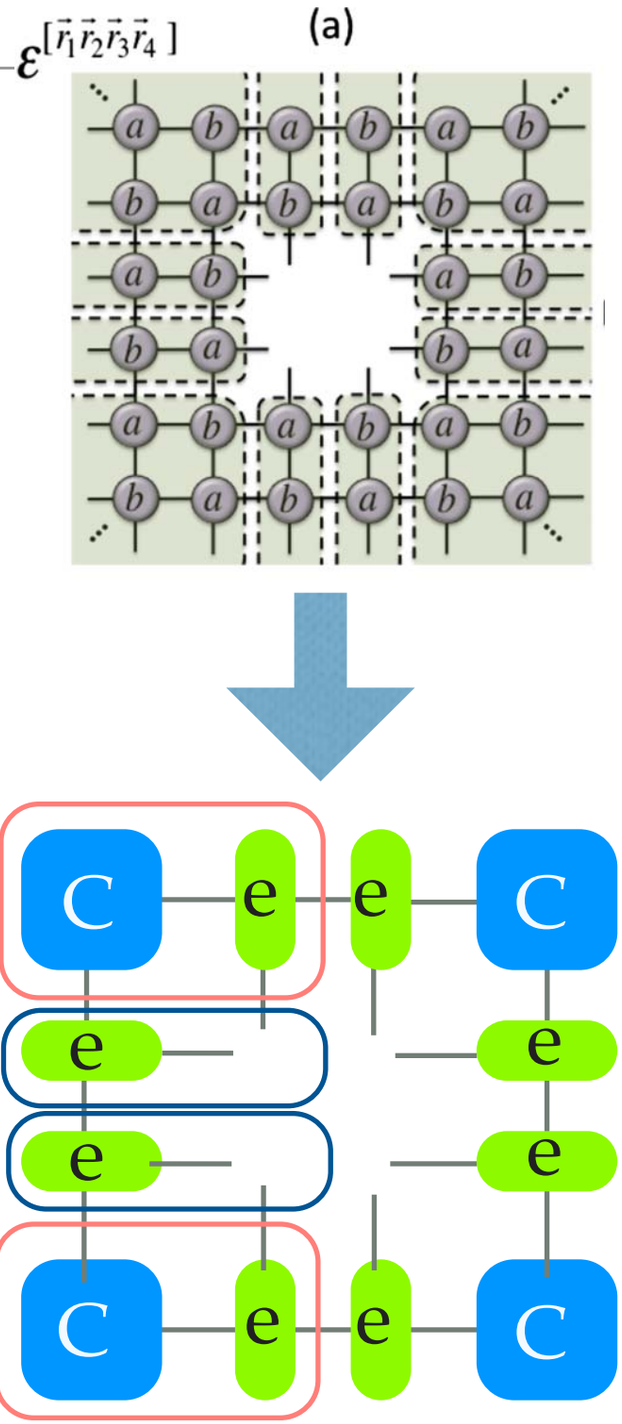




:Projector

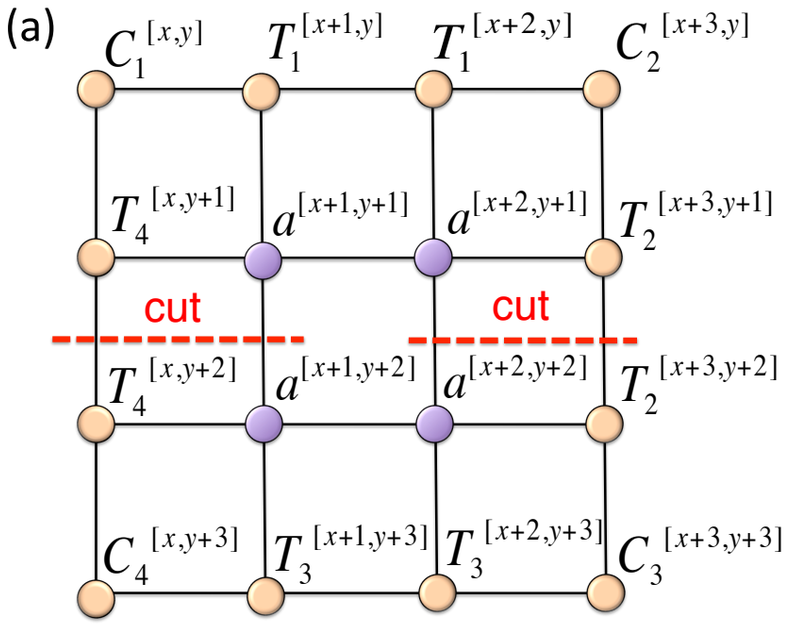
Same ways for right, top, bottom moves.

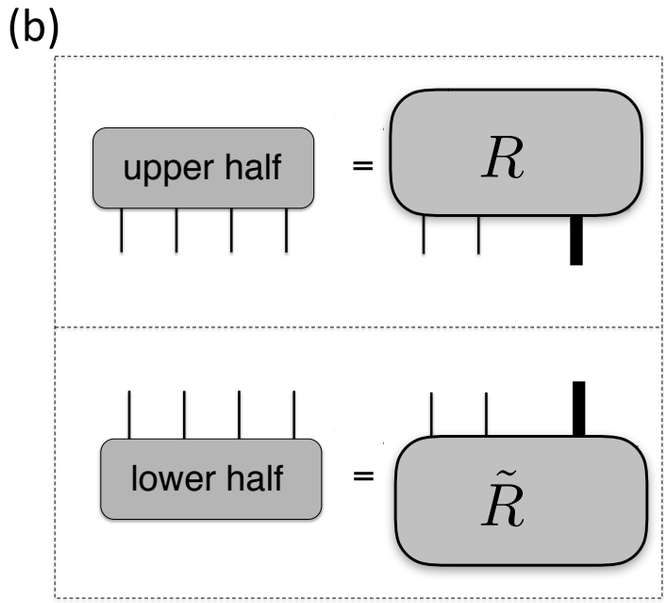
Repeat until convergence. (Typically several tens steps)

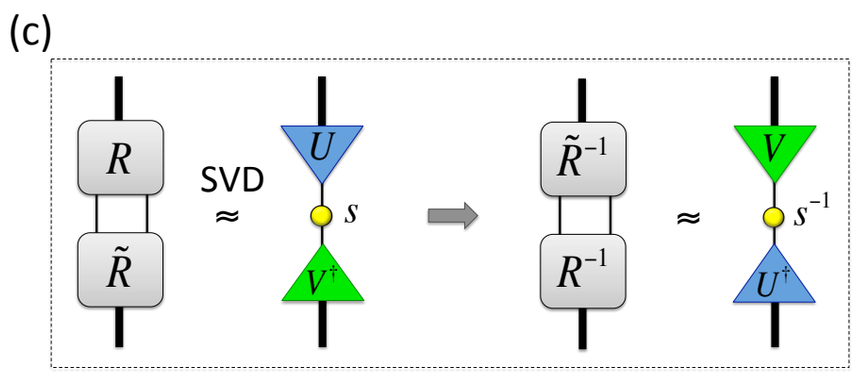


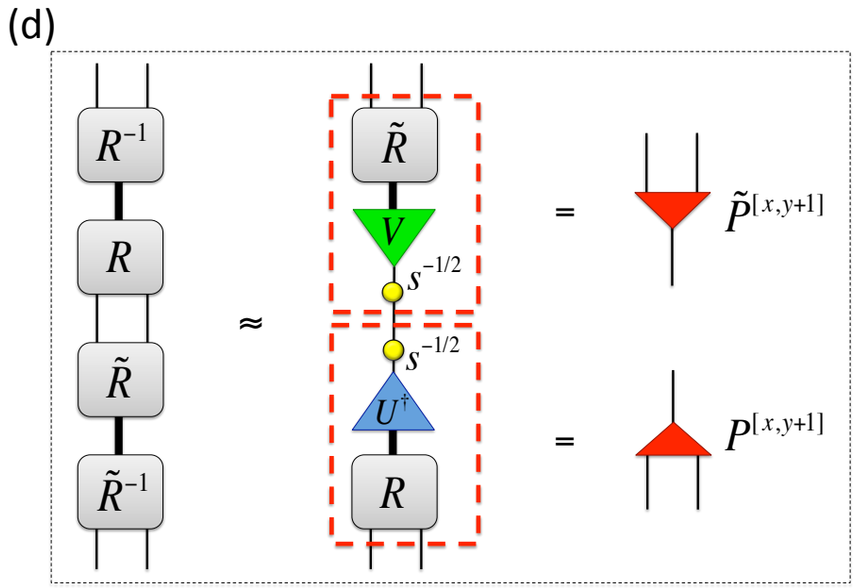
Calculation of projectors

(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: $O(\chi^3 D^6)$

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

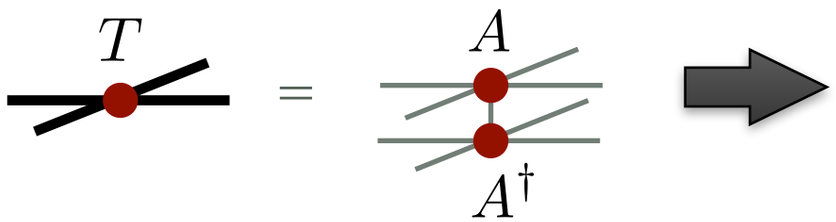
*Typically,

$\chi \geq D^2$ or $\chi \simeq D^2$

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.



In some case, we can reduce the contraction cost.

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.

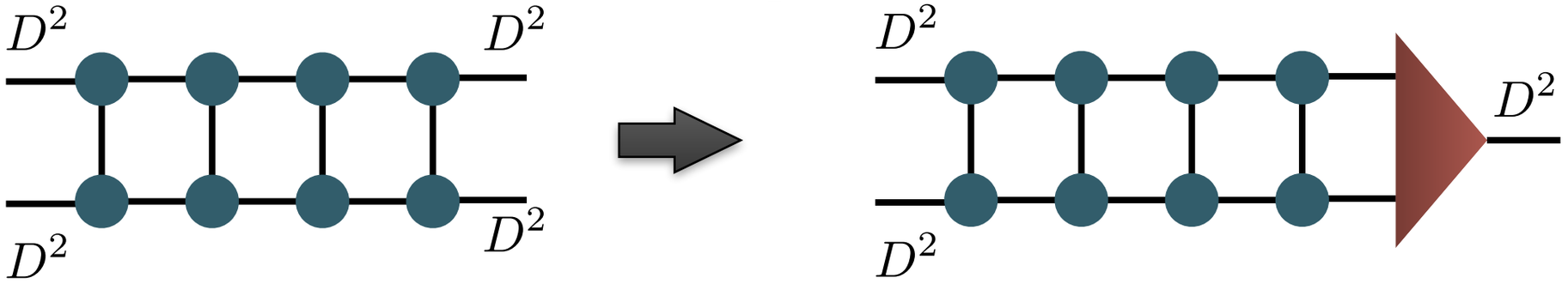
Full SVD: $O(D^{12})$ ⇒ Partial SVD: $O(D^{10})$

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.

* Same technique reduce the cost of TRG from $O(\chi^6)$ to $O(\chi^5)$.

*Example



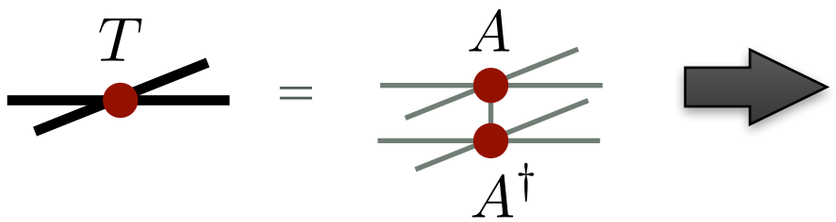
Contraction: $O(D^{12})$
Full SVD: $O(D^{12})$

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

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.



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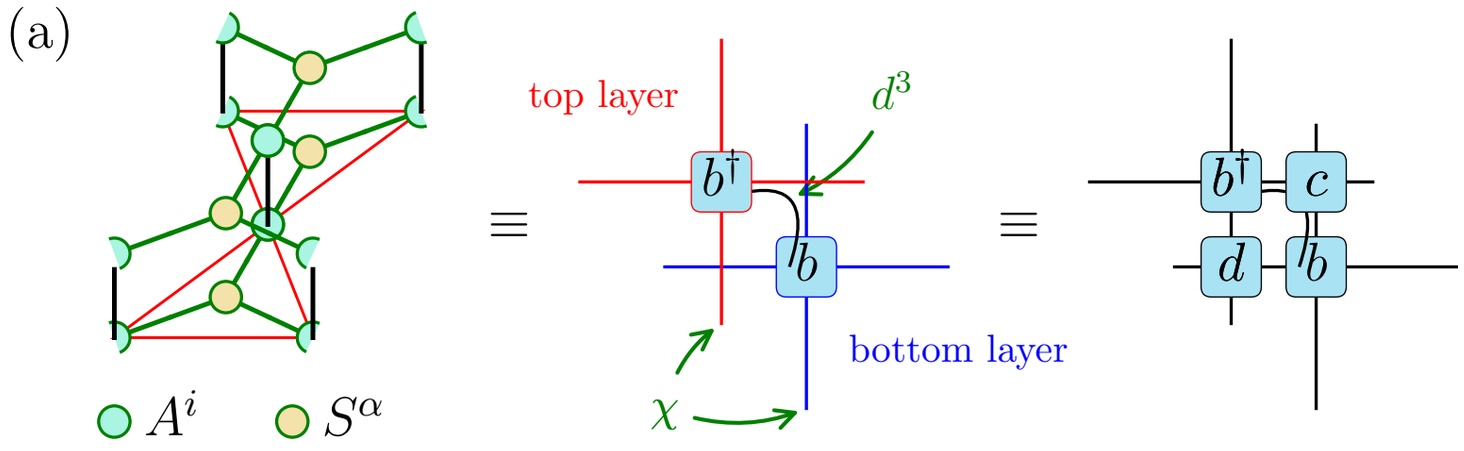
(2) Half-environment contraction: $O(\chi^3 D^6), O(\chi^2 D^8)$ ➡ not need

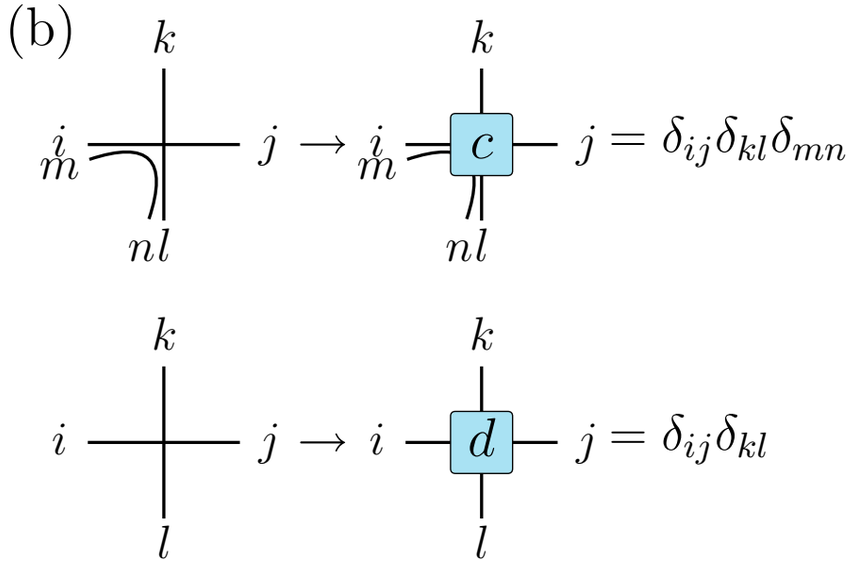
(3) SVD of RR matrix: $O(\chi^3 D^6)$ ➡ $O(\chi^2 D^6)$

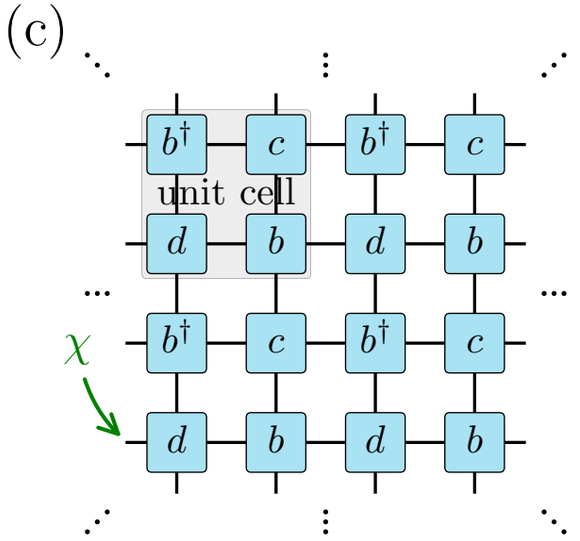
$O(D^{10})$

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 $O(D^8)$.

($\chi \sim D^2$)

Potential power of iTPS

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.)	$aL^{d-1} + \ln(\text{deg})$	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

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

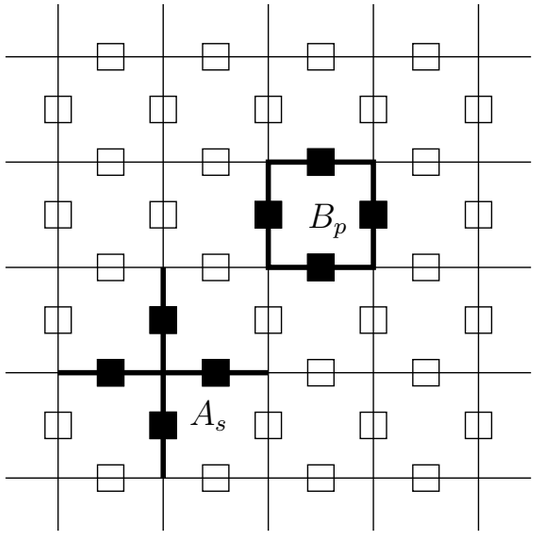
For d ≥ 2, leading contribution satisfies area low
even for gapless (critical) systems.

Example: Ground state represented by iTPS

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

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

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

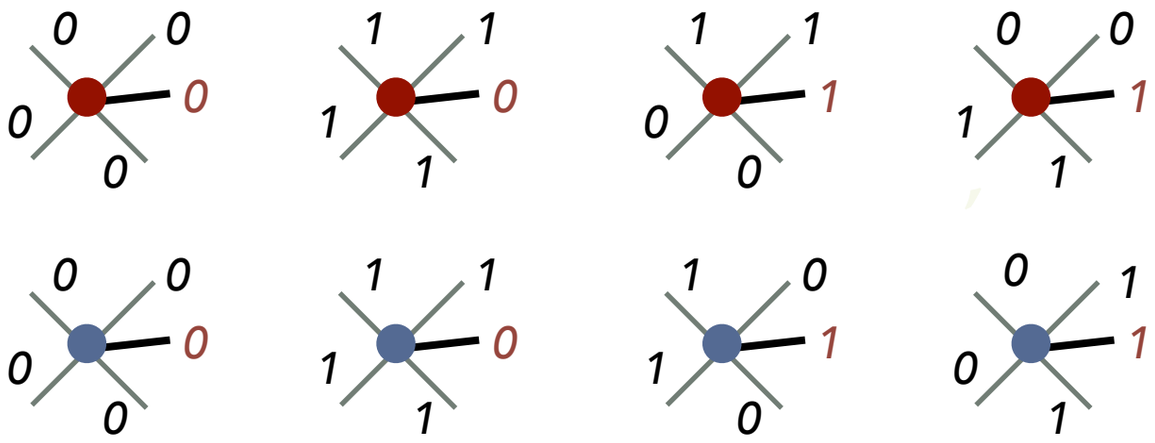


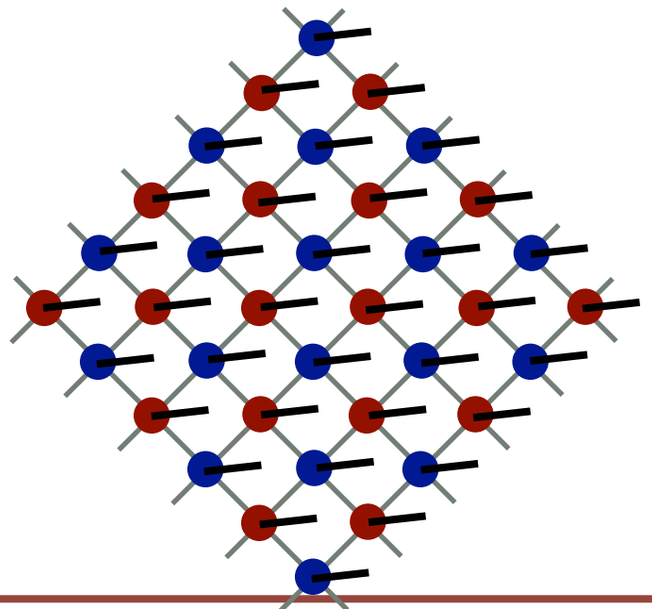
Its ground state is so called Z_2 spin liquid state.

"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)





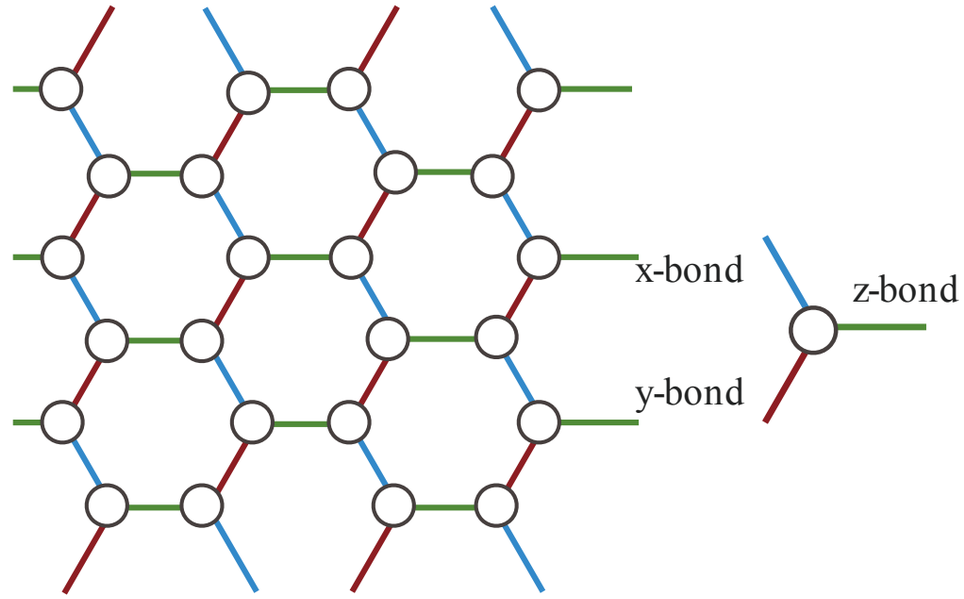
Example: Loop gas state for gapless Kitaev SL

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

$$\mathcal{H} = -\sum_{\gamma,\langle i,j\rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma$$

γ:bond direction

Ground states are spin liquids!



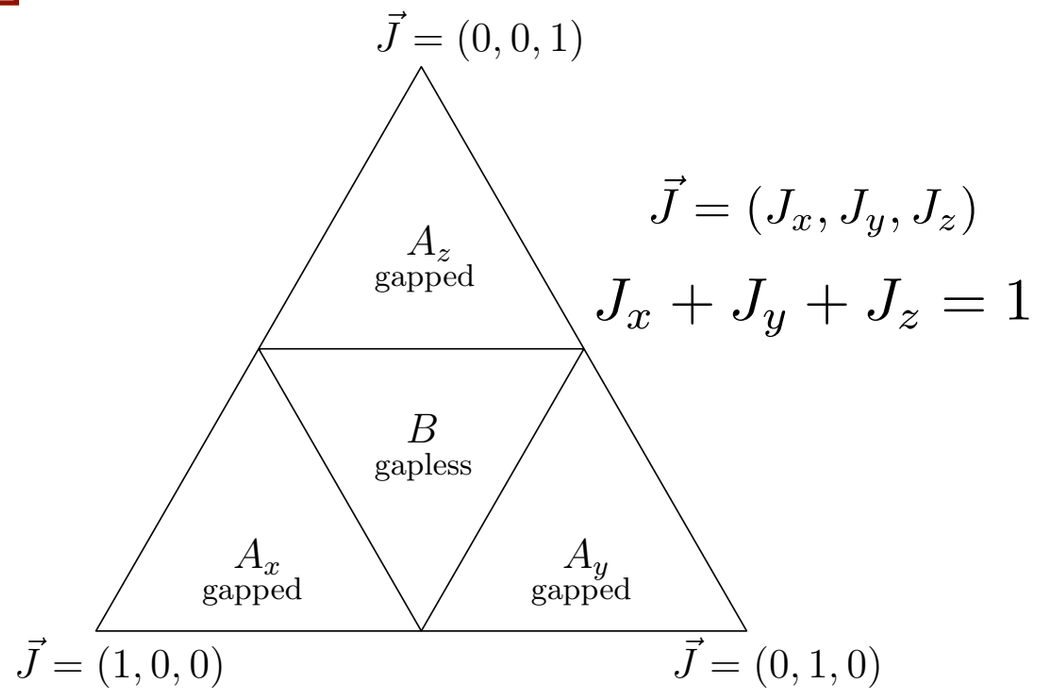
Anisotropic region (A) : gapped spin liquid

- 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



Example: Loop gas state for gapless Kitaev SL

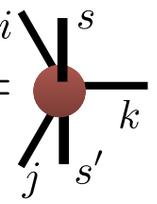
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, arXiv:1901.03614

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

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

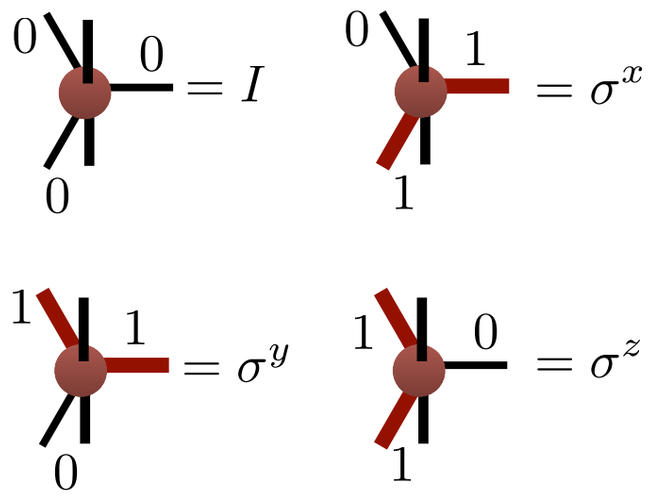
Ferromagnetic state pointing (1,1,1) direction.

(cf. Lee's seminar)

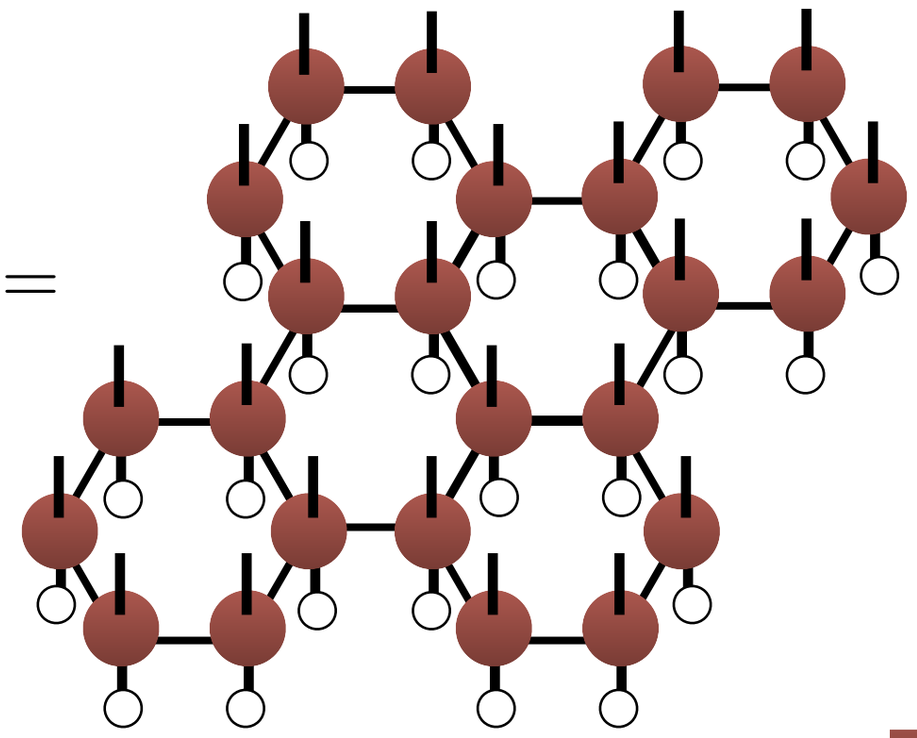
$Q^{ss'}_{ijk} =$ 

$i,j,k = 0,1$

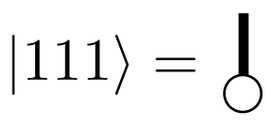
Non zero elements:



$|\mathrm{LGS}\rangle =$



D=2, TPS

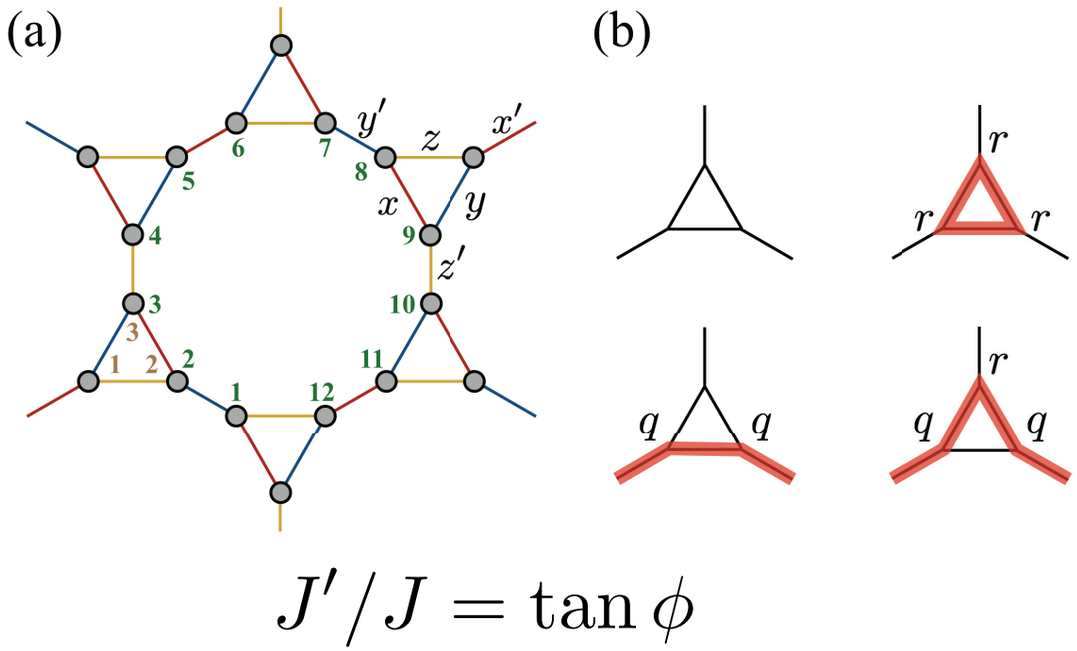
$|111\rangle =$ 

This LGS is critical,
with the Ising CFT universality.

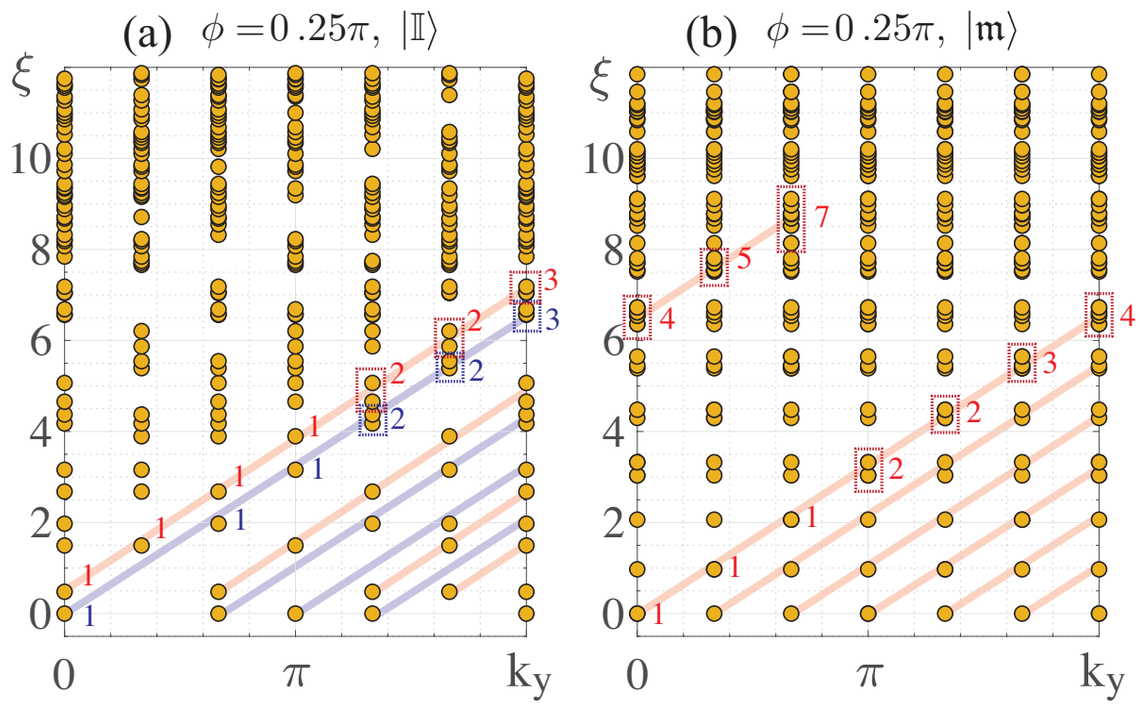
Example: chiral spin liquid on the star lattice

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, arXiv:1907.02268

(cf. Lee's symposium talk)



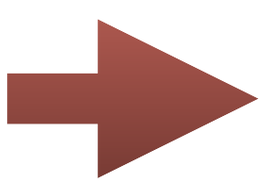
Entanglement spectrum



Similar LG construction gives us both of abelian and non-abelian chiral SL.

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.

Optimization of iTPS

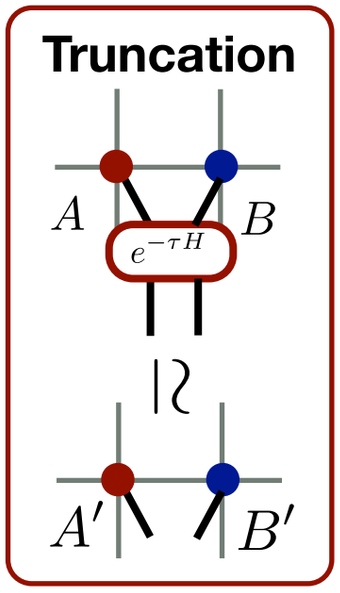
Typical optimization methods for iTPS

1. Imaginary time evolution

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

Suzuki-Torotter 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 ($O(D^8)$~$O(D^{10})$)
- 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. arXiv:1903:09650

cf. DMRG for MPS

Truncations in ITE

- Full update

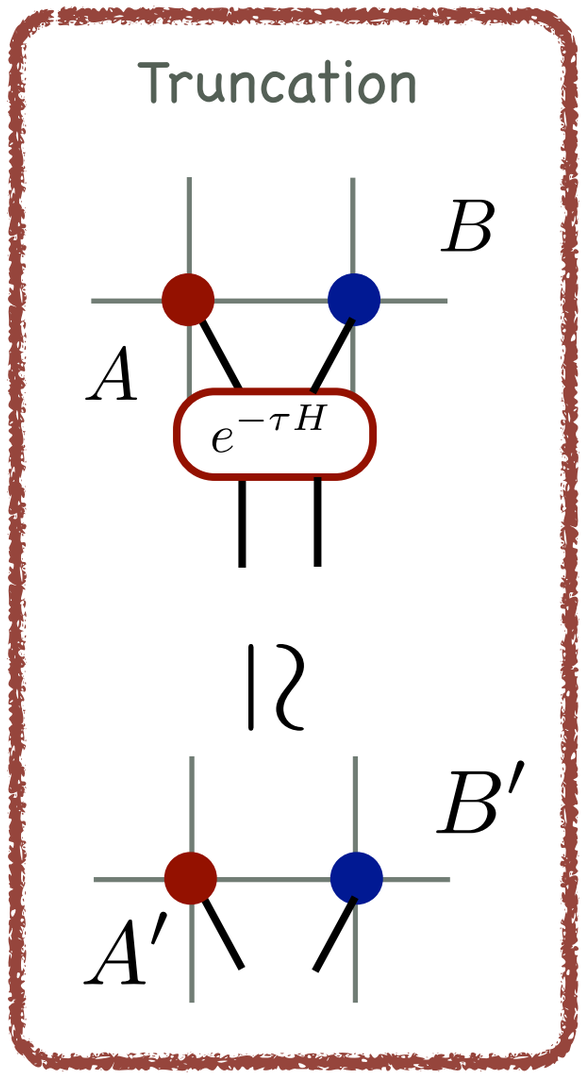
  Minimize the difference between two wave functions:

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

  $|\Psi\rangle$: 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

Simple update

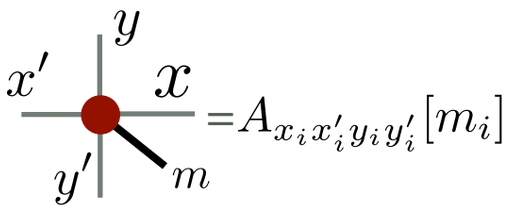
(H. G. Jiang *et al*, Phys. Rev. Lett. **101**, 090603 (2008))

Extended iTPS:

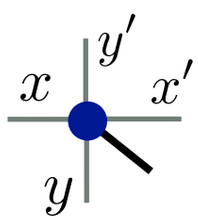
Insert (positive) diagonal matrix representing "weight" of bonds.

(cf. iTEBD)

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



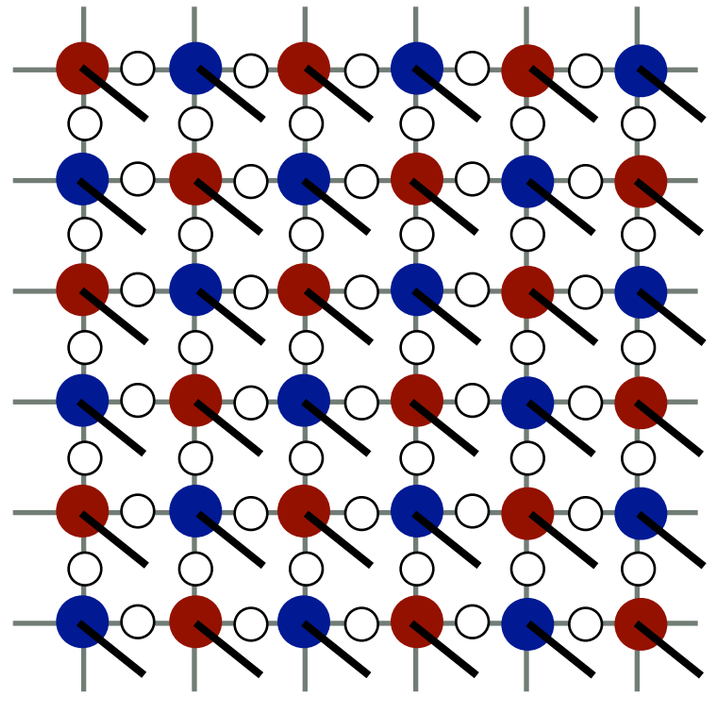
$= A_{x_i x'_i y_i y'_i}[m_i]$



$= B_{x_j x'_j y_j y'_j}[m_j]$ —○— $= \lambda$

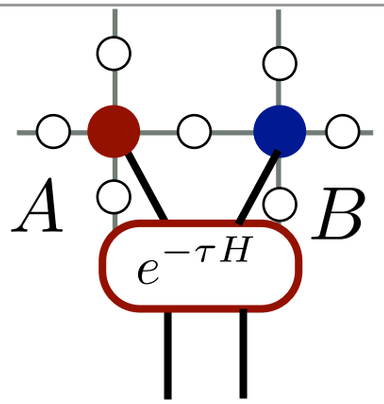
x,y,x',y' = 1,2, ... D

Extended PEPS



Simple update with naive SVD

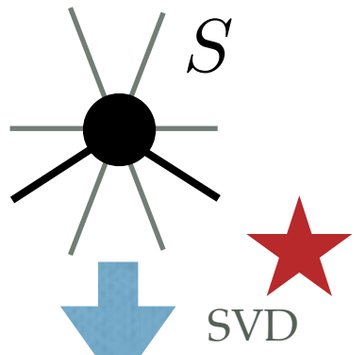
$$e^{-\tau H_x}|\Psi\rangle = \mathrm{Tr}\prod_{i\in A, j\in i+x}\sum_{m_i,m_j}\langle m_i' m_j'|e^{-\tau H_{ij}}|m_i m_j\rangle \lambda_{x_i}\lambda_{x_i'}\lambda_{y_i}\lambda_{y_i'}A_{x_i x_i' y_i y_i'}[m_i]B_{x_j x_j' y_j y_j'}[m_j]|m_i' m_j'\rangle$$



Truncation by SVD

1. Define a matrix "S"

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

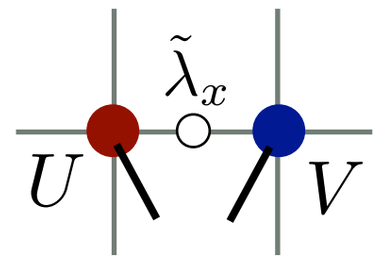


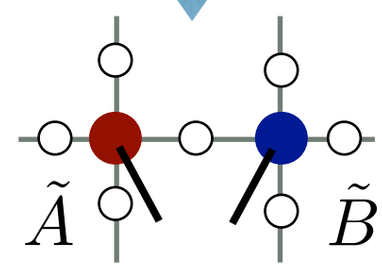
2. Do SVD ★

$$S_{y_i x_i' y_i' m_i, y_j x_j' y_j' m_j} = \sum_x U_{y_i x_i' y_i' m_i, x}\tilde{\lambda}_x V^T_{x, y_j x_j' y_j' m_j}$$

3. Truncate the matrix leaving upper D singular values

$$\tilde{A}_{x y_i x_i' y_i'}[m_i] = \lambda_{y_i}^{-1}\lambda_{x_i'}^{-1}\lambda_{y_i'}^{-1}U_{y_i x_i' y_i' m_i, x}$$
$$\tilde{B}_{x y_j x_j' y_j'}[m_j] = \lambda_{y_j}^{-1}\lambda_{x_j'}^{-1}\lambda_{y_j'}^{-1}V_{y_j x_j' y_j' m_j, x}$$





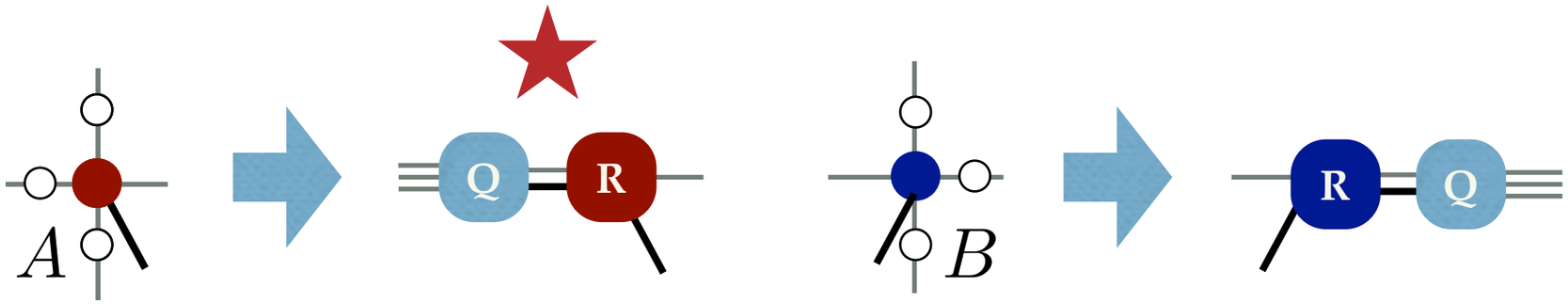
*** Meaning of λ**

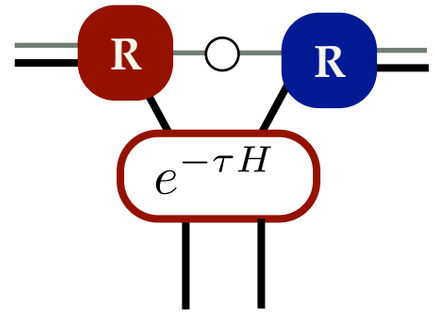
At SVD, λ provides information of local environment.

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

Simple update with QR decompositions

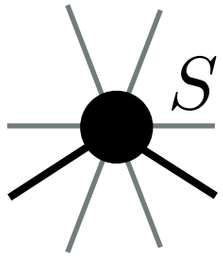
QR decomposition before SVD





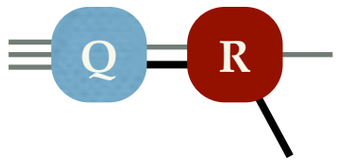
Calculation cost

Direct SVD:

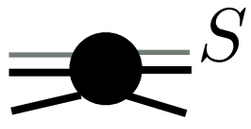


$O(D^9 m_d^3)$

QR decomposition:

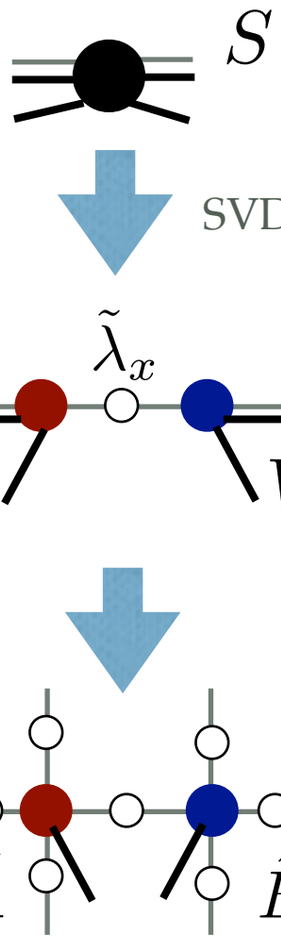


$O(D^5 m_d^2)$



$O(D^3 m_d^6)$

Usually D > m_d → QR method is cheaper.



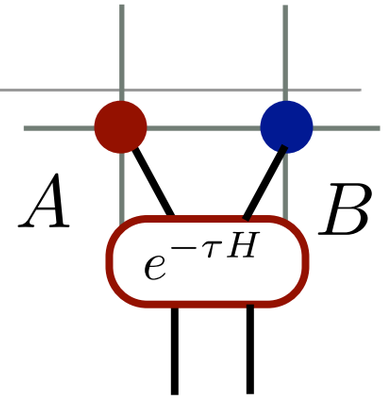
Full update

Minimize the difference between wave functions

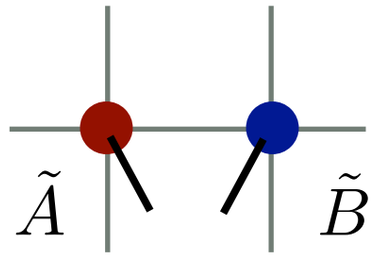
$$||\Psi\rangle - |\tilde{\Psi}\rangle||^2 = \langle\Psi|\Psi\rangle + \langle\tilde{\Psi}|\tilde{\Psi}\rangle - 2\mathrm{Re}\langle\Psi|\tilde{\Psi}\rangle = f$$

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

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



Necessary conditions for minimization $\dfrac{\partial f}{\partial \tilde{A}^*} = 0, \dfrac{\partial f}{\partial \tilde{B}^*} = 0$



Iterative calculation by solving linear equation

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

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

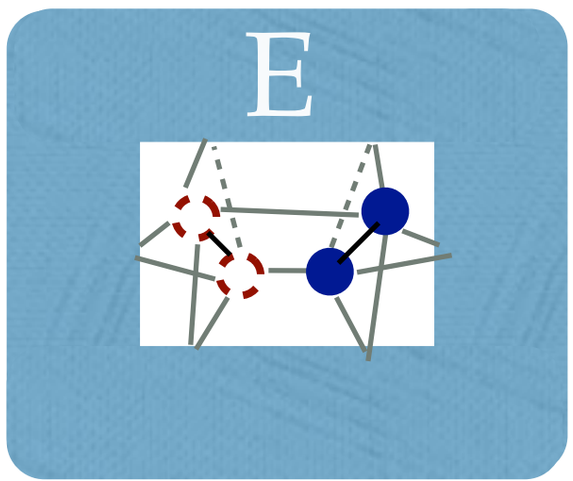
*Environment is fixed during the iteration

★$O(D^{12}m_d^3)$

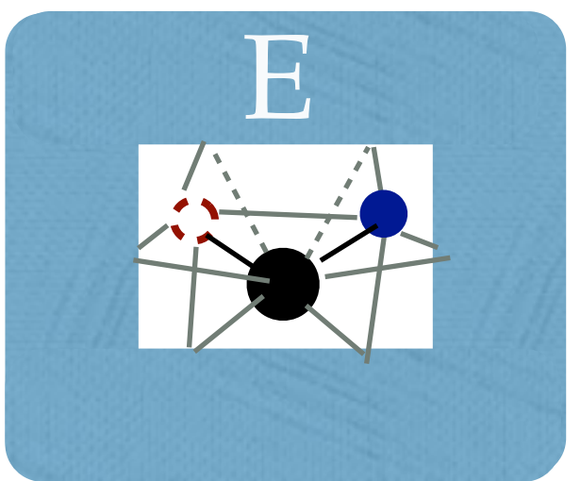
*Environment: $O(D^8) \sim O(D^{10})$

*Alternatively, we can also use the CG.

N_A, N_B :``Matrices"



W_A, W_B :``Vectors"



＊QR decomposition method:

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

★ linear equation $O(D^6m_d^6)$

Additional approximation for infinite system

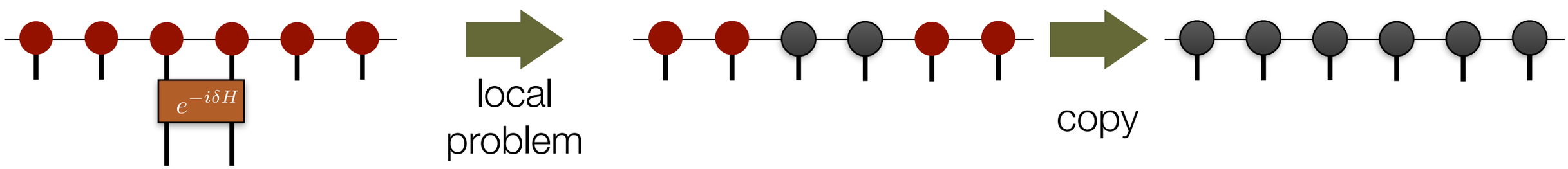
Even in full update, we actually consider iTPS locally:

We evaluate $||\Psi\rangle - |\tilde{\Psi}\rangle||^2 = \langle\Psi|\Psi\rangle + \langle\tilde{\Psi}|\tilde{\Psi}\rangle - 2\mathrm{Re}\langle\Psi|\tilde{\Psi}\rangle$

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.

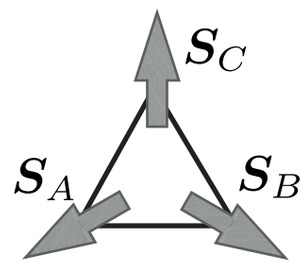


Applications of ITE updates

Kagome lattice Heisenberg model

Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_{i,z}$$



- Ground state at zero field

Classical GS: All states satisfying "120 degree structure"

→ Macroscopic degeneracy

Effect of thermal fluctuation: "order by disorder" mechanism

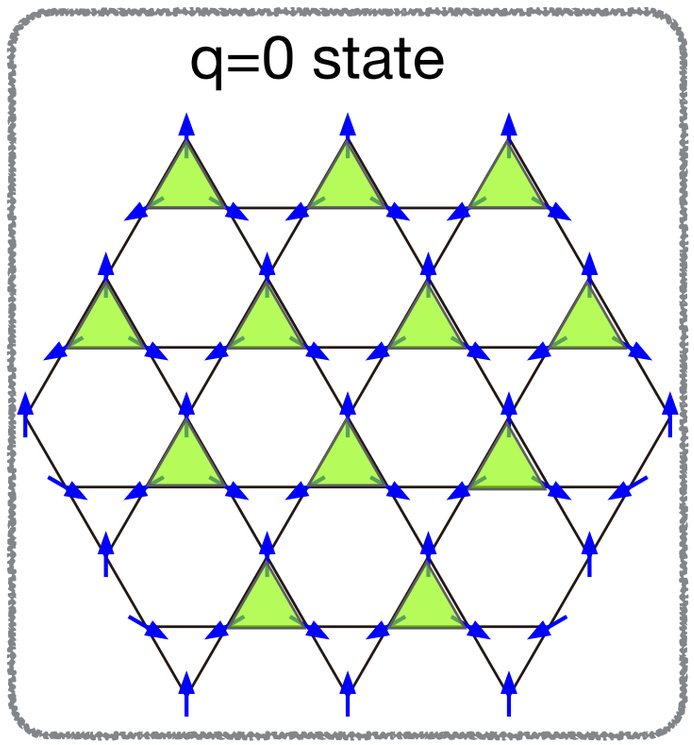
→selection of coplanar structure: q=0, √3 × √3

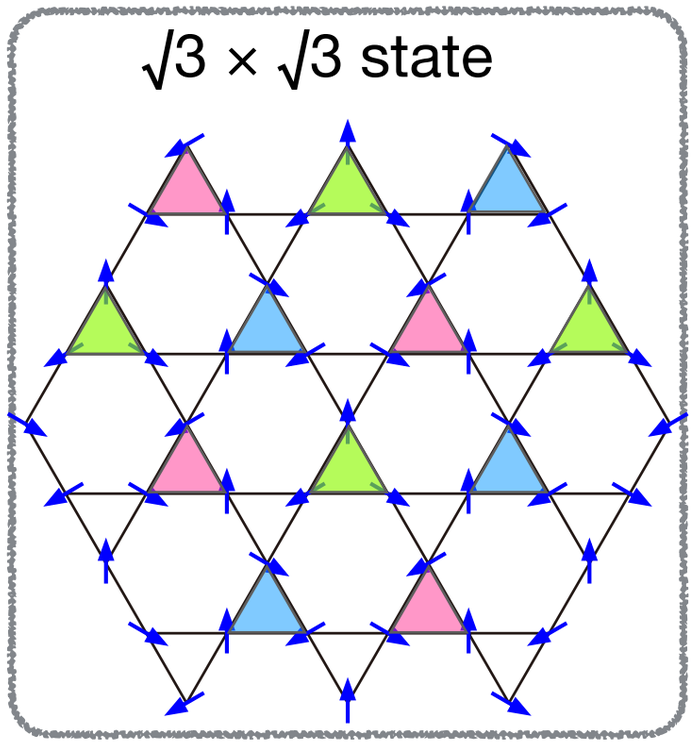
Quantum fluctuation:

S=1/2 quantum spin：

Spin liquid?

- Z_2 spin liquid
- U(1) spin liquid
- …





Magnetization process (S=1/2)

"Grand canonical" DMRG

(C. Hotta, *et al,* (2012, 2013), S.Nishimoto, *et al,* (2013)

Finite size system with modulation

→ Quantities in the thermodynamic limit

Four magnetization plateaus

M/M_{Sat} = 1/9, 1/3, 5/9, 7/9

Exact diagonalization ($N \leq 42$)

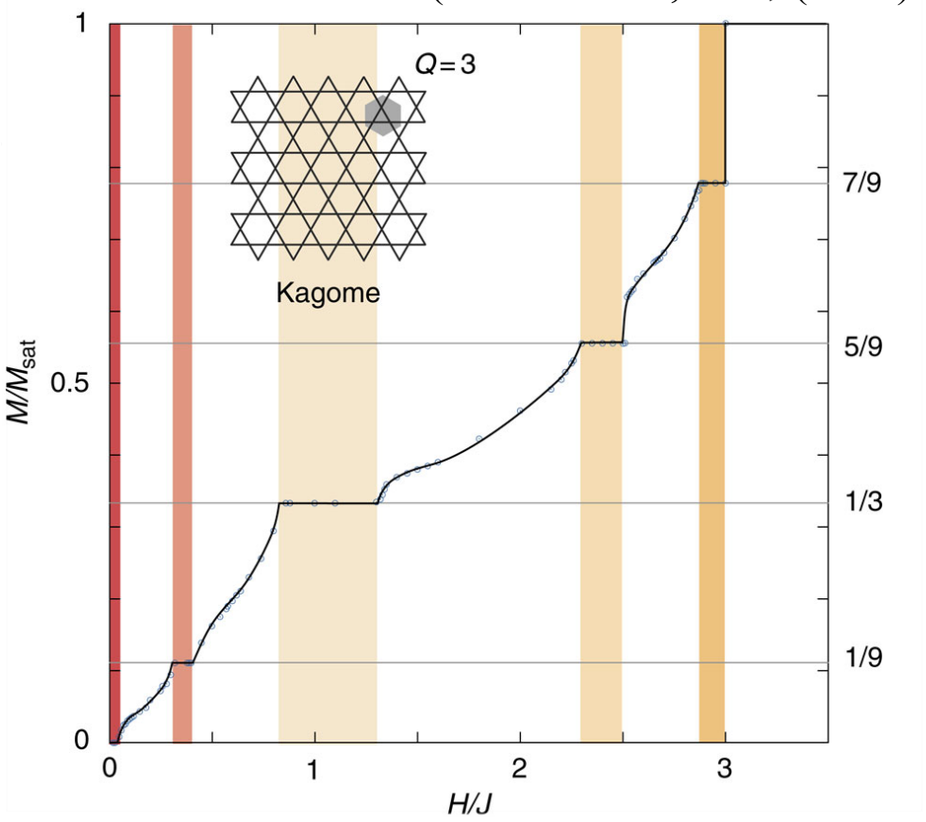
(H. Nakano, and T. Sakai (2012, 2014)

M/M_{sat}=1/3 is a "ramp"

- Anomalous critical exponents at the edge
- Plateau width could be infinitesimal

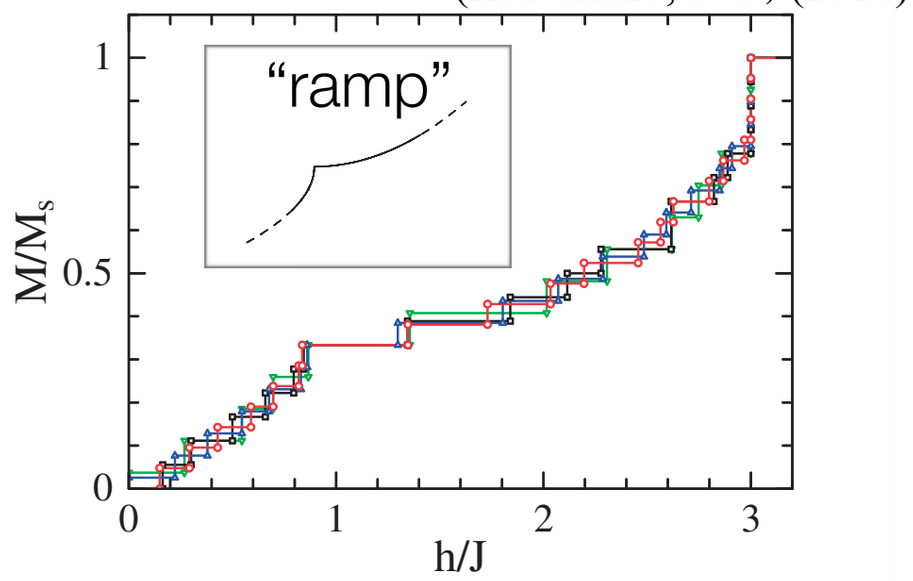
Magnetization by DMRG

(S.Nishimoto, *et al,* (2013)



Magnetization by ED

(H. Nakano, *et al,* (2014)



Magnetization process (S=1/2)

"Grand canoni

Exact [illegible]onalization (N ≤ 42)

(H. Nakano, and T. Sakai (2012, 2014)

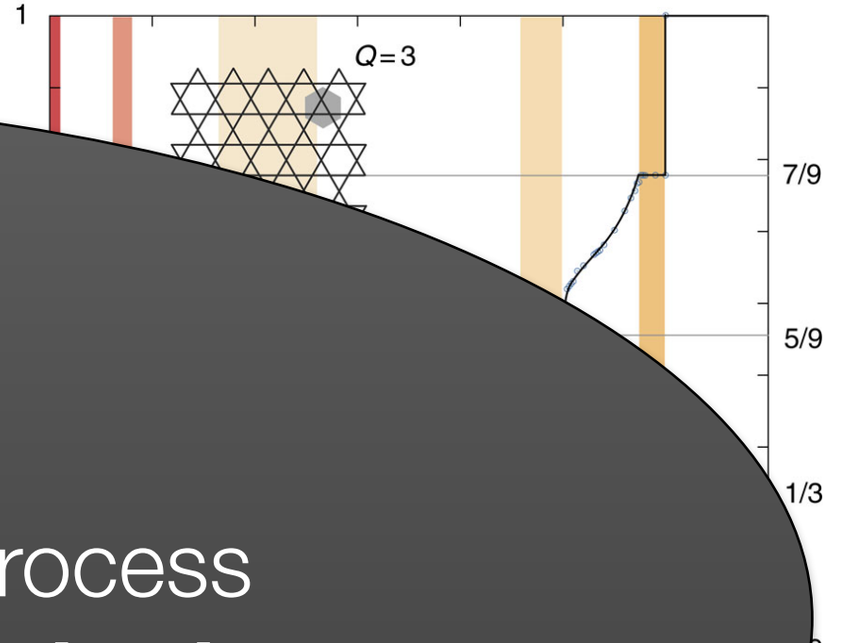
M/M_{sat}=1/3 is a "ramp"

- Anomalous critical exponents at the edge
- Plateau width could be infinitesimal

Aim:
Investigate magnetization process
using **tensor network method**
for infinite system

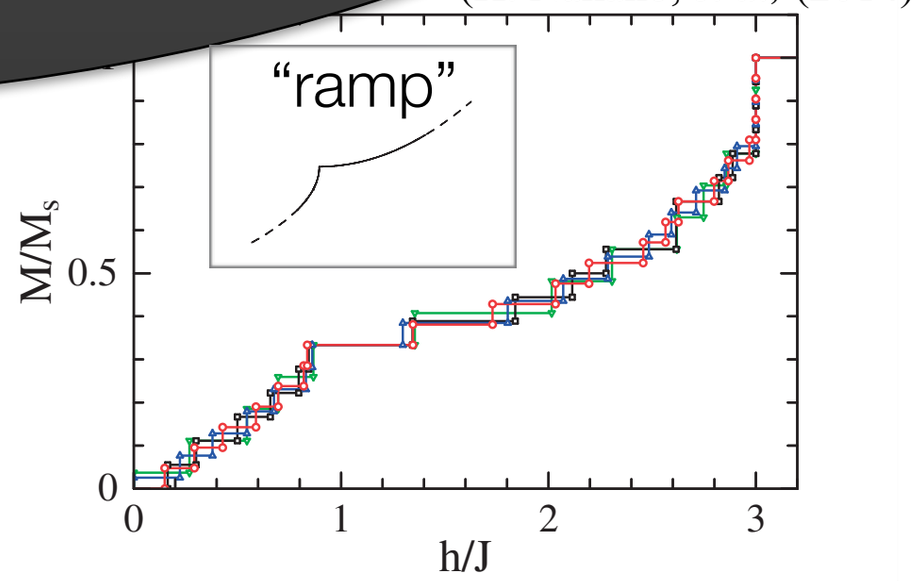
Magnetization by DMRG

(S.Nishimoto, *et al,* (2013)



[illegible]y ED

(H. Nakano, *et al,* (2014)

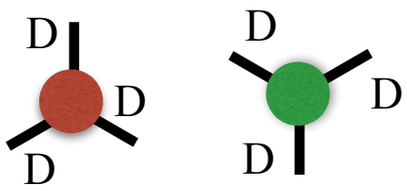


Extended PEPS for kagome lattice model

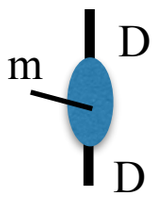
Extended PEPS (PESS)

D. Poilblanc et al, PRB 87, 140407(R) (2012)
Z. Y. Xie et al, PRX 4, 011025(2014))

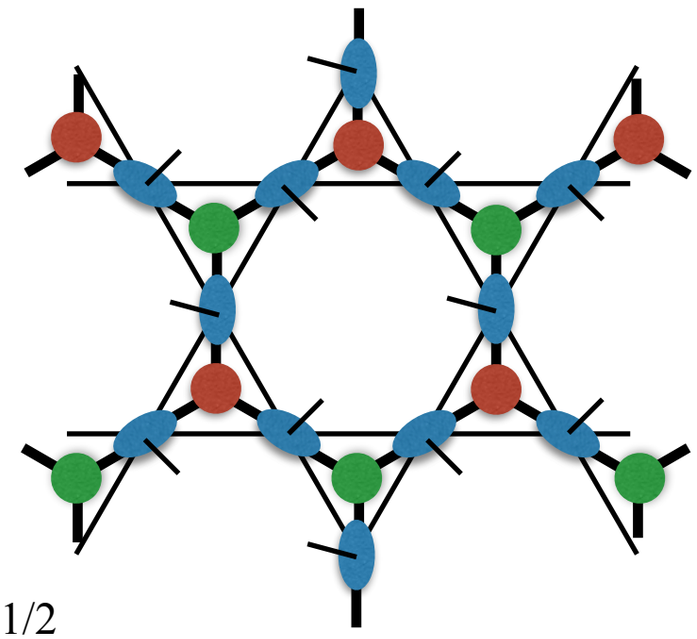
Tensors without spin



Tensors with spin

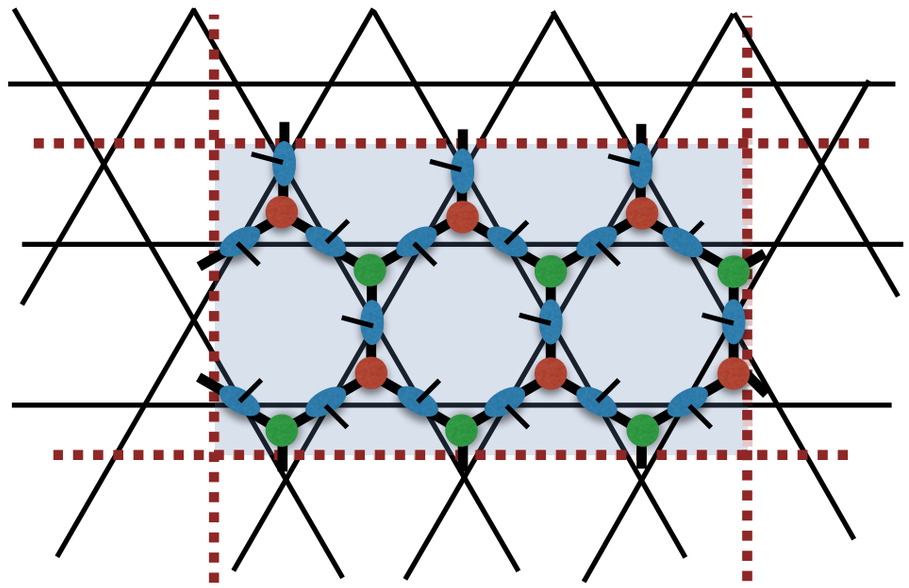


D: Bond dimension m: Sz = ±1/2



Infinite system with 18-sites unit cell

(Commensurate with √3 × √3 structure)



Two steps in the calculation

1. Optimization: optimize the tensor elements
   Truncation: Simple update (for two sites)
2. Evaluation of physical quantities:
   Approximation：Corner Transfer Matrix method

Differences from

T. Picot et al, PRB 93, 060407(R) (2016).

- Unit cell size
  They considered up to 9 sites
- Evaluation of physical quantities
  They used mean-field environment

Results：Magnetization curve

(R. Okuma, D. Nakamura, T. Okubo, et al, Nat. Commun. **10,** 1229 (2019))

Magnetization plateau

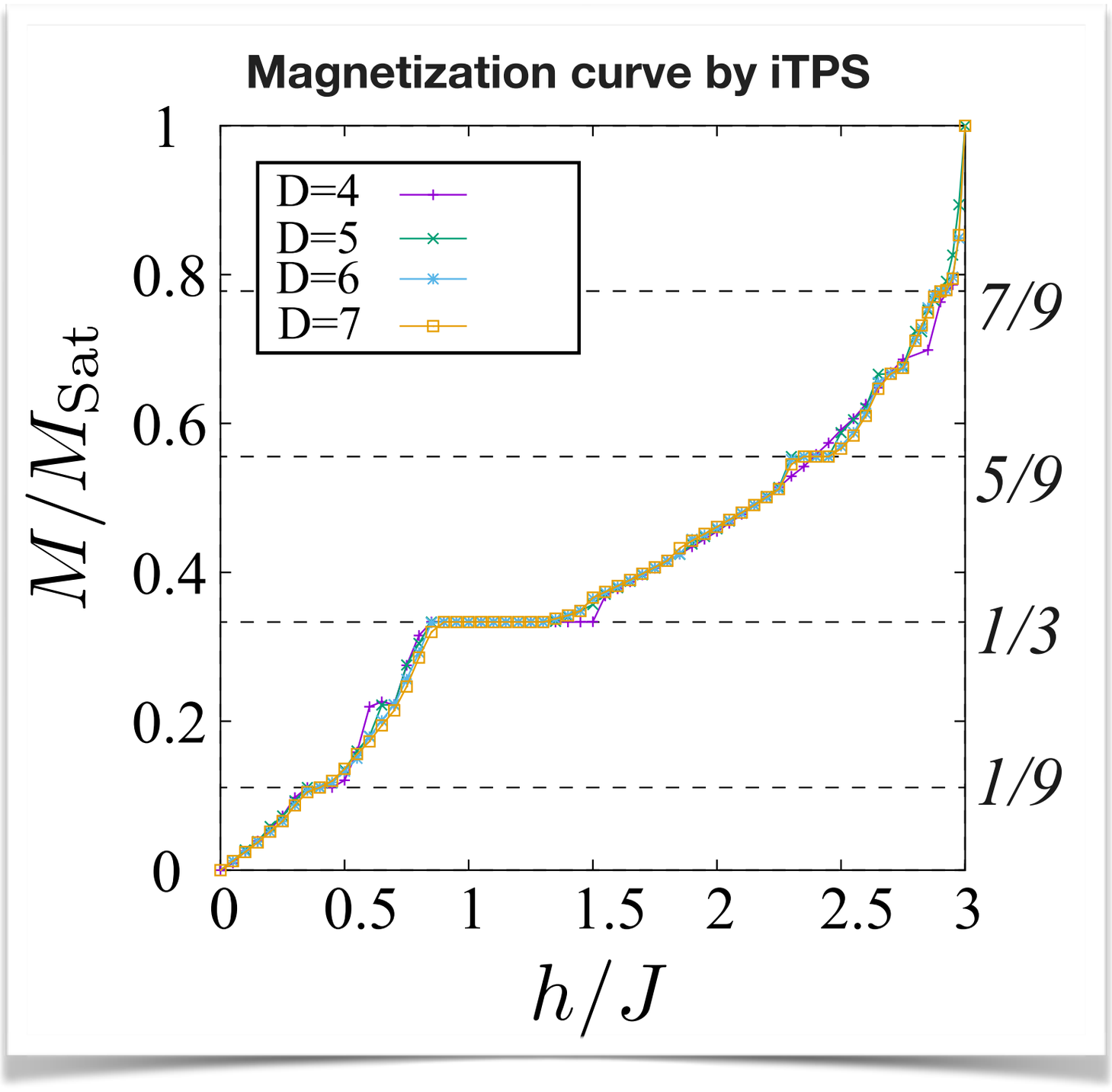
- Almost converged data up to D=7

1/9, 1/3, 5/9 :clear plateaus
7/9: weak anomaly

→ Consistent with DMRG

- Weak anomaly at 2/9, 6/9

→ They seem to vanish as D is increased.



Result：1/3 plateau state

Semi-classical UpUpDown

(Also observed in the study of T. Picot *et al*)

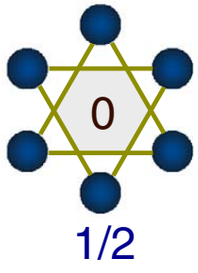
Depending on “initial states”
several types of pattern appear
Local minima!

(Lowest energy: √3 × √3)

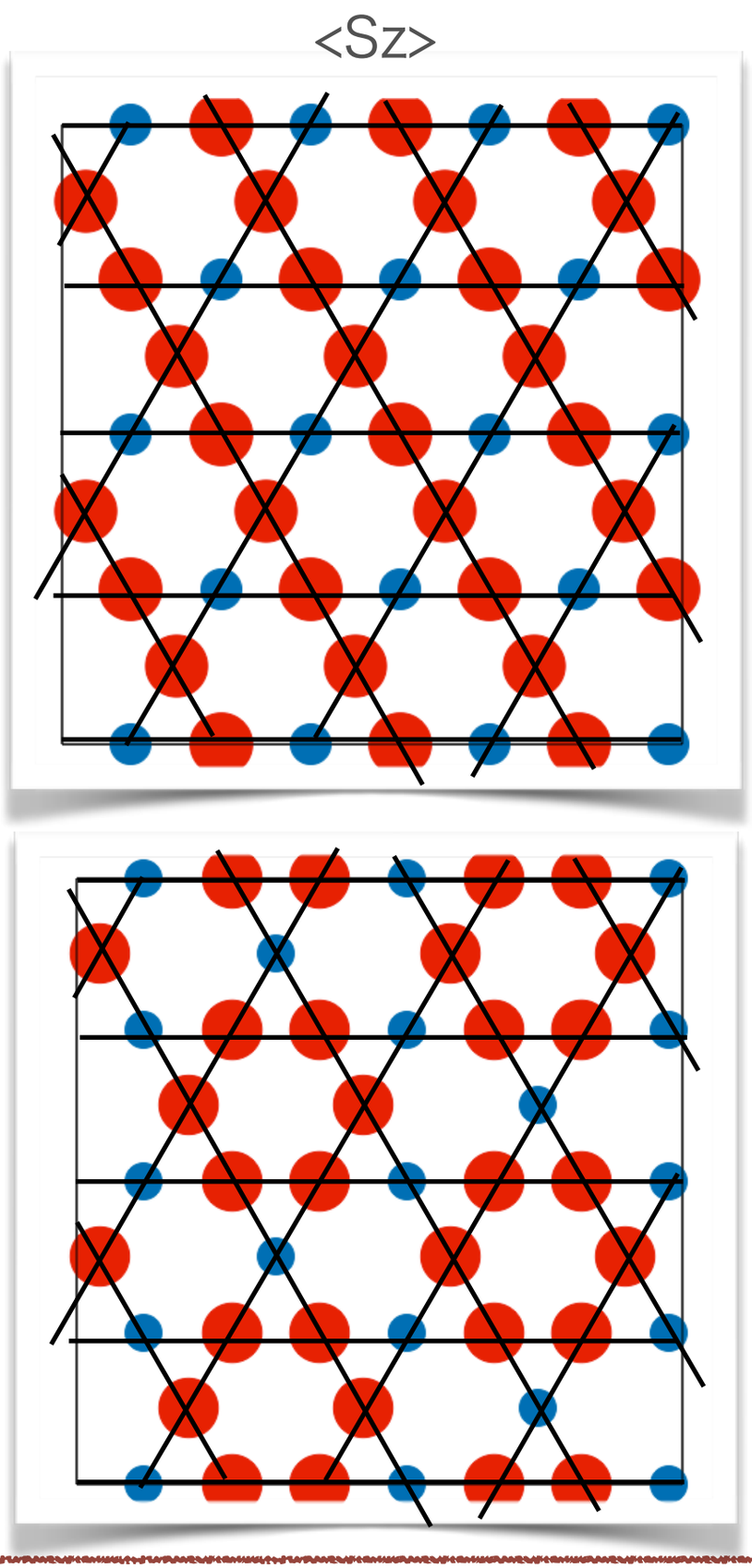
In DMRG, plaquette resonated state

Within D ≤ 7 and simple update,
It did not stabilized

More sophisticated optimization?



(S.Nishimoto, *et al,* (2013)

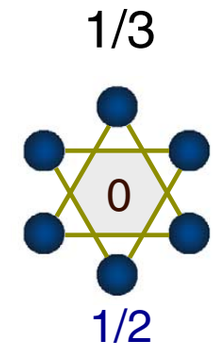


Hexagonal cluster update

Can we stabilize the resonated state observed in DMRG?

Correlation within a hexagon might be important.

Simple update: only two (or three) sites are updated simultaneously



Treat many-body correlations more accurately!

Hexagonal cluster update

Can we stabilize the resonated state observed in DMRG?

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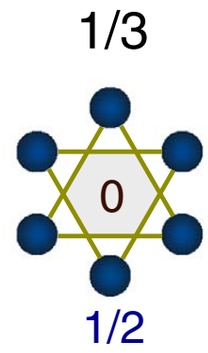
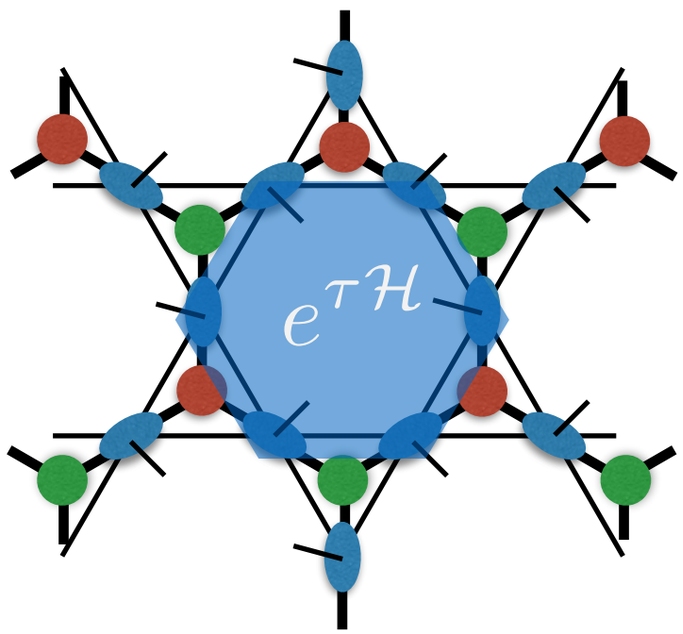
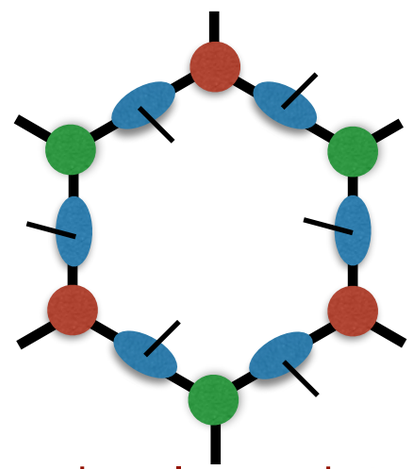


Treat many-body correlations more accurately!

Imaginary time evolution for a hexagon



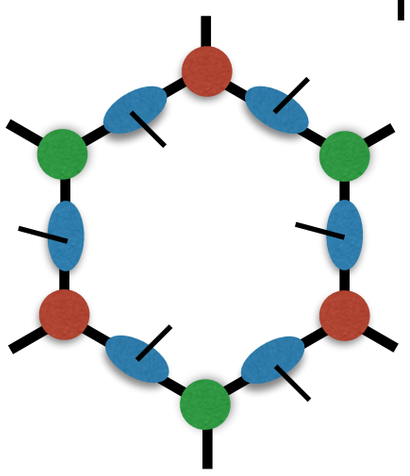
Update 12 tensors simultaneously

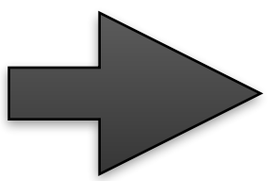


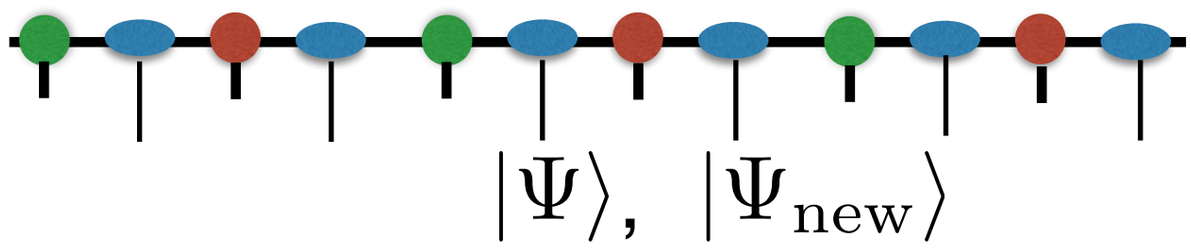
* Higher cost than the simple update,
* Lower cost than the environment calculation

Hexagonal cluster update：Basic idea

1 dimensional “MPS” with PBC.

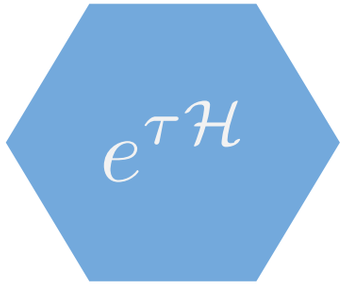


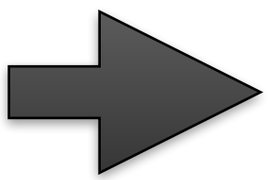


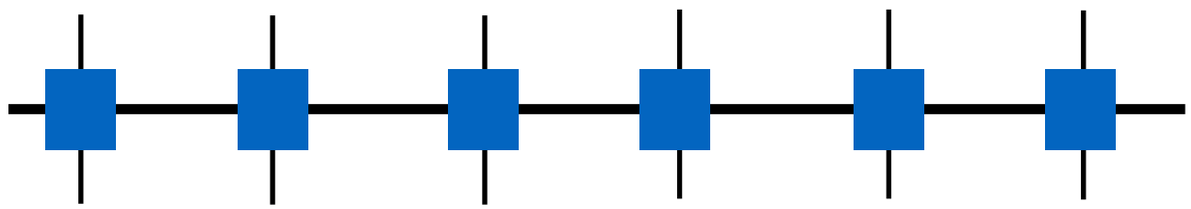


$|\Psi\rangle,\quad |\Psi_{\mathrm{new}}\rangle$

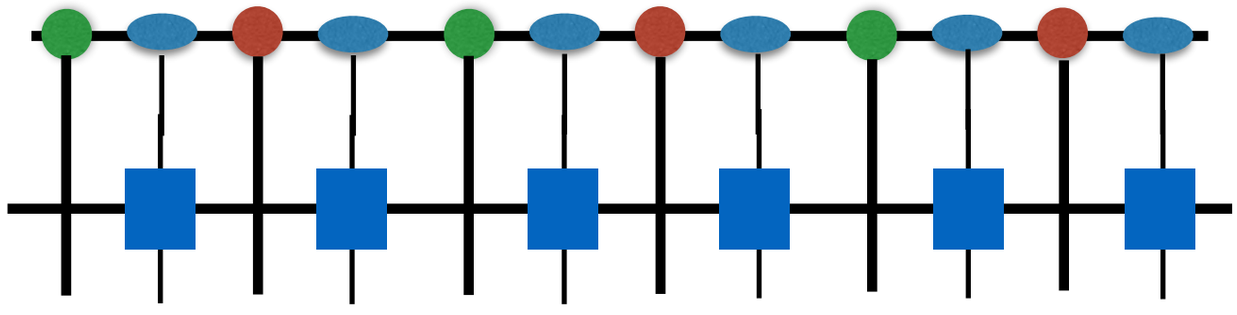
MPO representation







$$|\tilde{\Psi}\rangle = e^{\tau\mathcal{H}}|\Psi\rangle$$



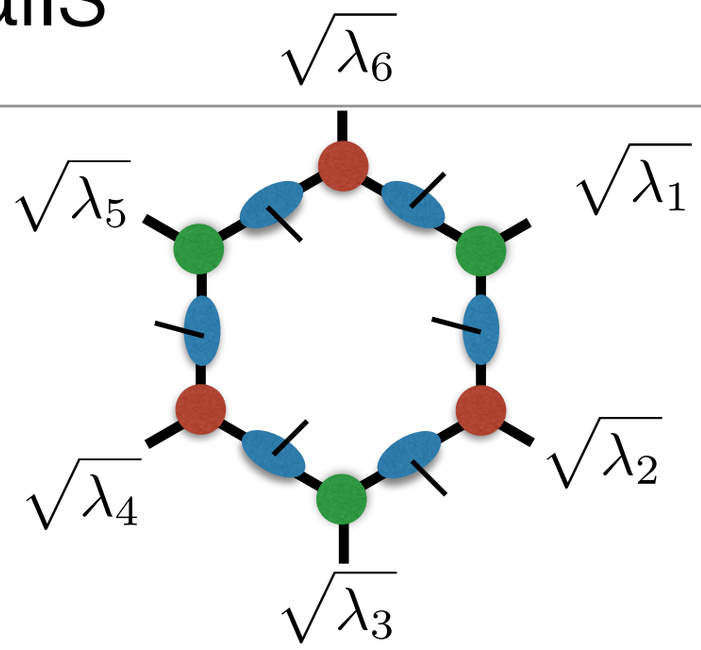
Minimize:

$$\||\tilde{\Psi}\rangle - |\Psi_{\mathrm{new}}\rangle\|^2$$

$|\Psi_{\mathrm{new}}\rangle$: MPS

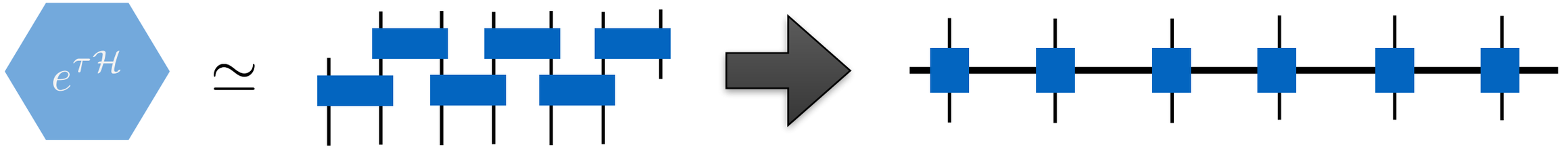
Hexagonal cluster update: Details

1. Insert λ into outside virtual bonds

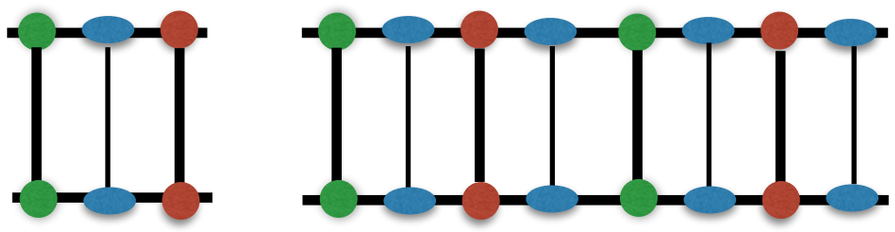


λ is important to obtain better energies

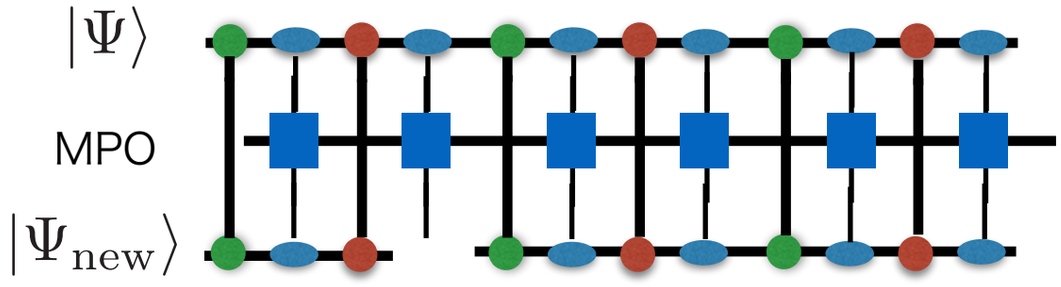
2. $e^{\tau H}$ is approximated by Suzuki-Trotter Decomposition



3. Minimization is performed iteratively $\left\| |\tilde{\Psi}\rangle - |\Psi_{\text{new}}\rangle \right\|^2$



N



$\vec{W}$

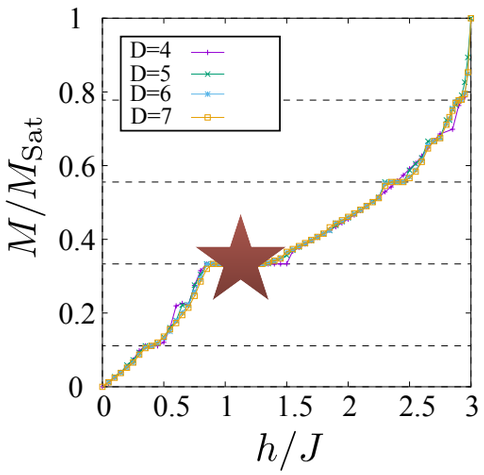
Solve linear equation: N = $\vec{W}$

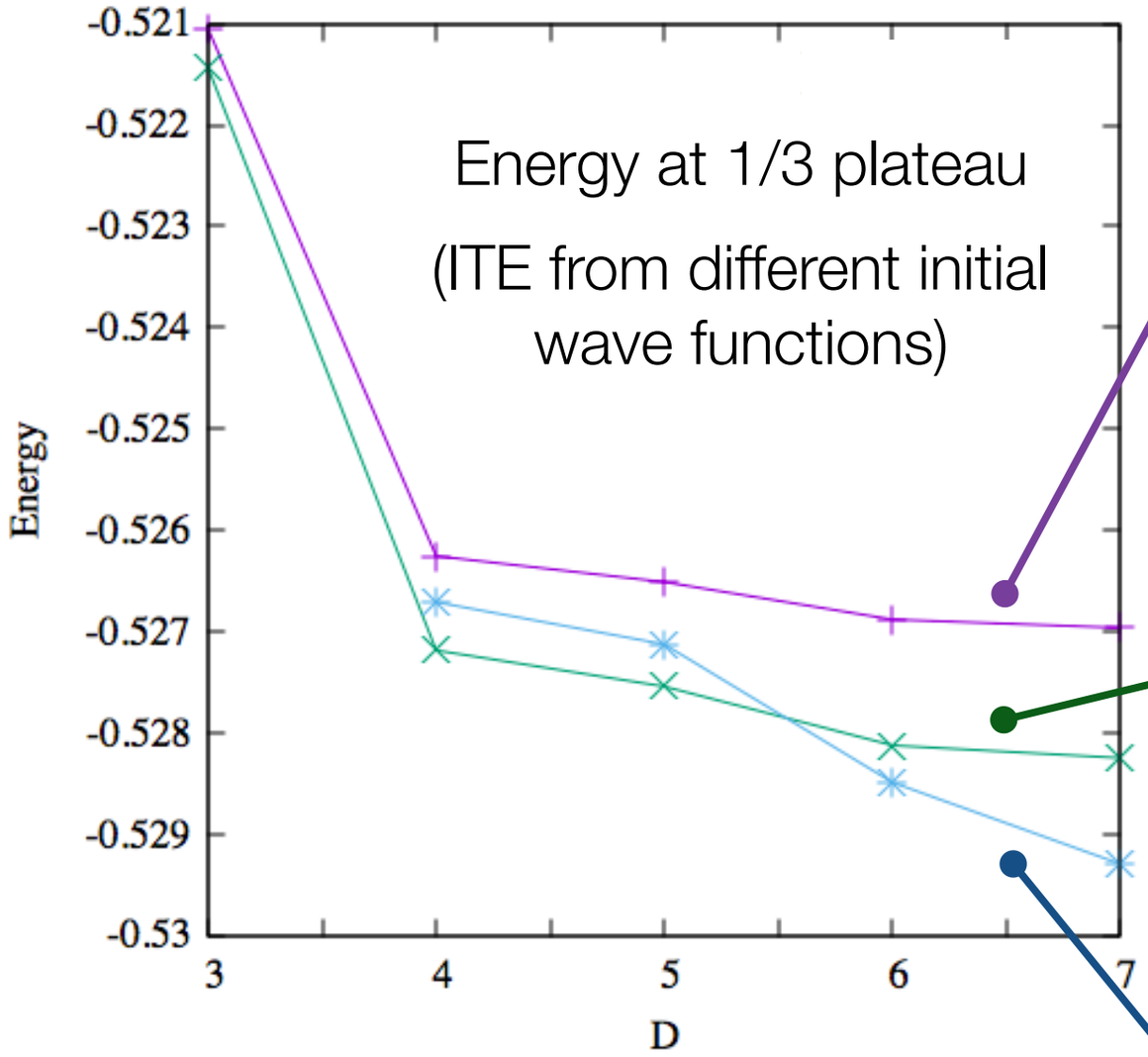
* Cost= O(D^6)

Result of hexagonal cluster update

(R. Okuma, D. Nakamura, T. Okubo, et al, Nat. Commun. **10,** 1229 (2019))

Hz = 1.1

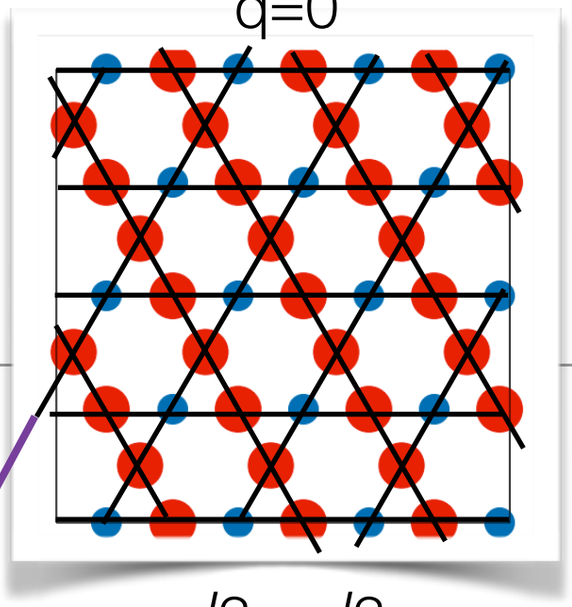




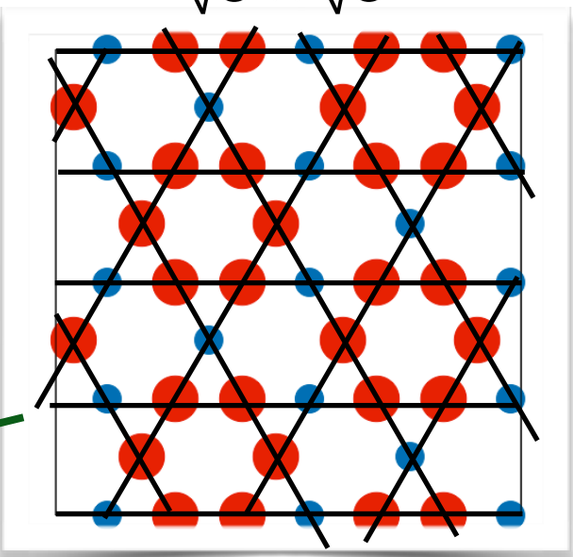
Energy at 1/3 plateau

(ITE from different initial wave functions)

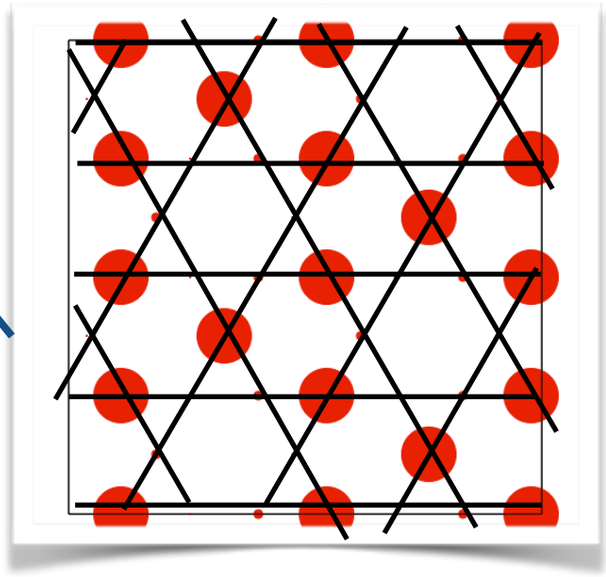
q=0



$\sqrt{3} \times \sqrt{3}$



Resonated

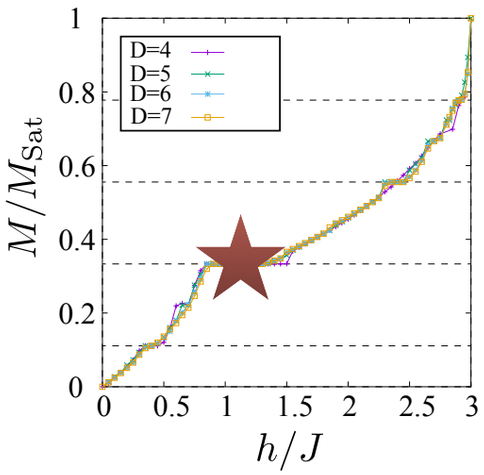


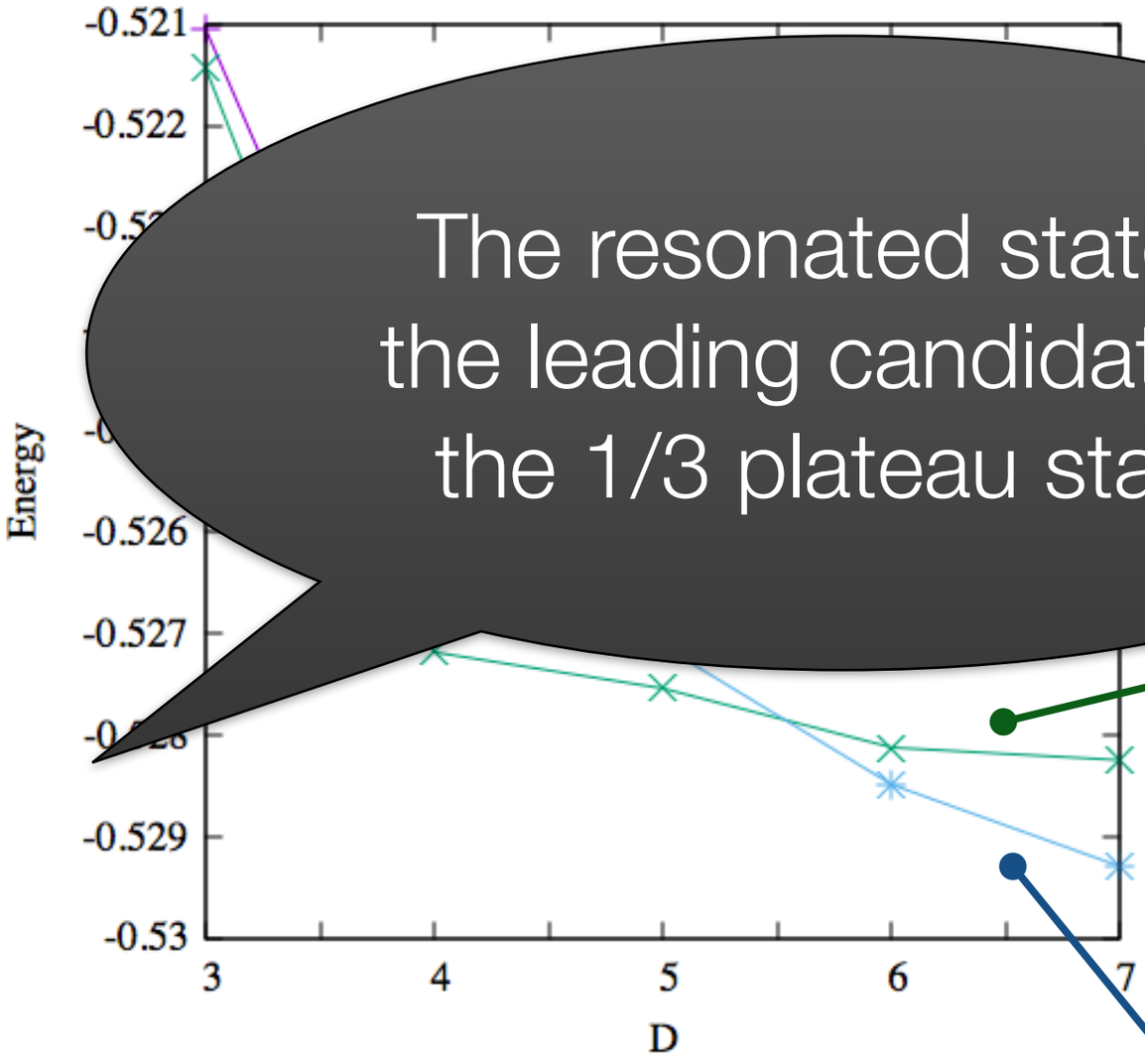
- By using the hexagonal cluster update, the resonated state is stabilized for D >= 4.
- Its energy becomes lower than up-up-down states, when we increase D.

Result of hexagonal cluster update

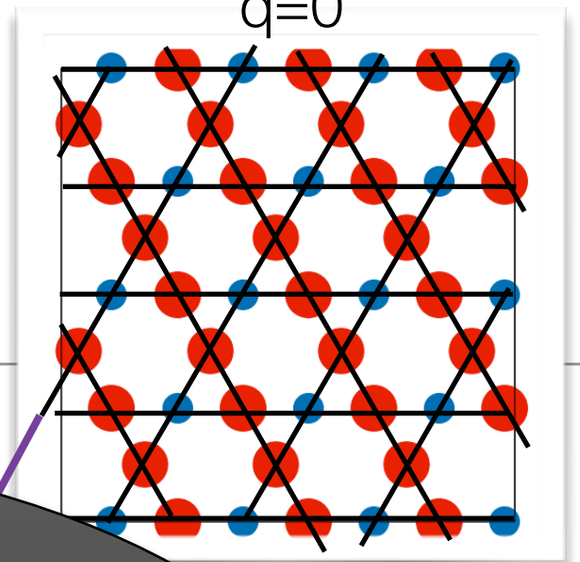
(R. Okuma, D. Nakamura, T. Okubo, et al, Nat. Commun. **10,** 1229 (2019))

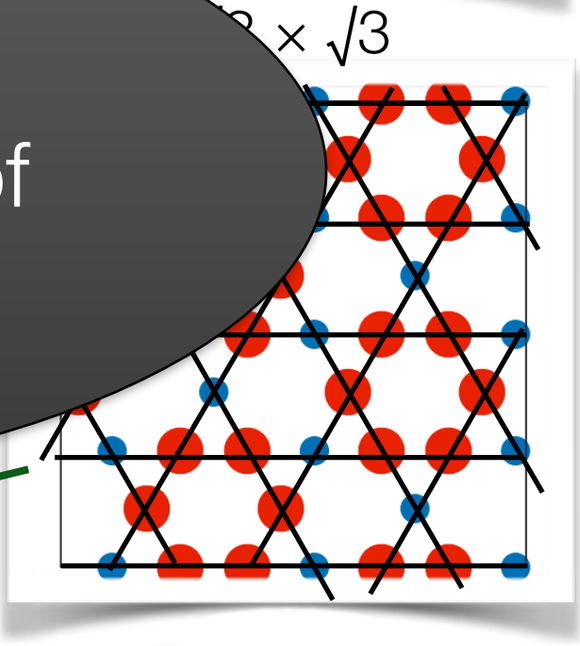
Hz = 1.1



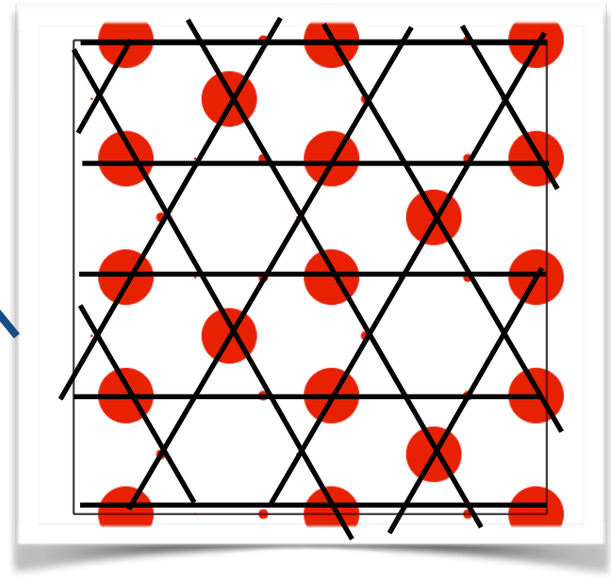


The resonated state is the leading candidate of the 1/3 plateau state!





Resonated



- By using the hexagonal cluster update, the resonated state is stabilized for D >= 4.
- Its energy becomes lower than up-up-down states, when we increase D.

Importance of variational optimization

Problems in imaginary time evolution

- States obtained by ITE tend to biased by the initial states.
  - It is not easy to obtain 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 increases along ITE.
  - It might be troublesome to pick up the lowest energy state.

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. arXiv:1903:09650)

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

Advantage:

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

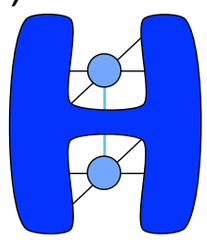
Variational optimization by using CTMRG

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

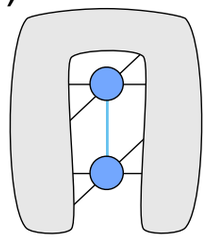
"Minimize Energy"

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

(a)

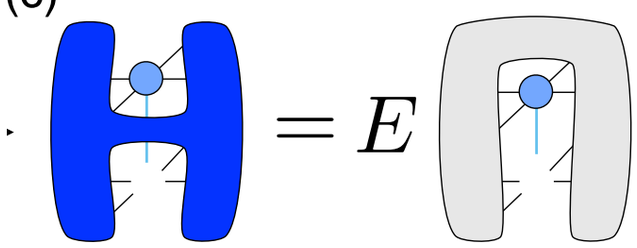
$\vec{A}^\dagger \mathbf{H} \vec{A} =$ 

(b)

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

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

(c)

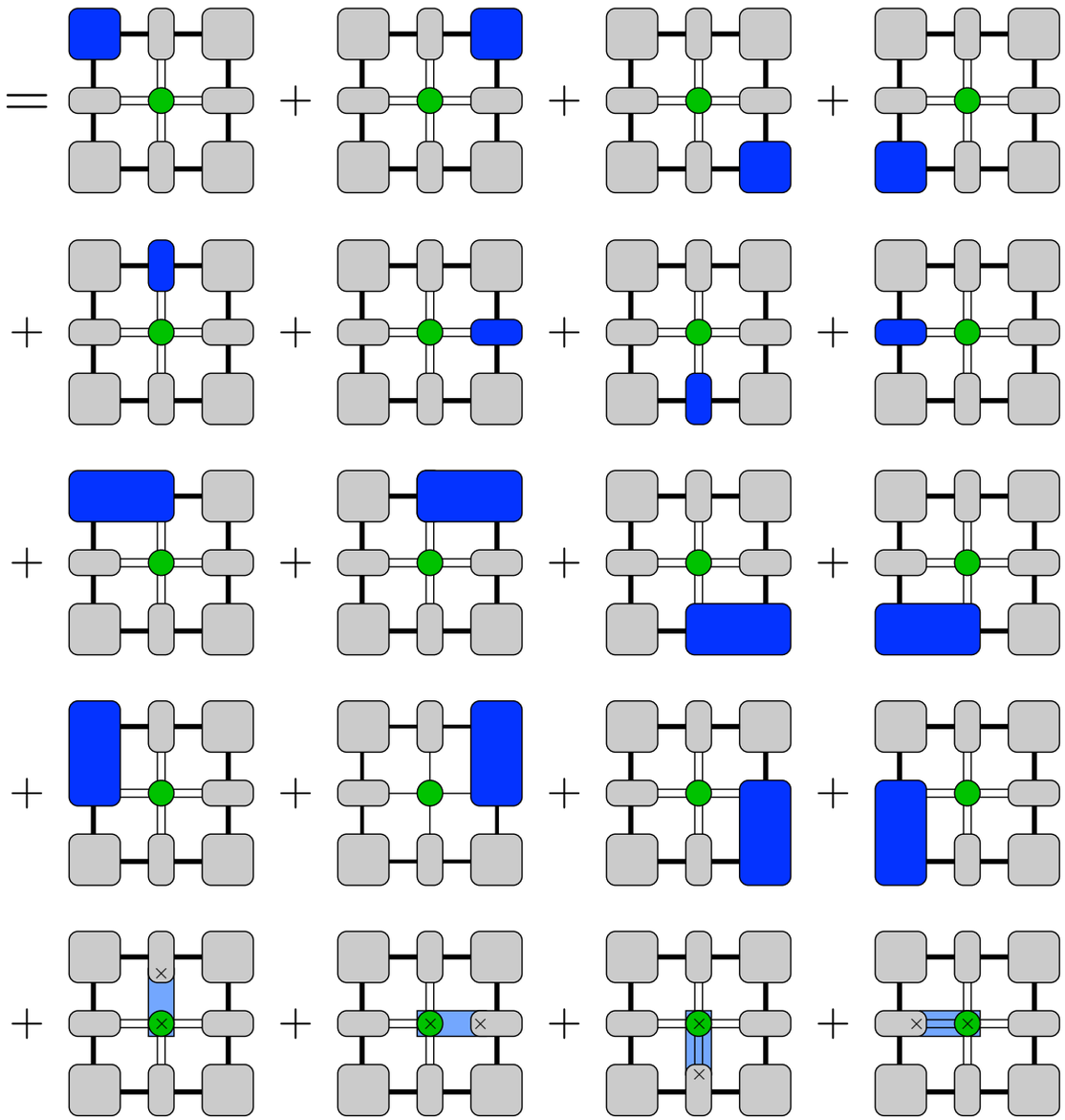


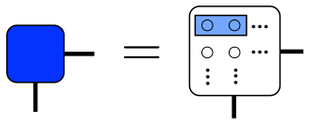
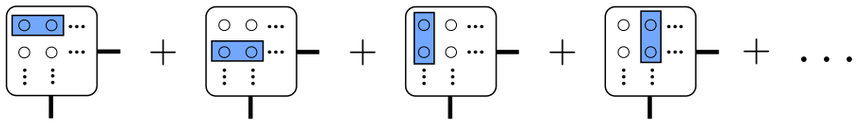
How to obtain H matrix in CTM

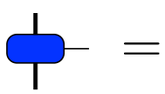
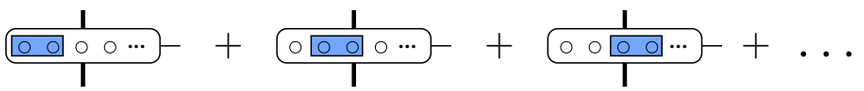
(P. Corboz, Phys. Rev. B **94**, 035133 (2016))

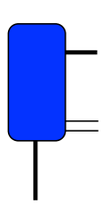
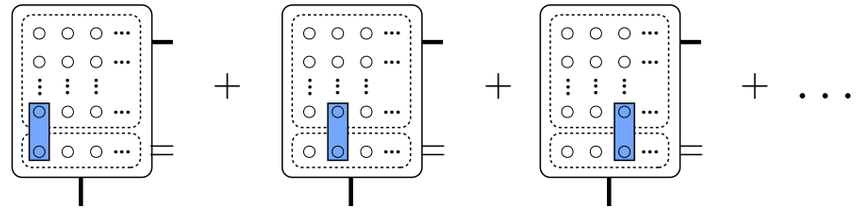
Systematic summation of Hamiltonian terms

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



$$\tilde{C}_1 =$$  $$= \quad + \quad + \quad + \quad + \ldots$$ 

$$\tilde{T}_4 =$$  $$= \quad + \quad + \quad + \ldots$$ 

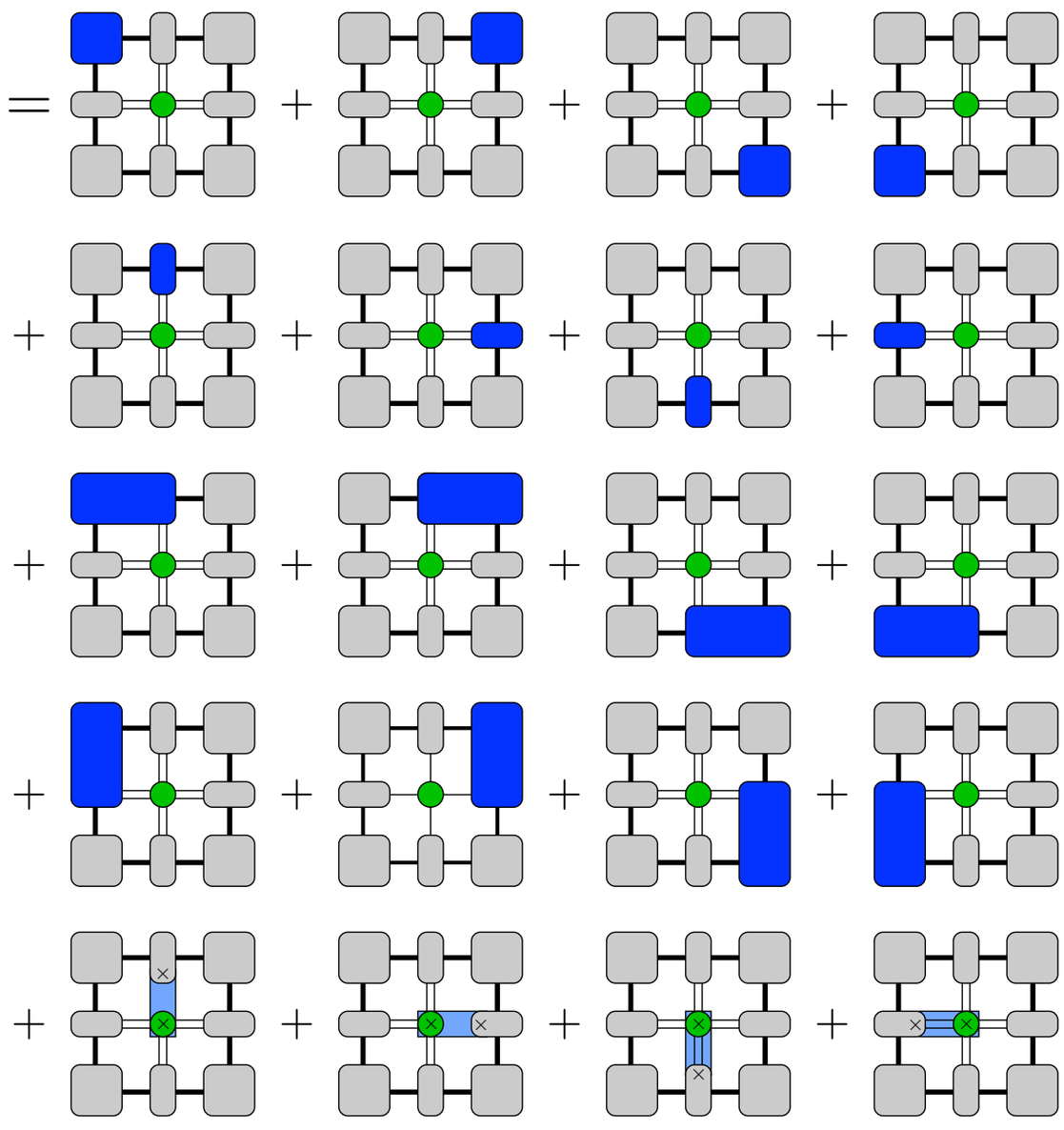
$$\tilde{C}_{v1} =$$  $$= \quad + \quad + \quad + \ldots$$ 

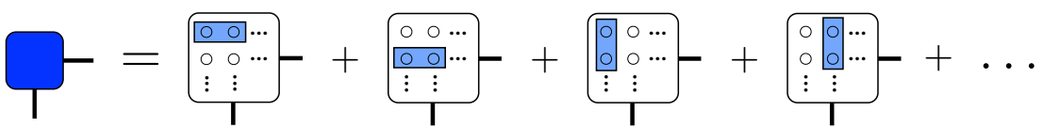
How to obtain H matrix in CTM

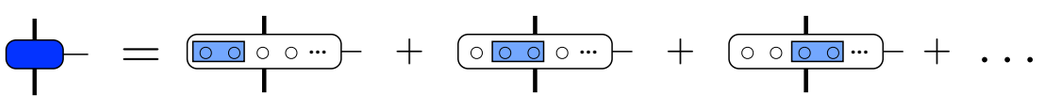
(P. Corboz, Phys. Rev. B **94**, 035133 (2016))

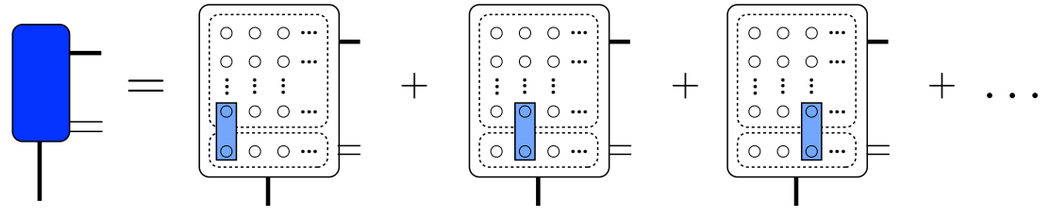
Systematic summation of Hamiltonian terms

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

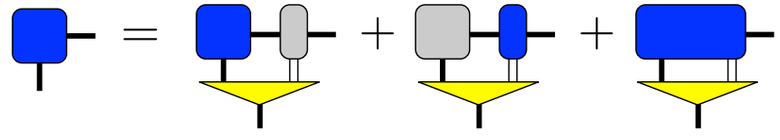


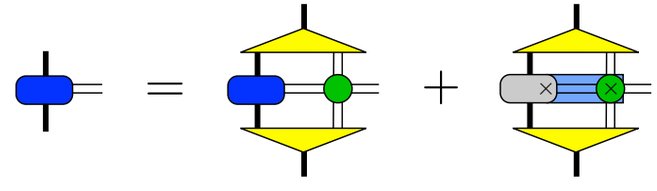
$\tilde{C}_1 =$ 

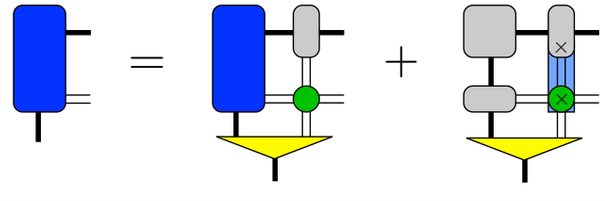
$\tilde{T}_4 =$ 

$\tilde{C}_{v1} =$ 

* Update is similar to standard CMT

$\tilde{C}'_1 =$ 

$\tilde{T}'_4 =$ 

$\tilde{C}'_{h1} =$ 

Applications: S=1/2 Heisenberg model

Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} S_i \cdot S_j$$

GS energy (from QMC):

$$E = -0.6694421(4)$$

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

Spontaneous magnetization

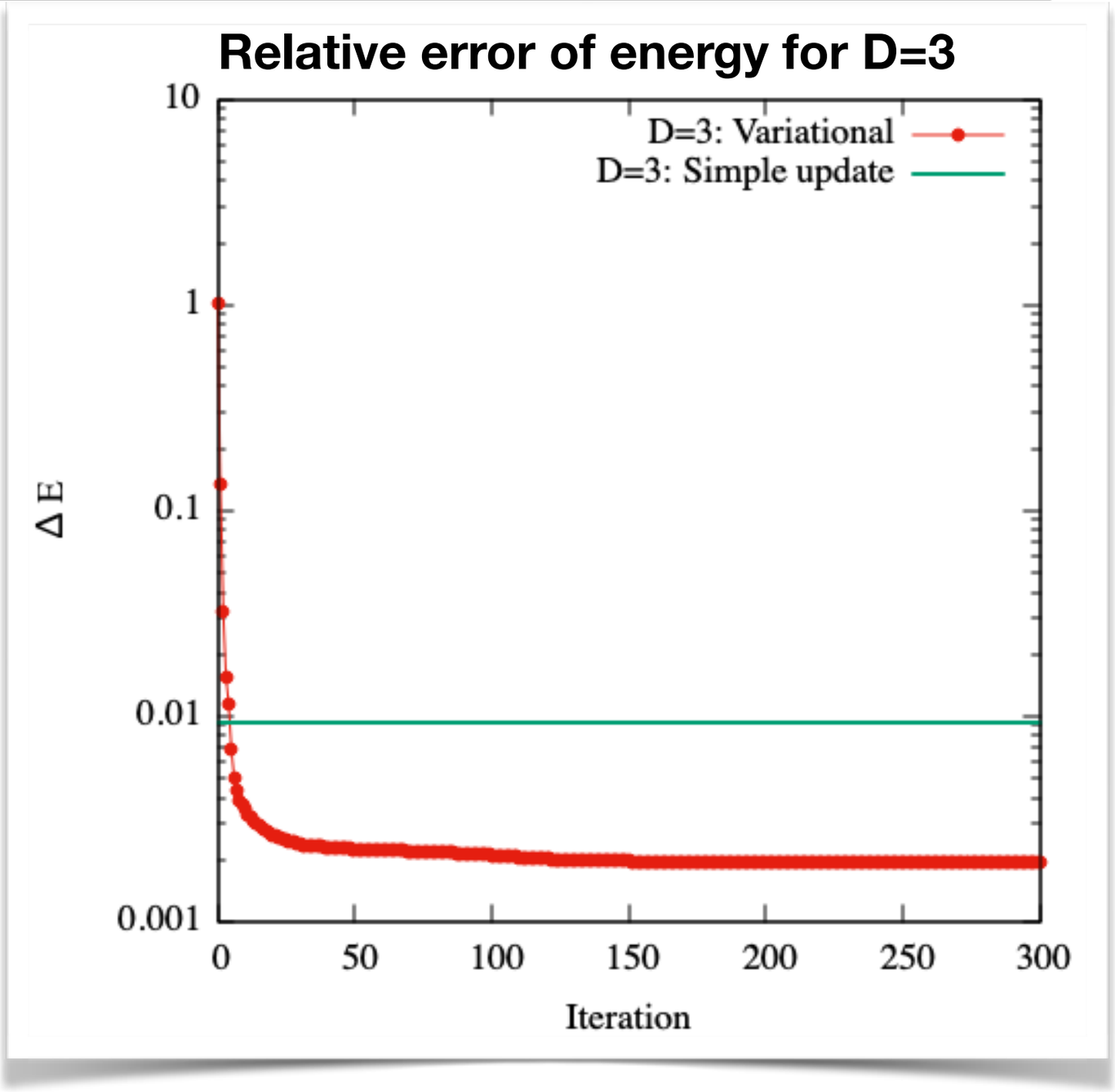
$$m_s = 0.3074$$

For D=3 iTPS

$m_s = 0.3769$ (Simple update)

$m_s \simeq 0.35$ (Full update from P. Corboz, Phys. Rev. B **94**, 035133 (2016))

$m_s = 0.3393$ (Variational)



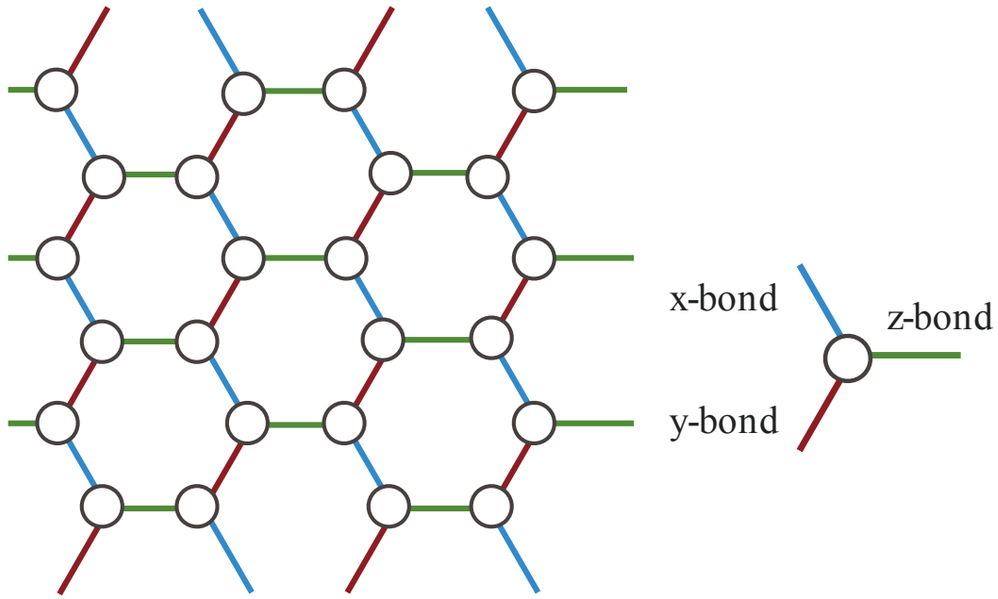
Application: Honeycomb lattice Kitaev Model

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

$$\mathcal{H} = -\sum_{\gamma,\langle i,j\rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma \qquad \left(S = \frac{1}{2}\right)$$

γ:bond direction

Depending on the bond direction,
only specific spin components interact.

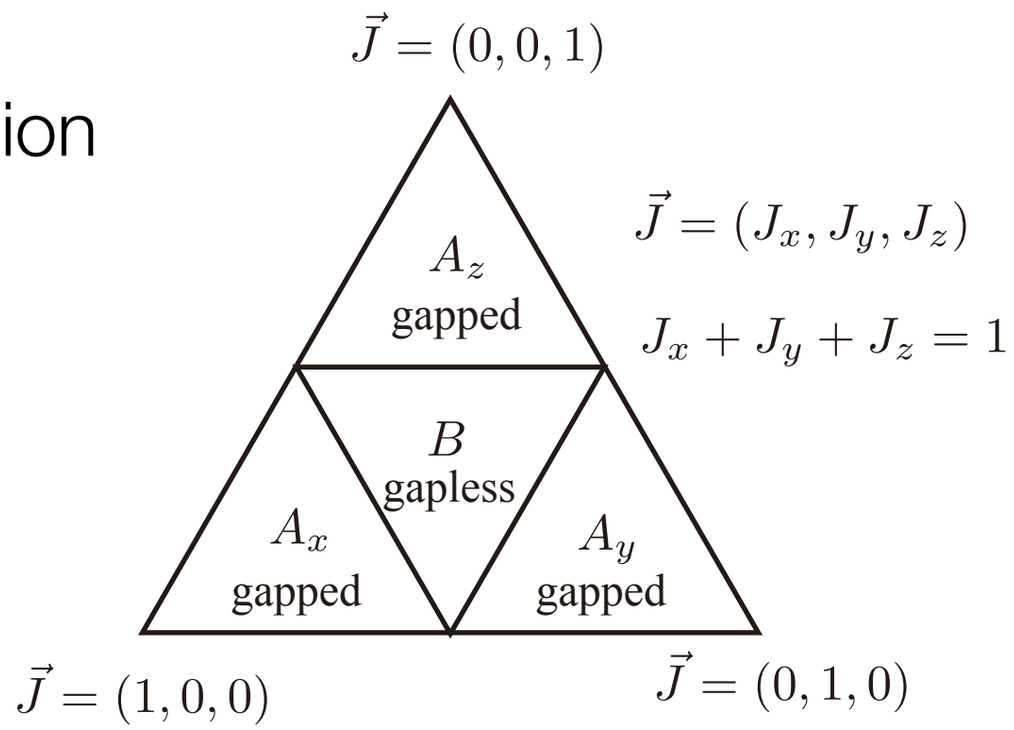


Exactly solvable by introducing Majorana fermion

Isotropic region (B) : gapless spin liquid

Anisotropic region (A) : gapped spin liquid

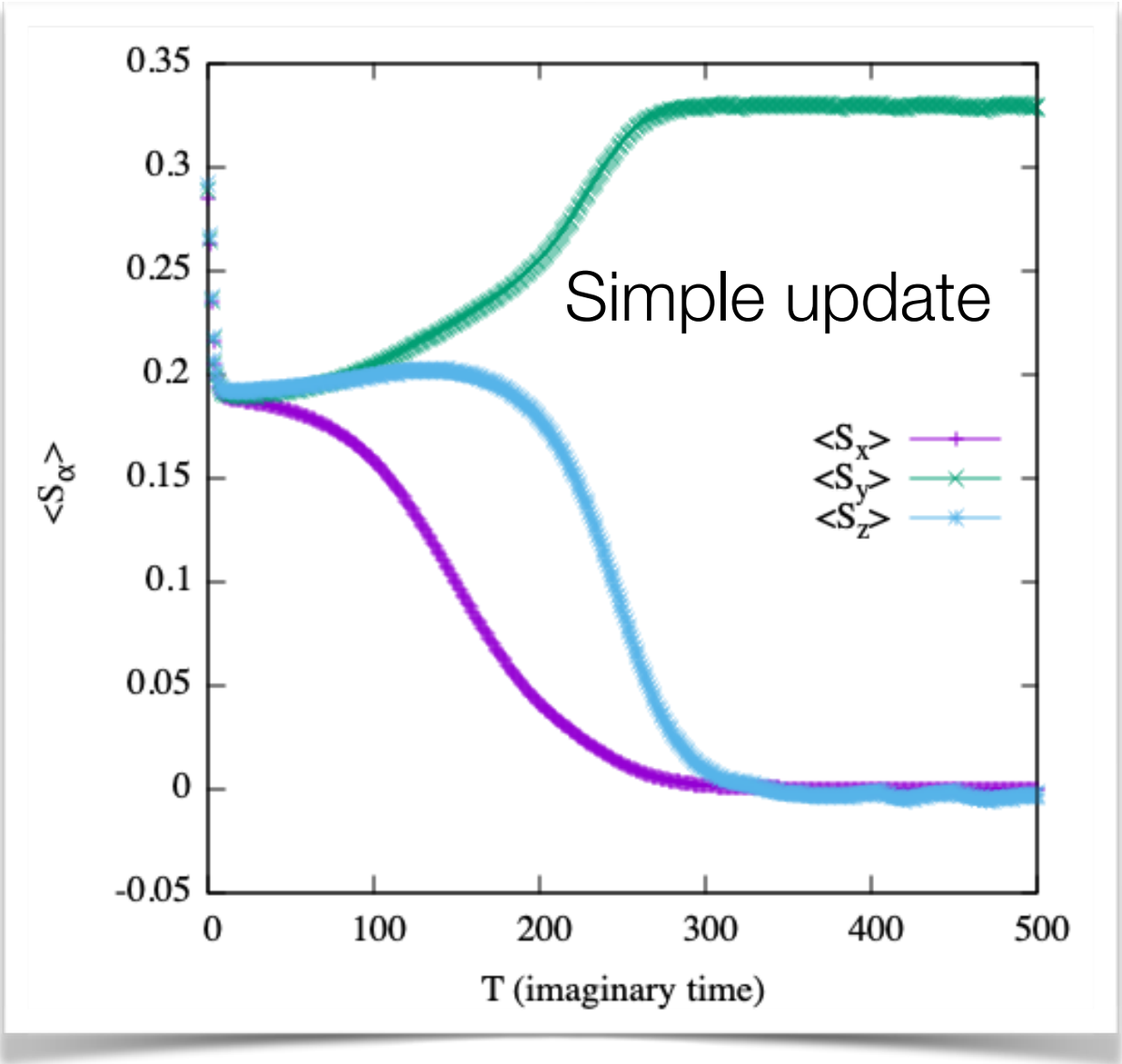
Phase diagram

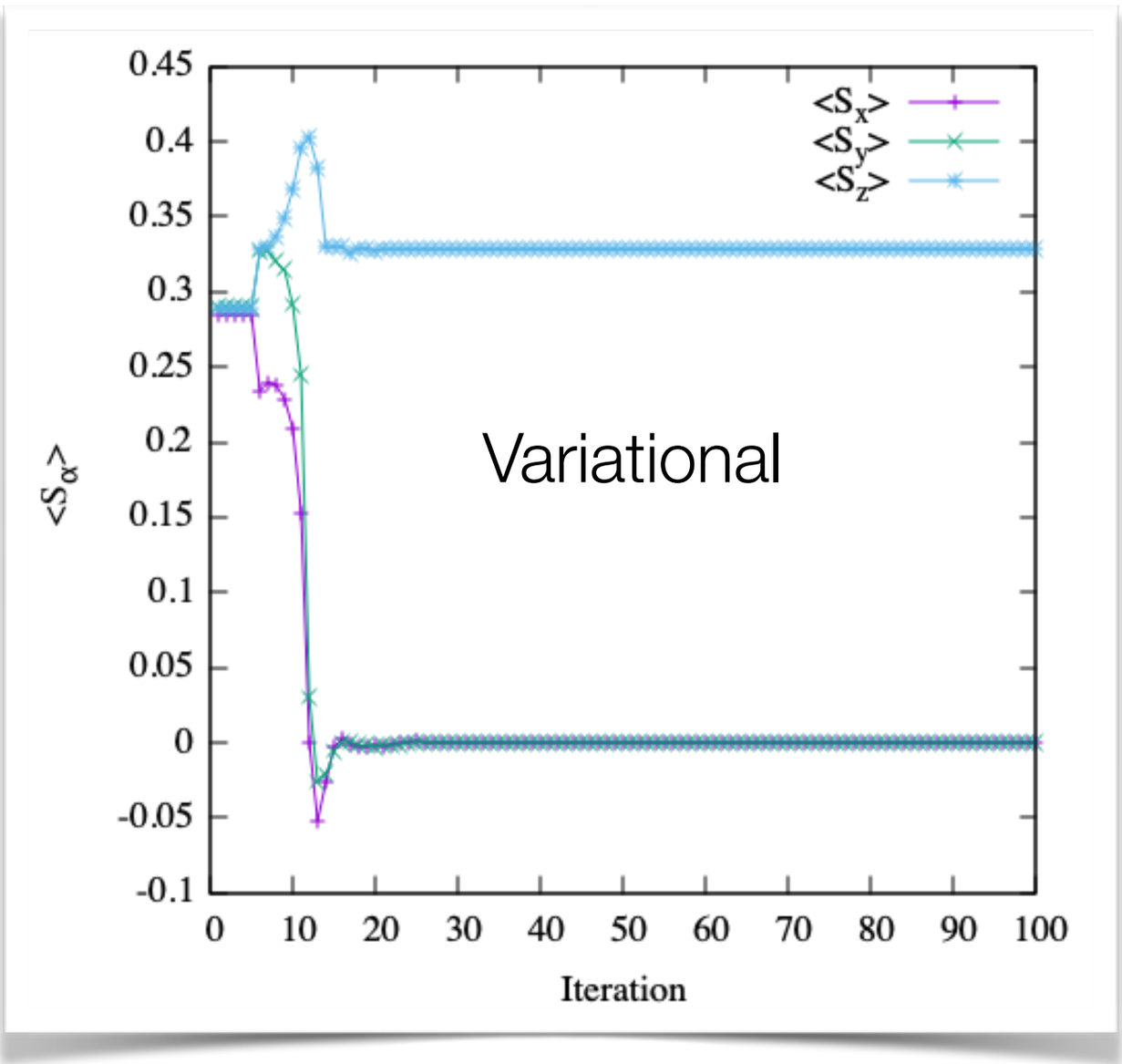


Applications: Kitaev model

At D=2: The lowest energy state is a ferromagnetic pointing (1,0,0) direction.
Starting from (1,1,1) FM state, it converges to (1,0,0) FM.

→ Variational optimization seems to have faster convergence.



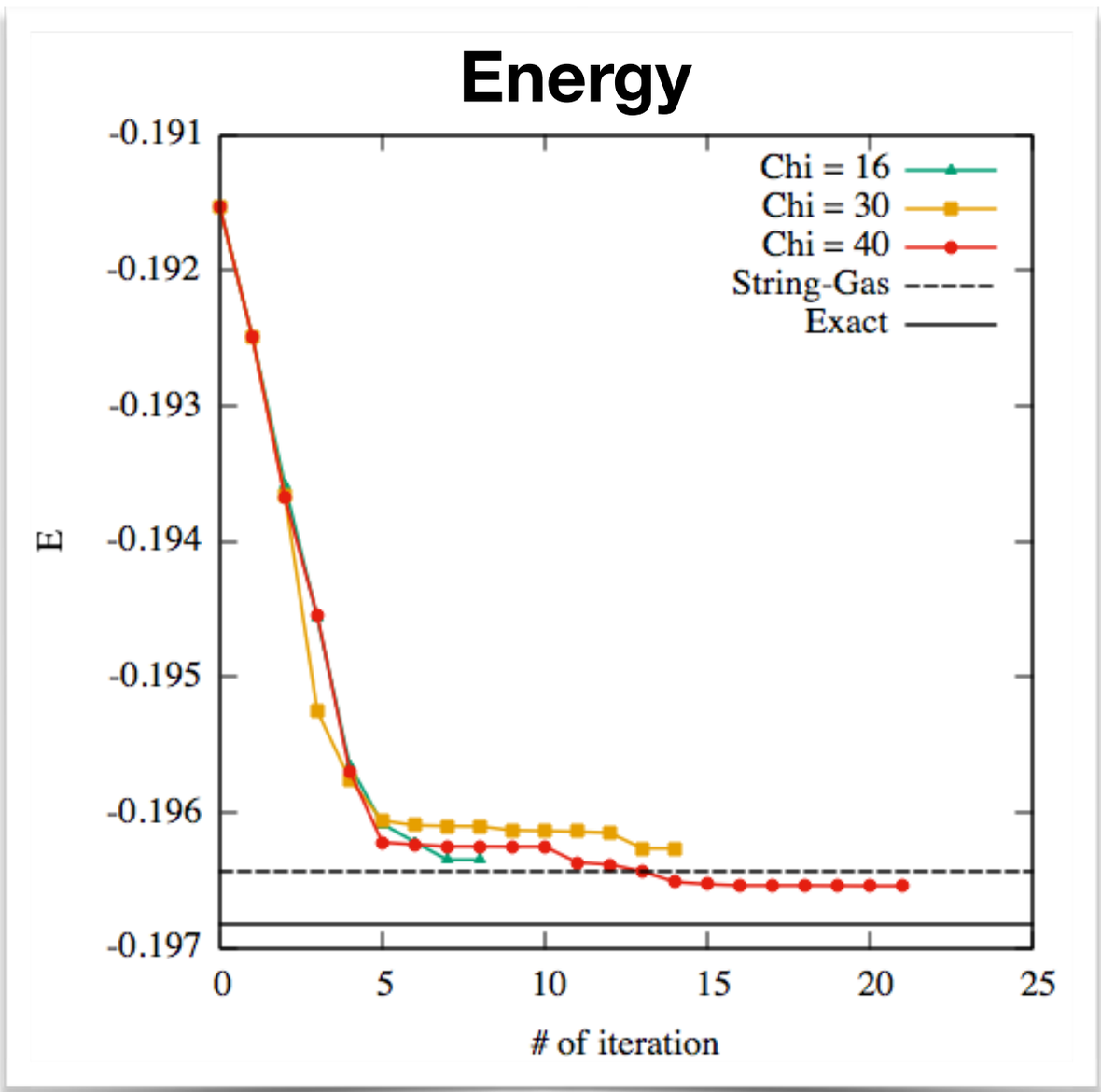


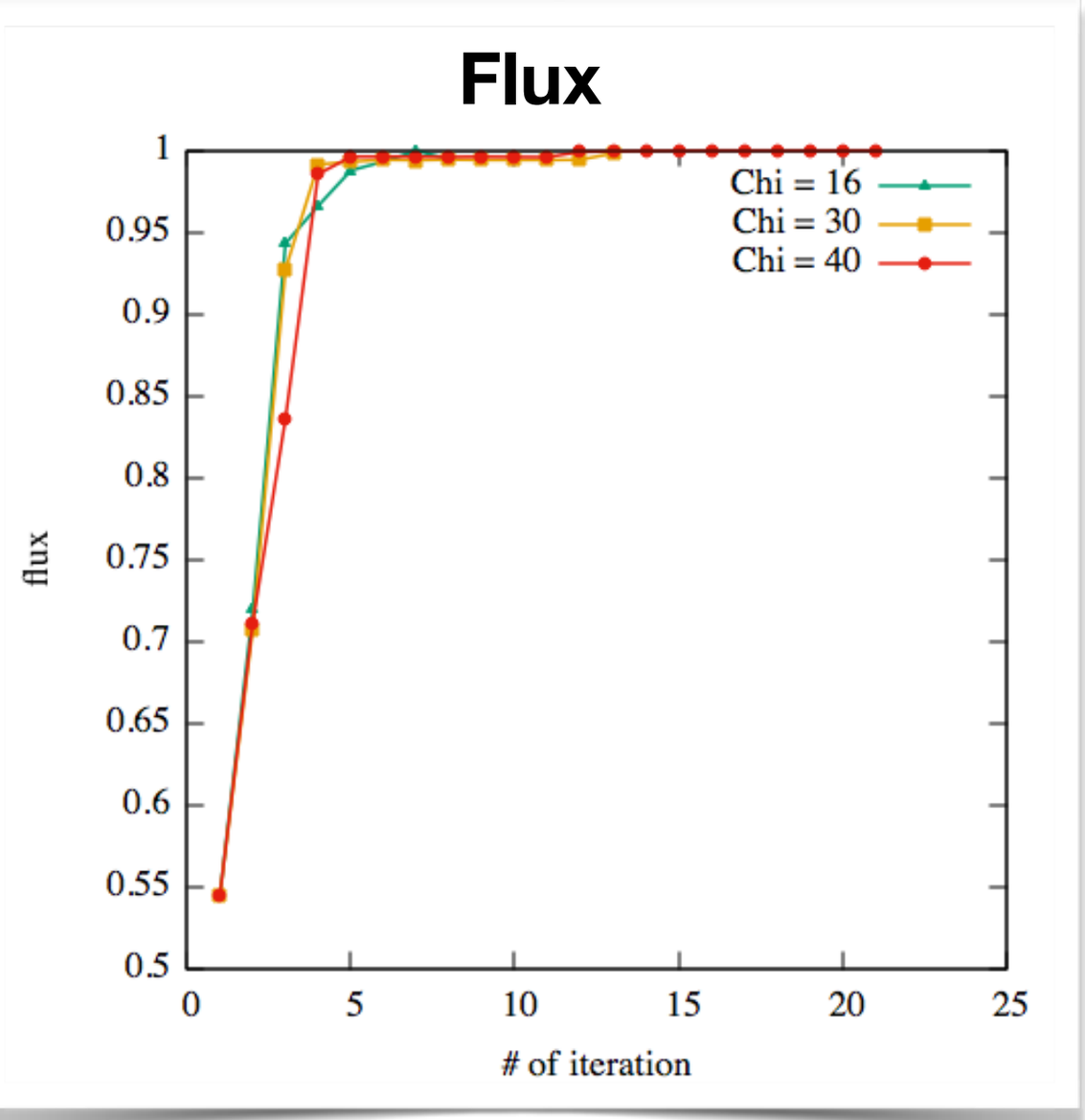
Applications: Kitaev model

Ref. H.-Y. Lee, R. Kaneko, T. Okubo and N. Kawashima, arXiv: 1901.05786

At D=3,4: For D=3, (1,1,1) FM seems to be the lowest energy state.

For D=4, starting from the final state of D=3,
we obtain very good Kitaev spin liquid state for after steps.





Summary

- By choosing proper tensor network structure, ground state wave functions can be approximated accurately.
  - To search good tensor networks, the area low of the entanglement entropy is important.
  - For one dimensional quantum system, matrix product states (MPS) works very well.
  - For two or higher dimensional systems, MPS breaks down. In these case, instead, tensor product states are good tensor networks.
- Owing to developments of algorithms and computers, tensor network methods become powerful method to investigate frustrated spin system in two dimensions.
  - iTPS can reproduce the Kitaev spin liquid accurately.
  - iTPS can be applicable to Kagome Heisenberg model.
- 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.