

計算科学における情報圧縮

Information Compression in Computational Science

2018.12.27

#12: テンソルネットワーク表現への発展

Tensor network representation

理学系研究科 物理学専攻 大久保 毅

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Outline

- How to use sample codes
- Breakdown of MPS representation
 - Critical system
 - Higher dimensional system
- Tensor Network for critical systems
 - Multi-scale Entanglement Renormalization Ansatz (**MERA**)
- Tensor Network for higher dimensions
 - Tensor Product State (**TPS**)
- Report problems

How to use sample codes

Exercise: examples of Schmidt decomposition

1-1: Random wave function (Sample code: Ex1-1.py or Ex1-1.ipynb)

- Make a random vector
- SVD it and see singular value spectrum and EE

1-2: Ground state of **S=1** Heisenberg chain (Sample code: Ex1-2.py or Ex1-2.ipynb)

$$\mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

- Calculate GS by diagonalizing Hamiltonian
- SVD it and see singular value spectrum and EE

*Note: the ground state of this model is gapped

show help: `python Ex1-2.py -h`

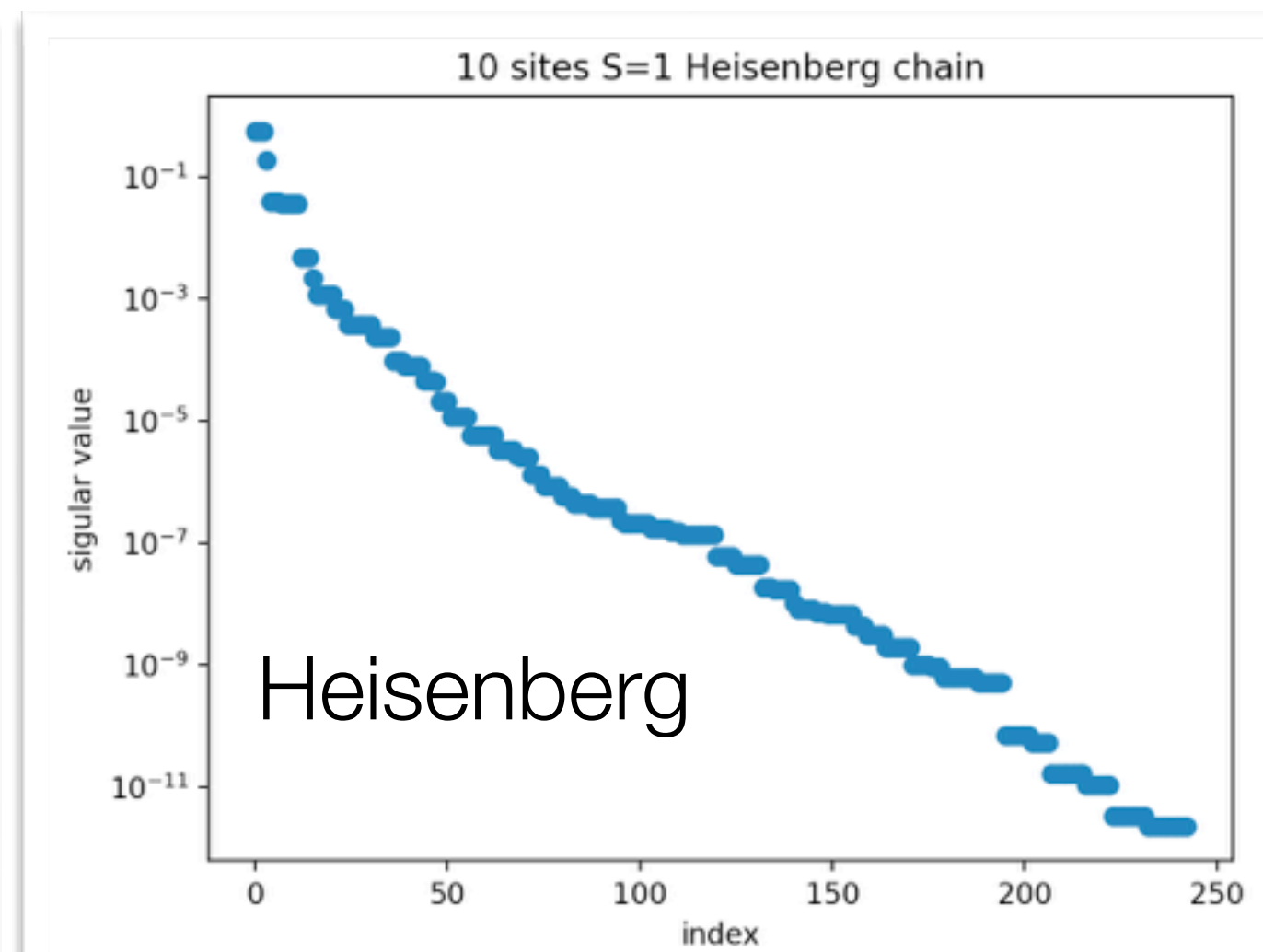
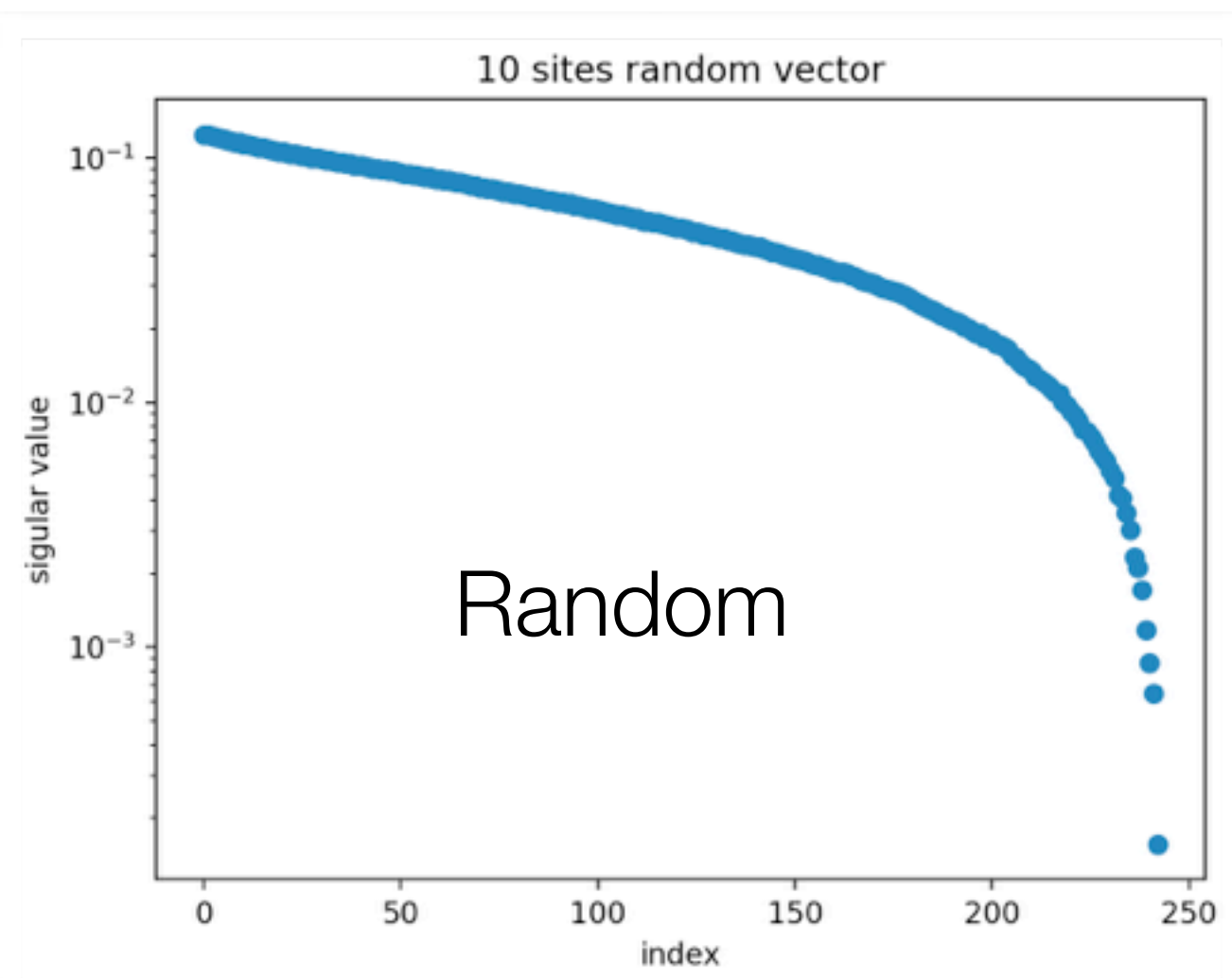
*** Try to simulate different system size "N"**
*** You can simulate other S by changing "m"**

Result: N=10 spectrum

$$\vec{\Psi} \in \mathbb{C}^{3^{10}}$$

A

B



Ground state wave function has lower entanglement!

Exercise 2: Make MPS and approximate it

2-1: Make exact MPS from GS wave function obtained by ED

(We can easily check that the MPS obtained by successive SVD satisfy the canonical condition.)

Sample code: Ex2-1.py or Ex2-1.ipynb

show help: *python Ex2-1.py -h*

2-2: Approximate the MPS by truncating singular values

- Calculate approximate GS energy and compare it with ED
- *Change χ_{max} and see energies*

Sample code: Ex2-2.py or Ex2-1.ipynb

show help: *python Ex2-2.py -h*

Exercise 3: (TEBD and) iTEBD simulation (ITE)

3-1: TEBD simulation

Simulate small finite size system and compare energy with ED

Sample code: Ex3-1.py or Ex3-1.ipynb

show help: *python Ex3-1.py -h*

3-2: iTEBD simulation

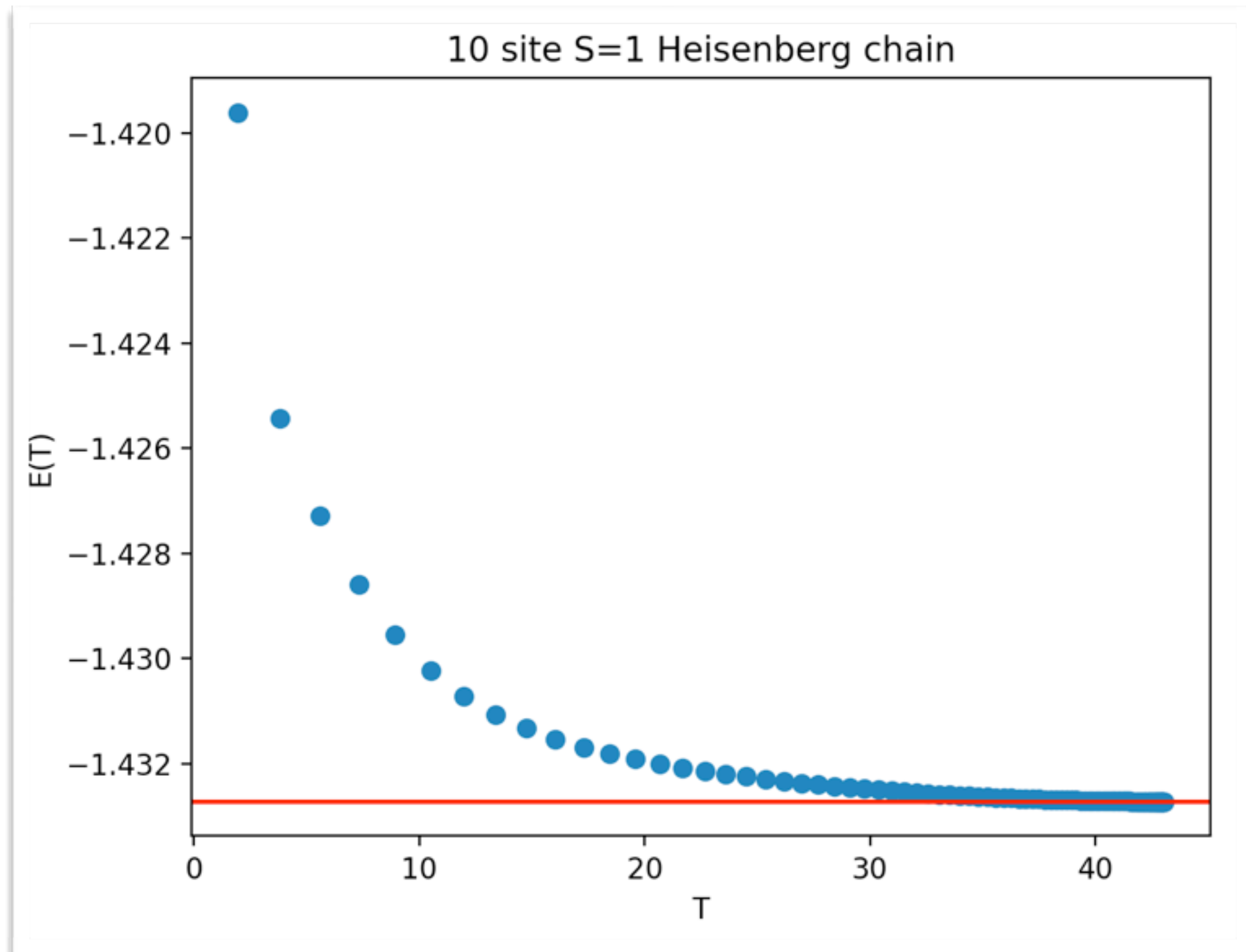
Simulate infinite system and calculate energy

Sample code: Ex3-2.py or Ex3-2.ipynb

show help: *python Ex3-2.py -h*

*** Try simulation with different "chi_max", "T_step"**

3-1: Energy dynamics in TEBD



Requirement for running sample scripts

File: Exercise_No10.zip

Python environment: `python2.7` or `python3`

Modules: `numpy`, `scipy` and `matplotlib`

Usage:

For jupyter notebook, type

`jupyter notebook`

and select `Ex?-?.ipynb` .

For python (command line), type

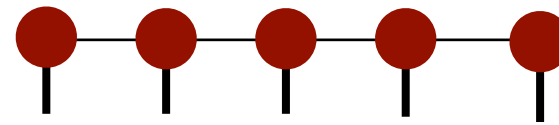
`python Ex?-?.py -h`

, then you can know how to change the parameters.

Breakdown of MPS representation

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 a^N



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

Phase transition

Transverse field Ising chain:

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

Ground state $|\Psi\rangle$

$h = 0$: Ferromagnetic state

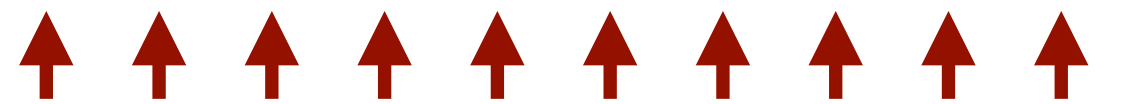
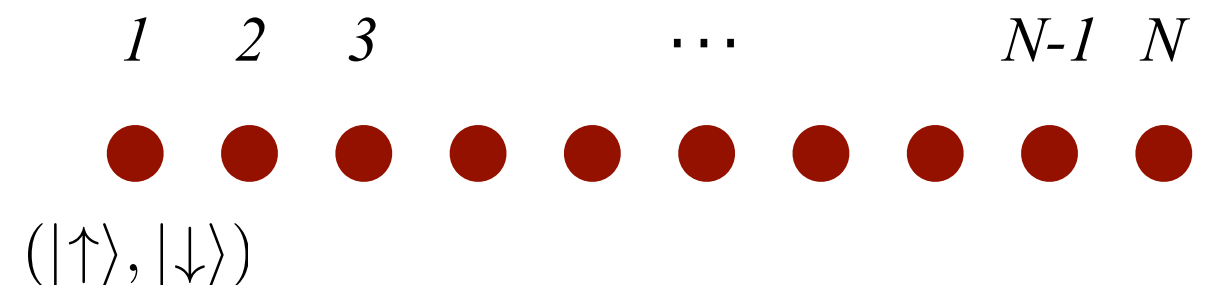
$h \rightarrow \infty$: Disordered state
(Field induced ferro)

In between these two limits,
there is a phase transition.

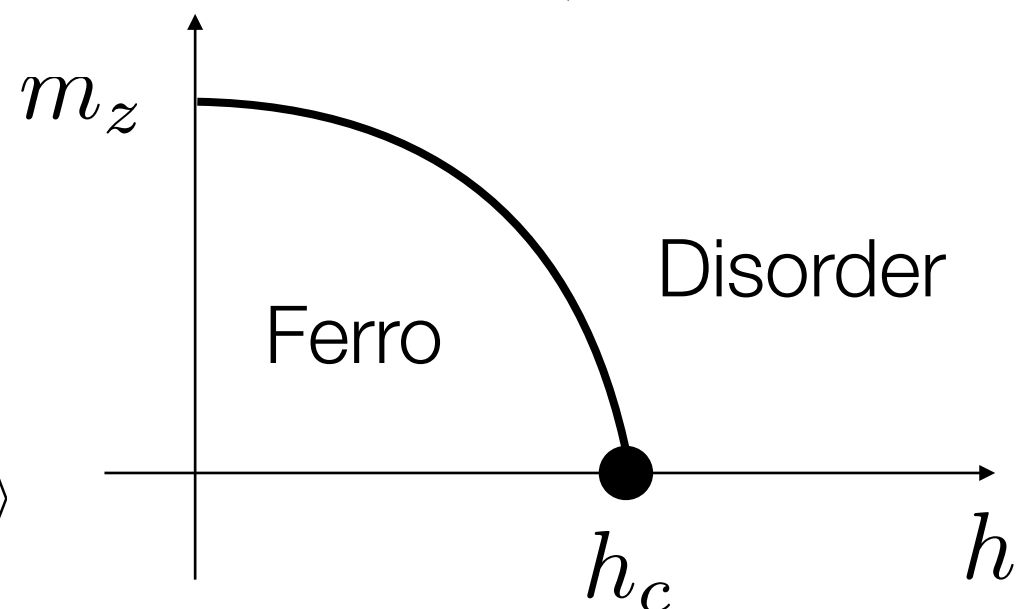
At the phase transition,
order parameter becomes zero.
(秩序変数)

(Spontaneous)
Magnetization
(自発磁化)

$$m_z = \frac{1}{N} \sum_i \langle \Psi | S_i^z | \Psi \rangle$$



$$\rightarrow = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle)$$



Critical point and correlation length

$h = h_c$: Critical point (臨界点)

Behavior of a correlation function:

$0 \leq h < h_c$: Ferromagnetic state

$$\langle \Psi | S_i^z S_{i+r}^z | \Psi \rangle \sim C e^{-\frac{r}{\xi}} + m_z^2$$

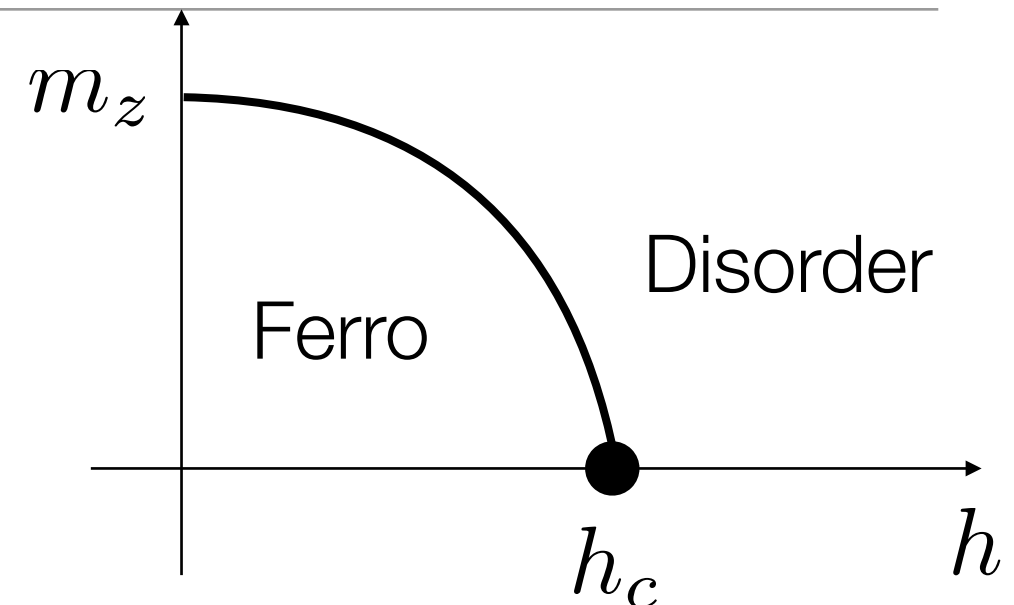
$h_c < h$: Disordered state

$$\langle \Psi | S_i^z S_{i+r}^z | \Psi \rangle \sim e^{-\frac{r}{\xi}}$$

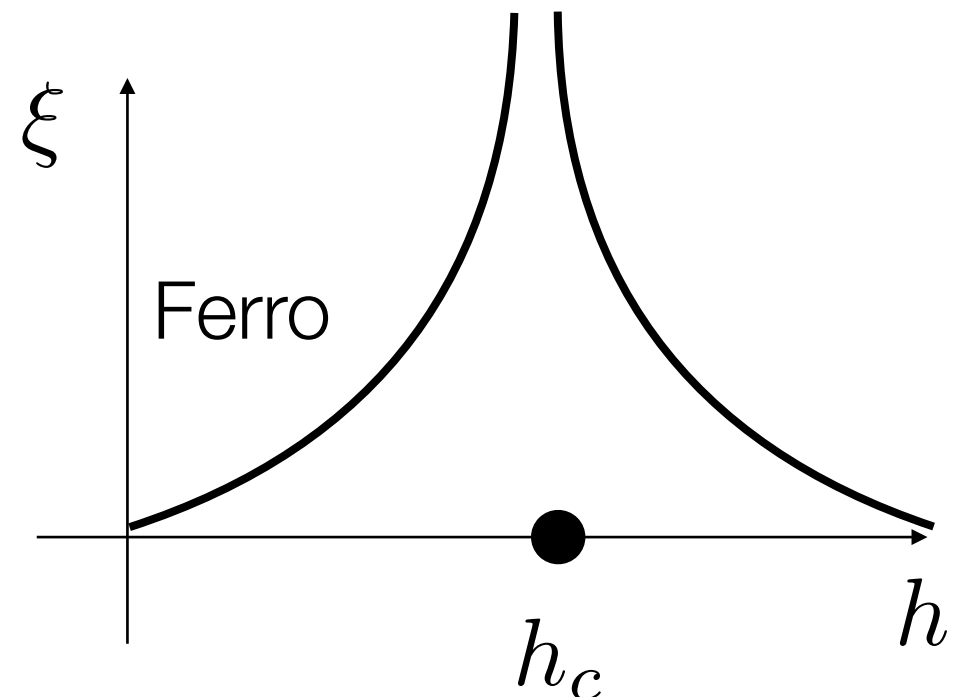
$h = h_c$: Critical point

$$\langle \Psi | S_i^z S_{i+r}^z | \Psi \rangle \sim r^{-2p}$$

Correlation length **diverges** at critical point!



$\xi = \xi(h)$: Correlation length (相関長)



Scale invariance at the critical point

$h = h_c$: Critical point (臨界点)

$$C(r) \equiv \langle \Psi | S_i^z S_{i+r}^z | \Psi \rangle \sim r^{-2p} \quad \text{Power law decay!}$$

After a scale transformation $r' = br$

$$\Rightarrow C(r') = C(br) = b^{-2p} C(r)$$

Change in the correlation function is only a constant factor.

\Rightarrow If we scale spins as $\tilde{S}_i^z = b^p S_i^z$
the correlation function becomes

$$\tilde{C}(r') \equiv \langle \Psi | \tilde{S}_i^z \tilde{S}_{i+r'}^z | \Psi \rangle = C(r)$$

This property is called as "scale invariance". (スケール不変性)

Physics (properties) in different scale is essentially same.

DMRG (variational MPS) calculation of TFI model

Ö. Legeze, and G. Fáth, Phys. Rev. B **53**, 14349 (1996)

Errors of the ground and the 1st excited states energies **varying system size N** .

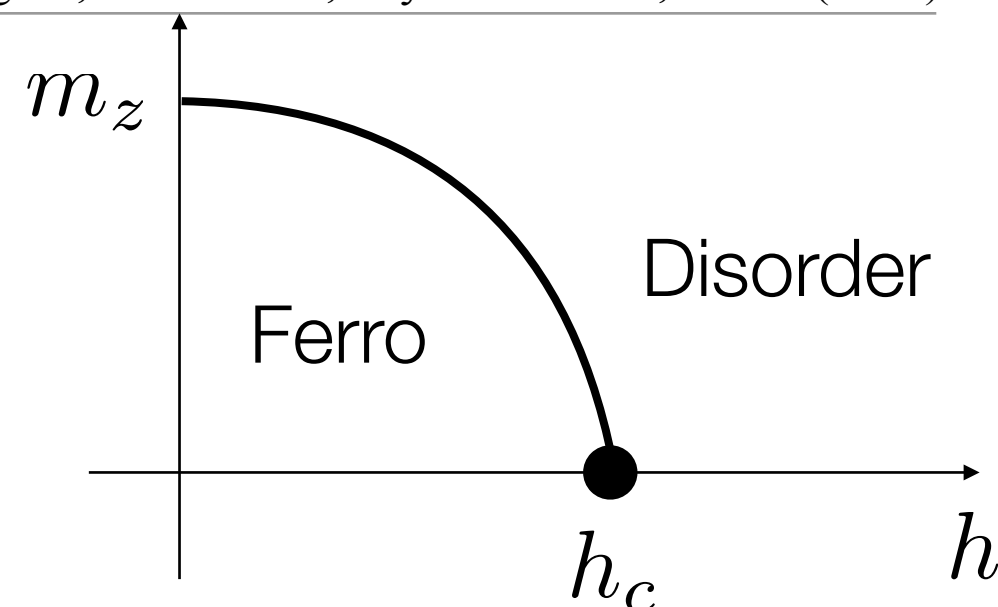
For a fixed dimension m ,

Ferro and disordered states:

The errors are **almost independent of N** .

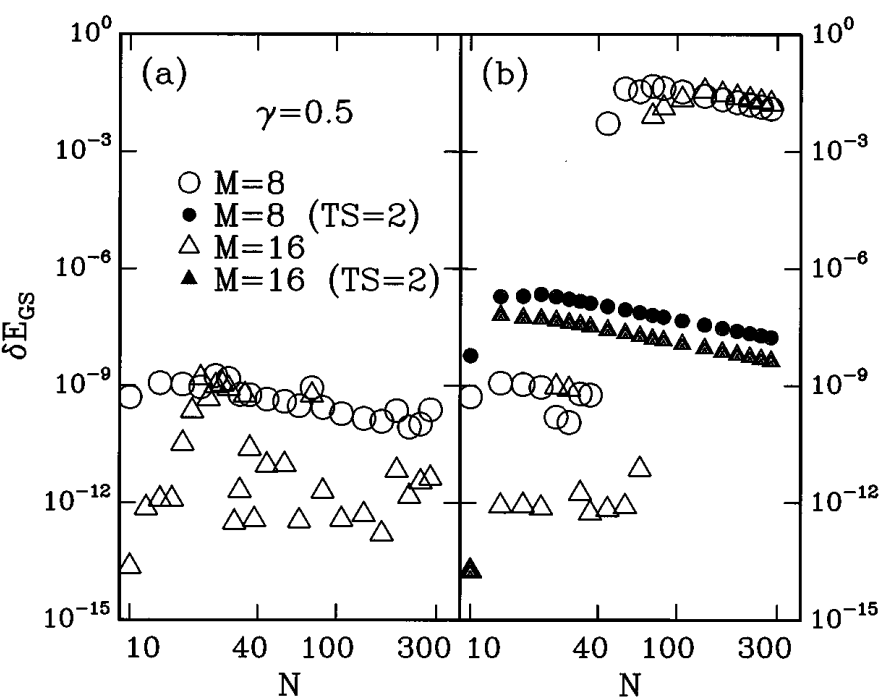
Critical point:

The errors **gradually increases as increase N** .



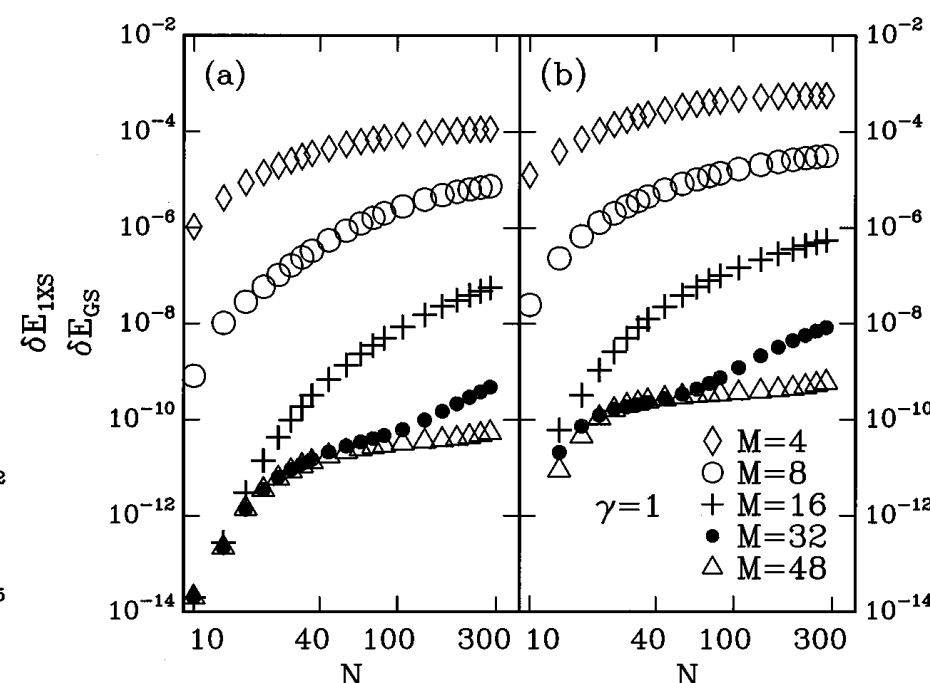
$$0 \leq h < h_c$$

$$h = 0.25$$



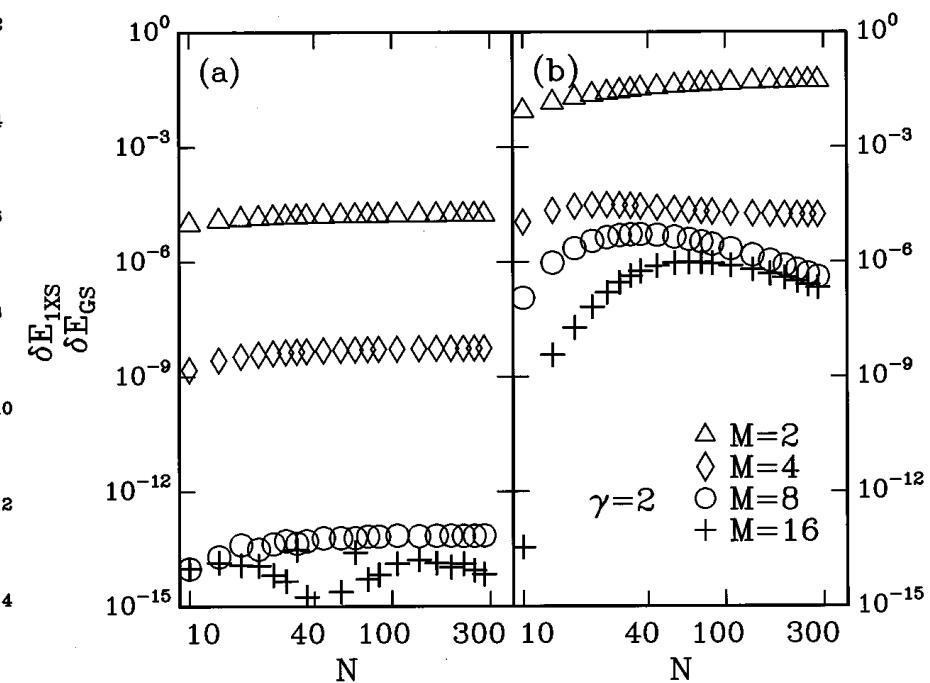
$$h = h_c$$

$$h = 0.5$$



$$h_c < h$$

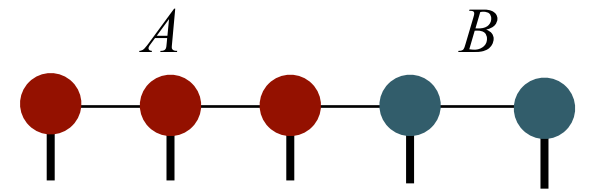
$$h = 1.0$$



Entanglement entropy of TFI model

Entanglement entropy:

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



State	EE of the original vector	Required bond dimension
Ferro or Disordered	$S_A = O(1)$	$\chi = O(1)$
Critical	$S_A = O(\log N)$	$\chi = O(N^\alpha)$

We need **polynomially large** bond dimension for critical system!

➡ More efficient tensor network for critical systems?

Key point: **Scale invariance** of the system

Higer dimensional system

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

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

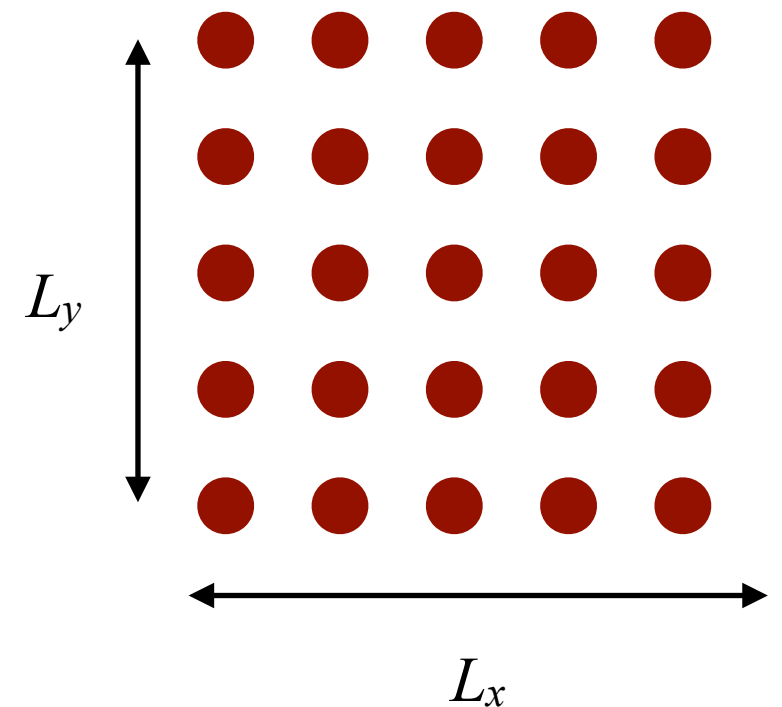
$\sum_{\langle i,j \rangle}$:Summation over the
nearest neighbor pair

Area law

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

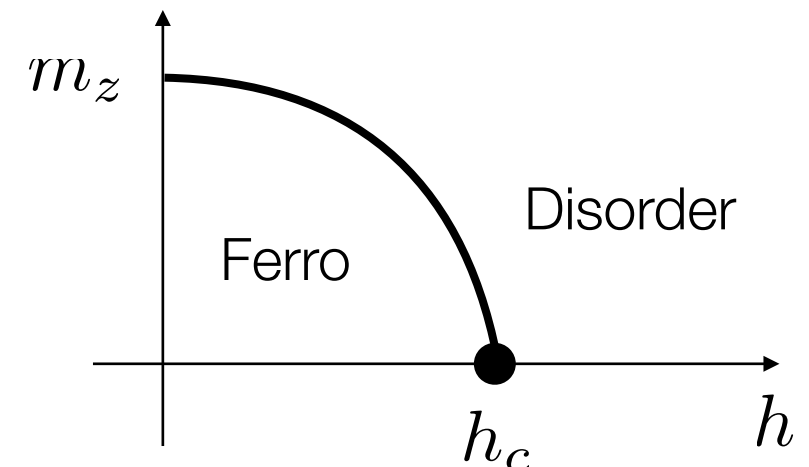
$$S_A \sim \sqrt{N} = L$$

Two-dimensional array



$$N = L_x \times L_y$$

Phase diagram

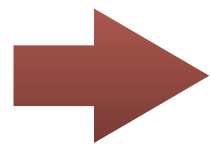


MPS for two-dimensional system

When we apply MPS representation for a square lattice system:

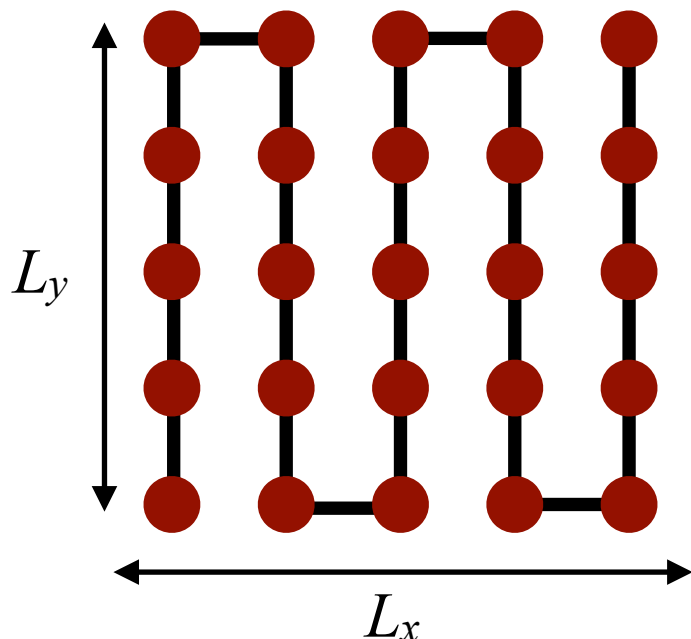
Setting **(1)** $S_A \leq L_x \log \chi$:Satisfying area law?

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



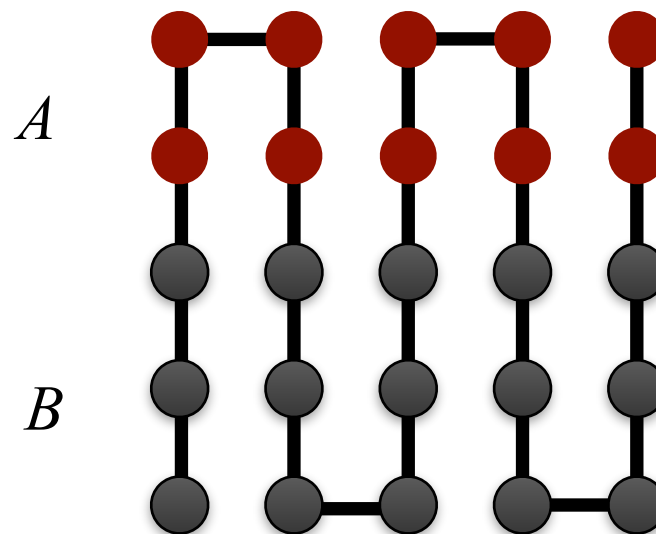
MPS cannot cover the area law of the entanglement entropy in higher (d =2,3, ...) dimensions.

Possible MPS
(Snake form)

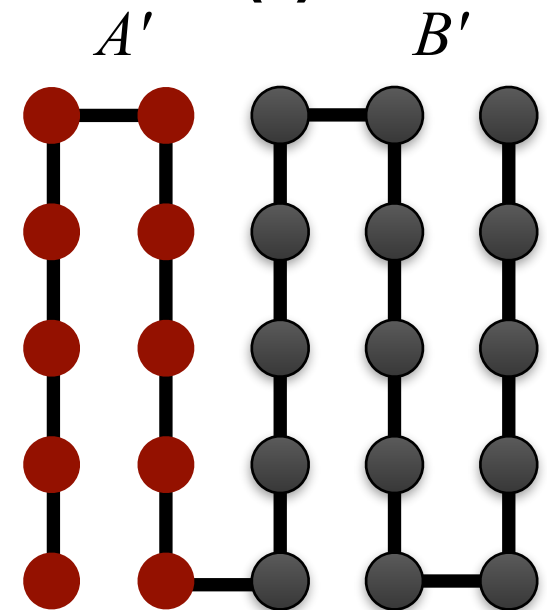


Two settings of **system** and **environment**

(1)



(2)



MPS for two-dimensional system: comment

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

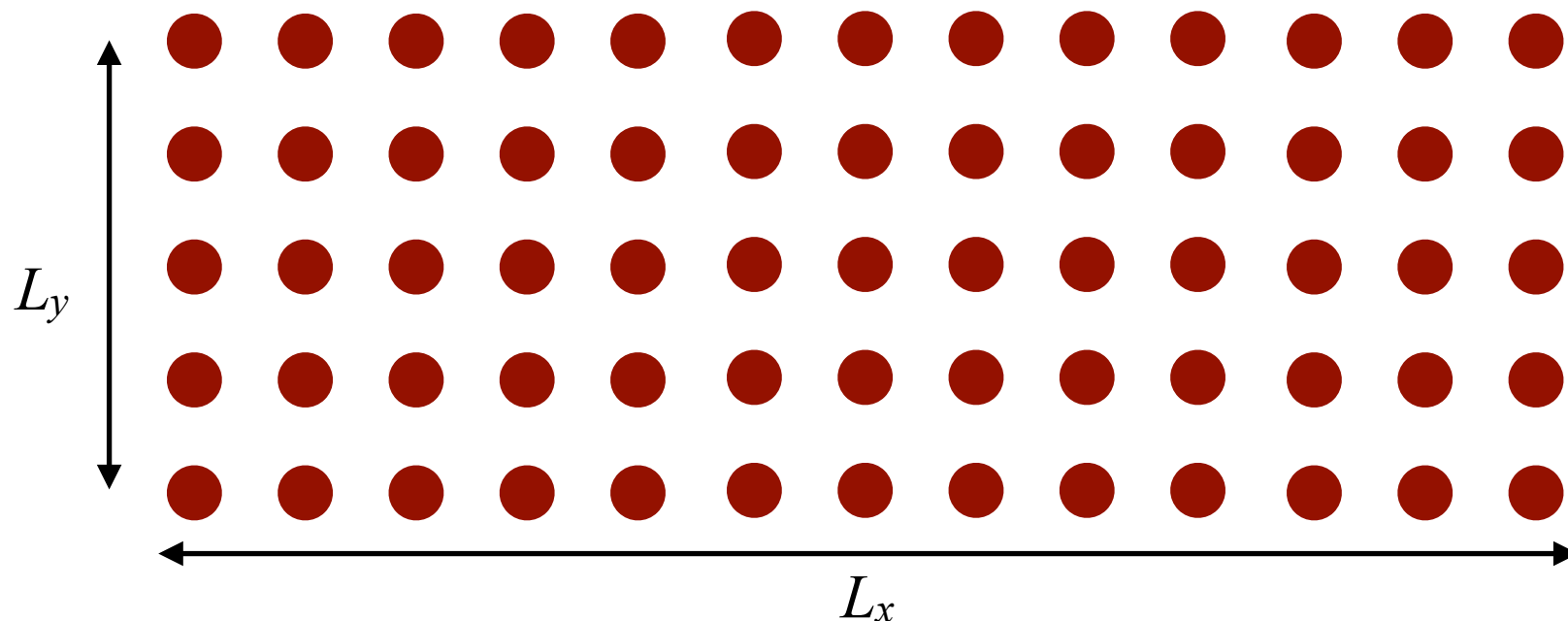
In setting (1), MPS can satisfy the area law **partially**.

➡ We can **increase** L_x easily with **keeping** L_y constant.

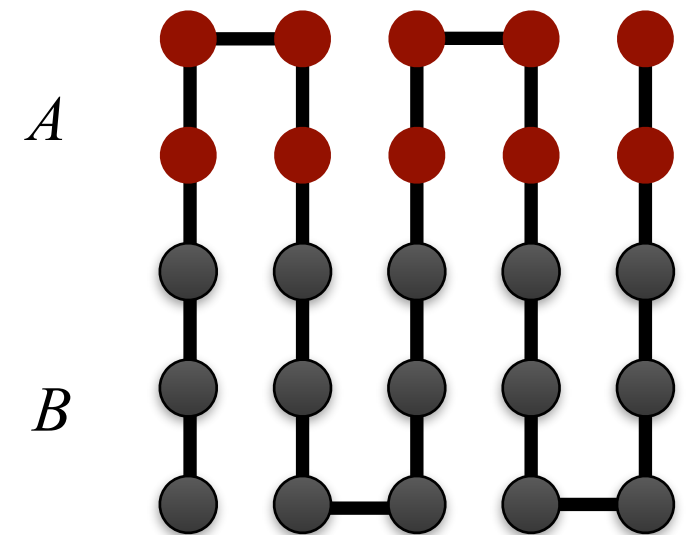
$$\chi = O(e^{L_y})$$

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

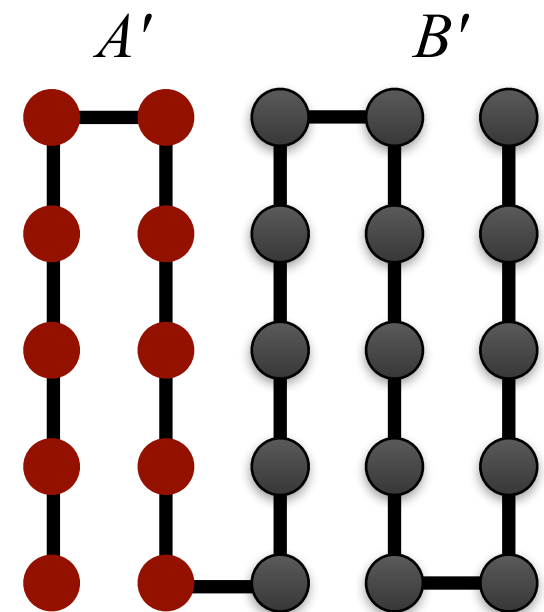
Quasi one dimensional system ("strip" or "cylinder")



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




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

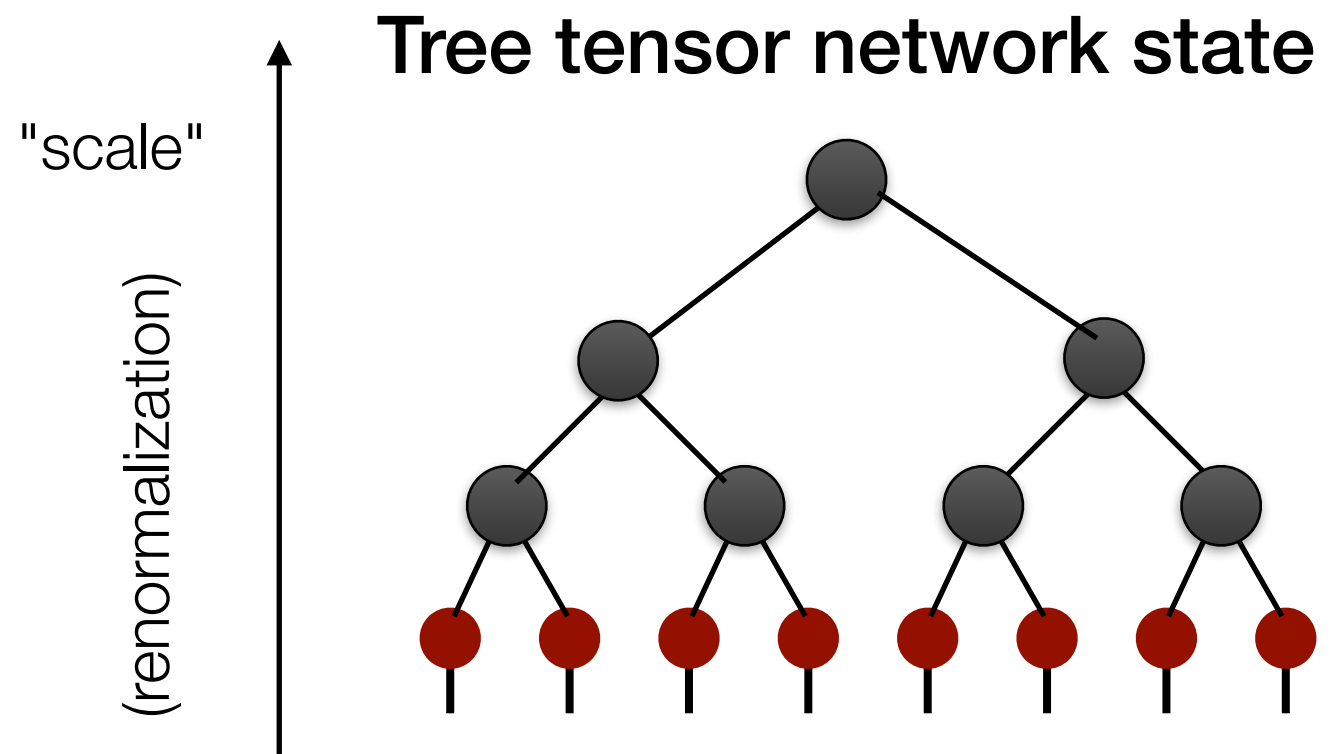
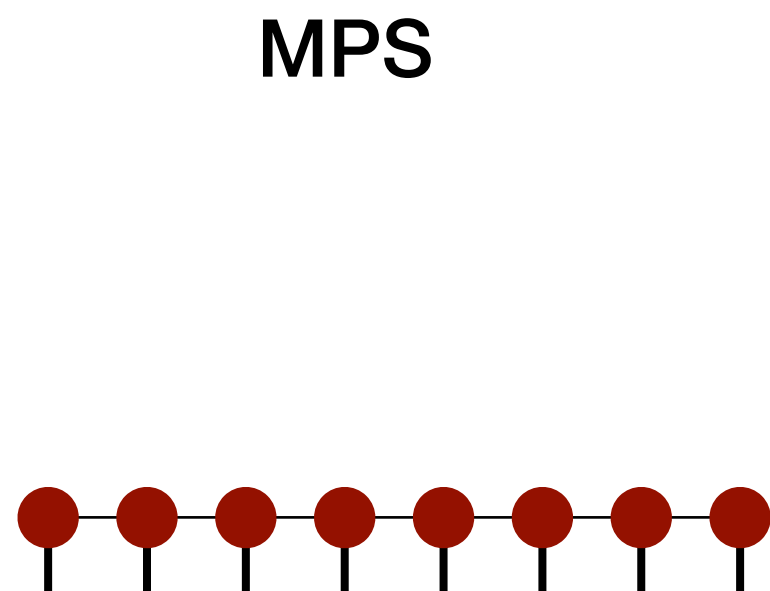


Tensor network for critical systems:
Multi-scale Entanglement Renormalization Ansatz

Hierarchical structure: tree tensor network

Critical system  Scale invariance

A simple scale invariant tensor network: **tree tensor network**



Notice:

Unitary tensors

Unitary tensor

$$U_{ij}^{kl} = \begin{array}{c} |k\rangle \quad |l\rangle \\ \boxed{U} \\ |i\rangle \quad |j\rangle \end{array}$$

$$(U^\dagger)_{kl}^{ij} = (U_{ij}^{kl})^*$$

$$\sum_{i,j} U_{ij}^{kl} (U^\dagger)_{k'l'}^{ij} = \delta_{kk'} \delta_{ll'}$$

$$\begin{array}{c} |k\rangle \quad |l\rangle \\ \boxed{U} \\ |k'\rangle \quad |l'\rangle \end{array} \quad \boxed{U^\dagger} \quad \begin{array}{c} |k\rangle \quad |l\rangle \\ |k'\rangle \quad |l'\rangle \end{array} = \begin{array}{c} |k\rangle \quad |l\rangle \\ |k'\rangle \quad |l'\rangle \end{array}$$

$$\sum_{k,l} (U^\dagger)_{kl}^{ij} U_{i'j'}^{kl} = \delta_{ii'} \delta_{jj'}$$

$$\begin{array}{c} |i\rangle \quad |j\rangle \\ \boxed{U^\dagger} \\ |i'\rangle \quad |j'\rangle \end{array} \quad \boxed{U} \quad \begin{array}{c} |i\rangle \quad |j\rangle \\ |i'\rangle \quad |j'\rangle \end{array} = \begin{array}{c} |i\rangle \quad |j\rangle \\ |i'\rangle \quad |j'\rangle \end{array}$$

Isometric tensors

Isometric tensor (half unitary tensor) = Isometry

$$W_{ij}^k = \text{triangle diagram} \quad \sum_{i,j} W_{ij}^k (W^\dagger)_{k'}^{ij} = \delta_{kk'} \quad \text{stacked triangles} = \text{vertical line}$$

The diagram shows the definition of an isometric tensor W_{ij}^k as a triangle with a top leg labeled k and two bottom legs labeled i and j . It then shows the unitarity condition for the bottom legs: $\sum_{i,j} W_{ij}^k (W^\dagger)_{k'}^{ij} = \delta_{kk'}$. This is represented by two stacked triangles (one pointing up, one pointing down) with legs labeled k and k' , which is equal to a single vertical line with legs labeled k and k' .

Unitarity condition only for "bottom" legs.

Isometry works as a "projector" from the bottom space to the top space.

$$\dim(\text{bottom}) \geq \dim(\text{top})$$

It is also related to the "renormalization" of degree of freedoms.

We pick up "important" degree of freedoms by isometries.

Isometric tree tensor network and its scale invariance

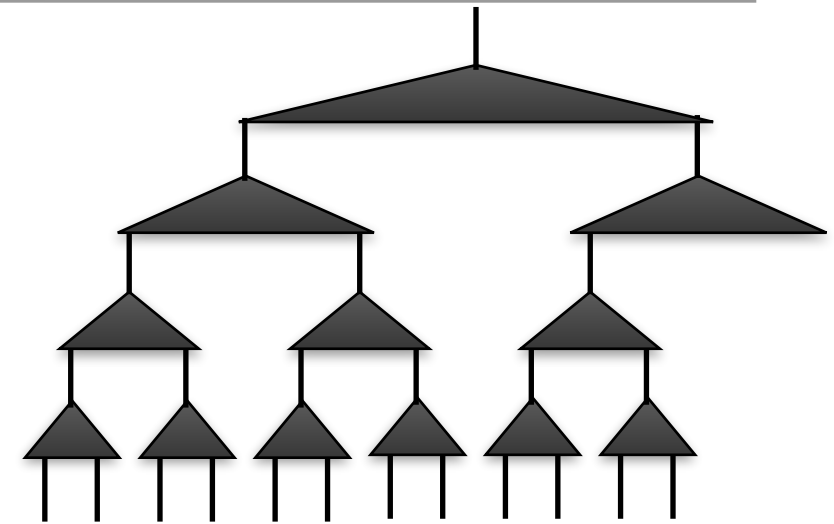
Consider an (infinite) tree tensor network consists of **identical isometries** as a wave function.

Properties:

1. It is normalized as $\langle \Psi | \Psi \rangle = 1$
(Trivial from the definition of the isometry)

2. It can be scale invariant.

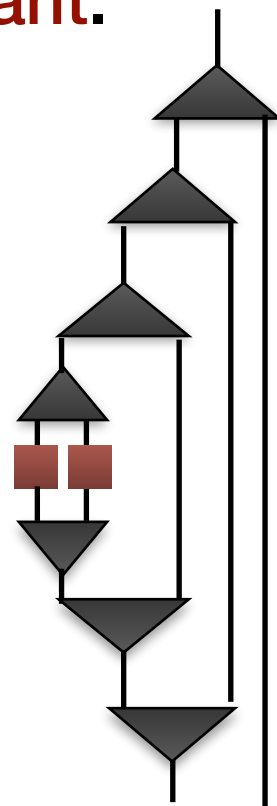
$$|\Psi\rangle =$$



$$C(1) \equiv \langle \Psi | S_1^z S_2^z | \Psi \rangle =$$

$$S_i^z =$$

spin

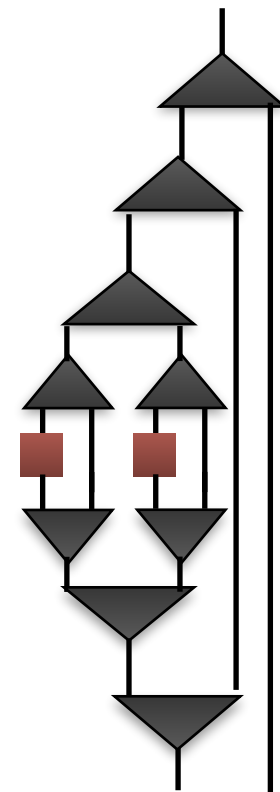


...

$$C(2) \equiv \langle \Psi | S_1^z S_3^z | \Psi \rangle =$$

$$(S_i^z)' =$$

"renormalized" spin



...

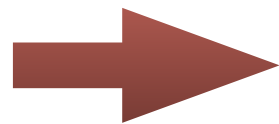
➡ If $(S_i^z)' = 2^{-p} S_i^z$, then $C(2r) = 2^{-2p} C(r)$

Scale invariant!

Entanglement entropy of TTN

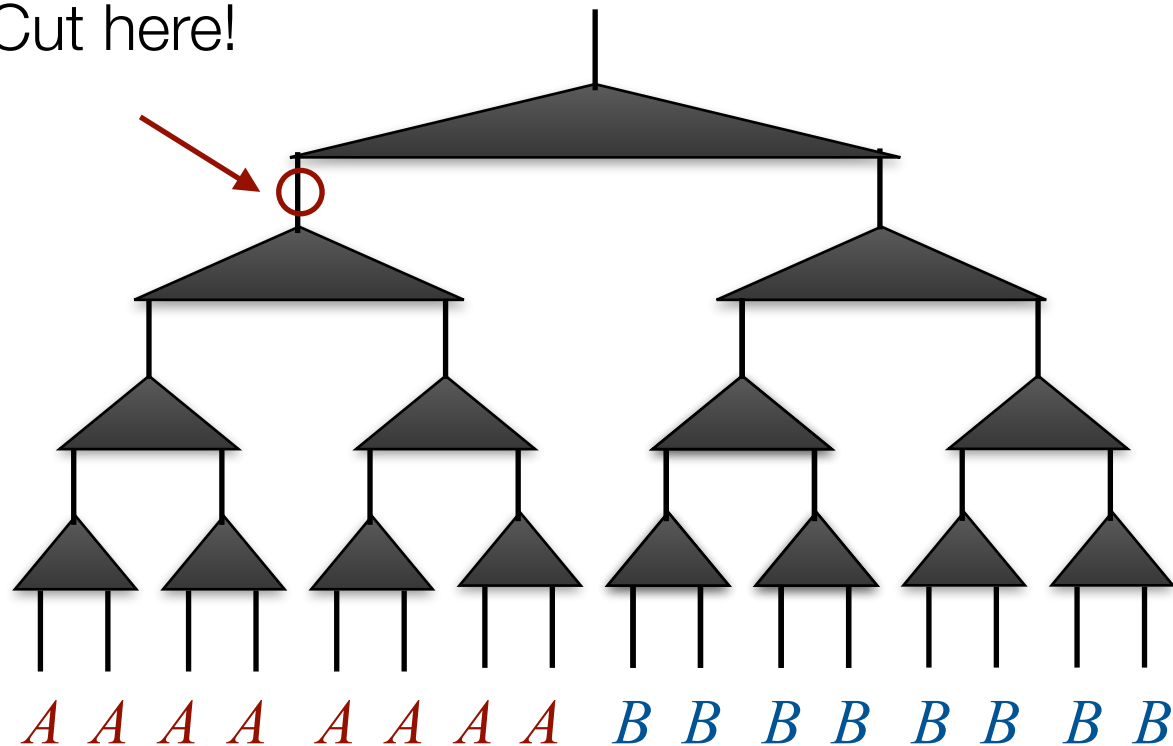
Entanglement entropy of tree tensor networks (TTN):

Due to the tree structure, two regions are connected by only "one bond".
(or a few)

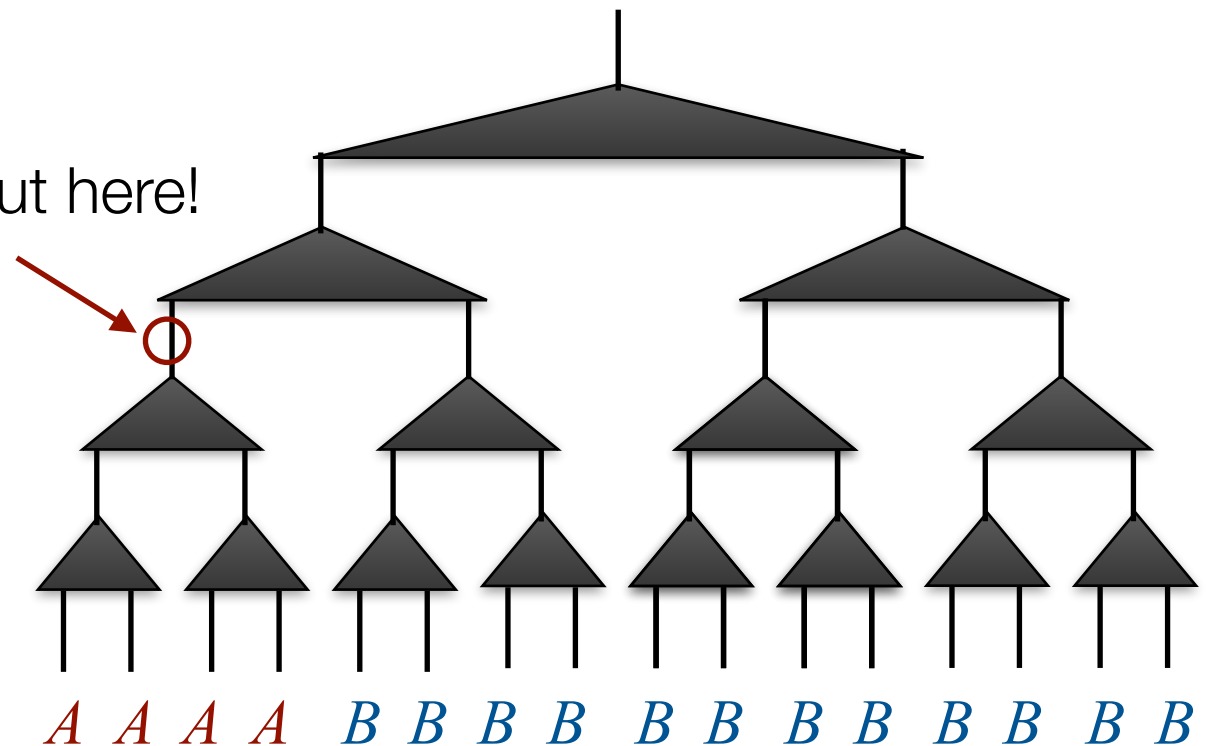


$$S_A = -\text{Tr } \rho_A \log \rho_A \leq \log \chi$$

Cut here!



Cut here!



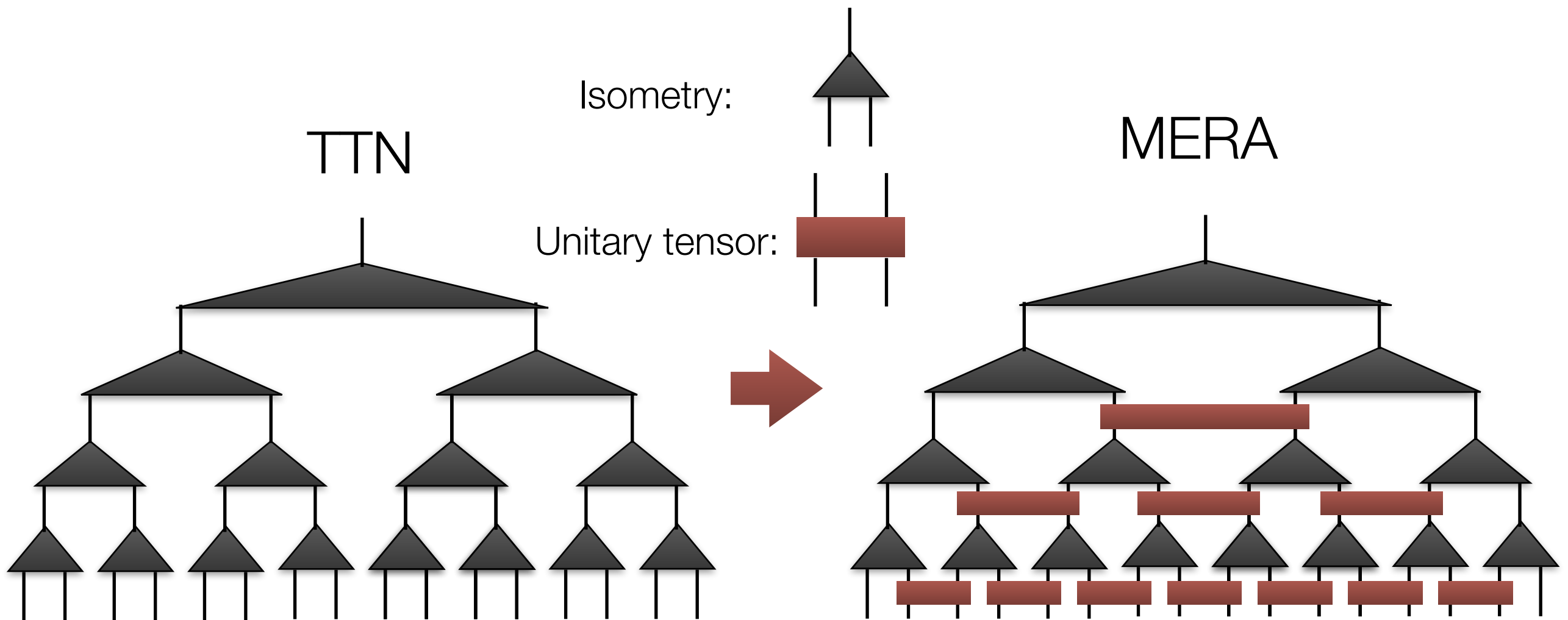
MERA

(G. Vidal, Phys. Rev. Lett. **99**, 220405 (2007))

(G. Vidal, Phys. Rev. Lett. **101**, 110501 (2008))

Multi-scale Entanglement Renormalization Ansatz (**MERA**)

Before applying isometry, insert a **unitary tensor**.

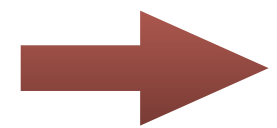


☒ Normalization

☒ Scale invariance (if we set the identical tensors)

Entanglement entropy of MERA

Due to the unitary matrices, # of bonds connecting **two regions** **logarithmically increase**.

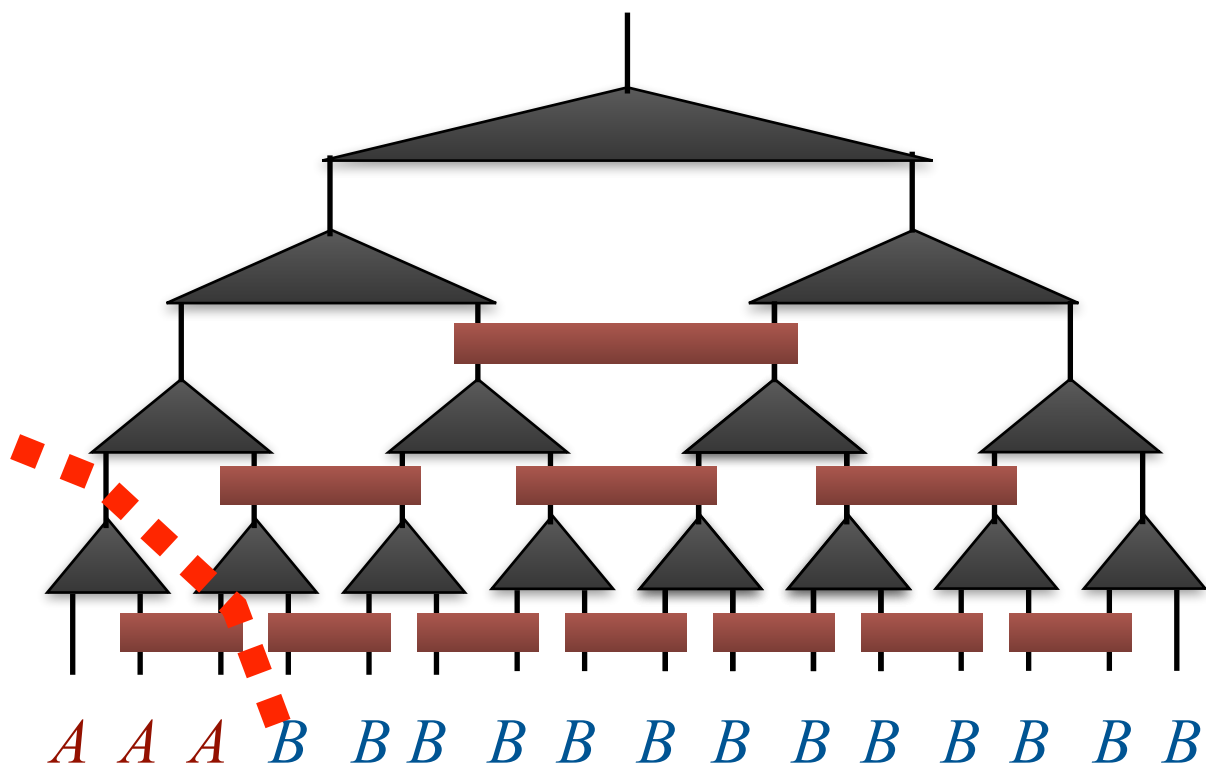


$$\text{rank } \rho_A \leq \chi^{N_c(N)} \sim \chi^{\log N}$$

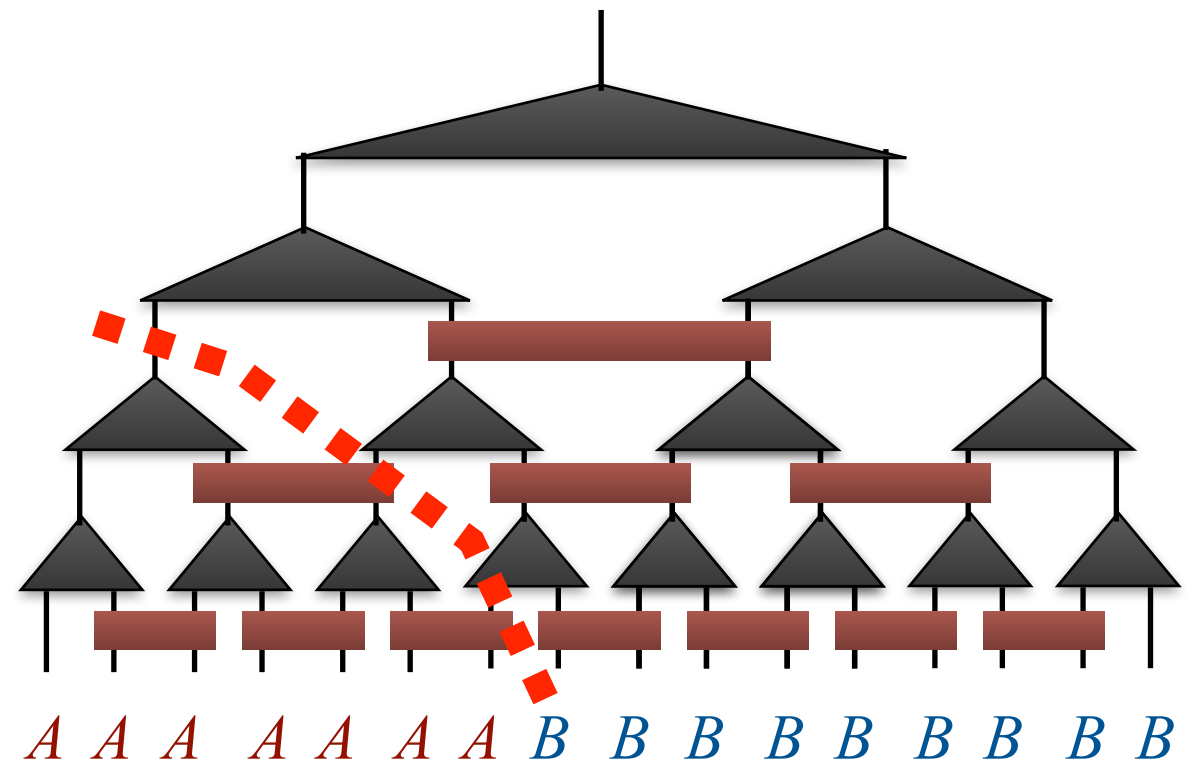
$$S_A = -\text{Tr } \rho_A \log \rho_A \leq (\log \chi) \log N$$

$N_c(N)$

of minimum cut
for a N -site region



Minimum # of cuts = 2



Minimum # of cuts = 3

Application of MERA

Transverse field Ising chain:

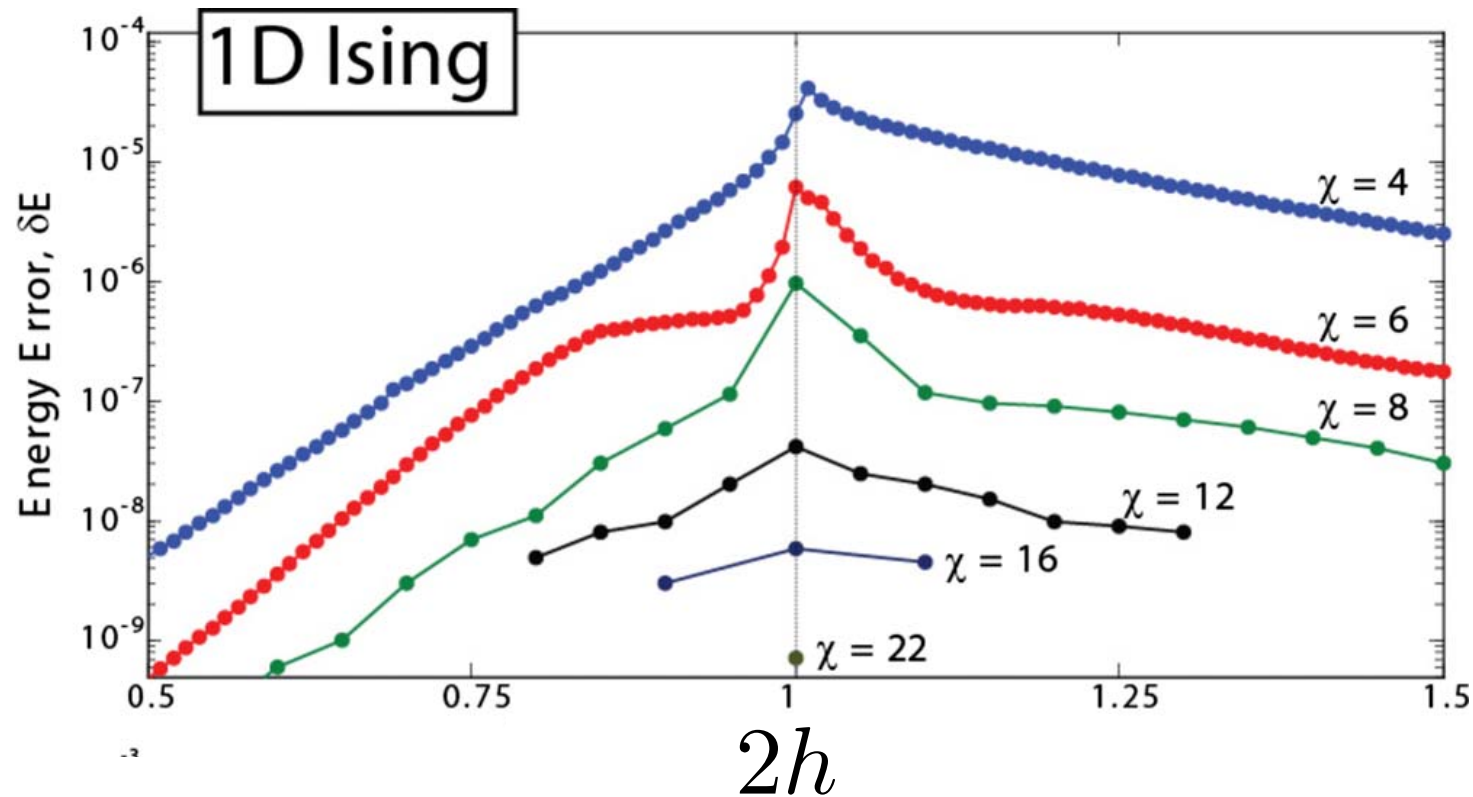
$$\mathcal{H} = - \sum_{i=1}^{N-1} S_i^z S_{i+1}^z - h \sum_{i=1}^N S_i^x$$

MERA can represent
very large (Infinite)
critical system!

Energy errors:

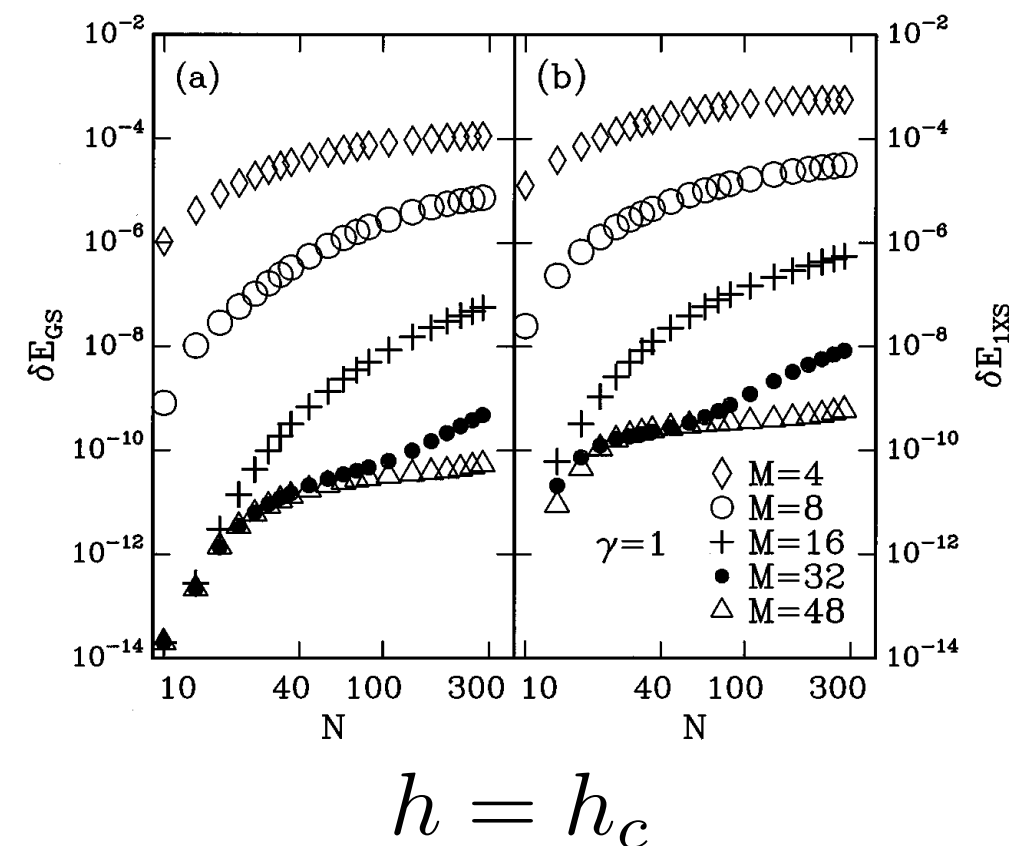
MERA (Infinite chain)

(G. Evenbly and G. Vidal, Phys. Rev. B. **79**, 144108 (2009))



DMRG (finite chain)

Ö. Legeze, and G. Fáth (1996)



Interesting topics related to MERA

- By using scale invariance of MERA, we can calculate **properties of critical system** accurately.
(G. Evenbly and G. Vidal, Phys. Rev. B. **79**, 144108 (2009))
(R.N.C. Pfeifer, (G. Evenbly and G. Vidal, Phys. Rev. A. **79**, 040301(R) (2009))
 - Critical exponents and Operator product expansion coefficients in the Conformal Field Theory (CFT)
- We can consider MERA in higher dimensions
 - It is scale invariant **but satisfies the area law**
(G. Evenbly and G. Vidal, Phys. Rev. Lett. **102**, 180406 (2009))
 - For the system **with logarithmic correction** in the EE, such as **metal**, "branching MERA" has been proposed.
(G. Evenbly and G. Vidal, Phys. Rev. Lett. **112**, 220502 (2014))
(G. Evenbly and G. Vidal, Phys. Rev. B. **89**, 235113 (2014))
- Relation between MERA and other fields
 - Wavelet transform (G. Evenbly and S. R. White, Phys. Rev. Lett. **112**, 140403 (2016))
 - AdS/CFT (quantum gravity, black hole)
(M. Nozaki, S. Ryu, and T. Takayanagi, J. High Energy Phys. **10**, 193 (2012))

Tensor network for higher dimensional systems:
Tensor Product State
(Projected Entangled Pair State)

Entanglement entropy in higher dimensions

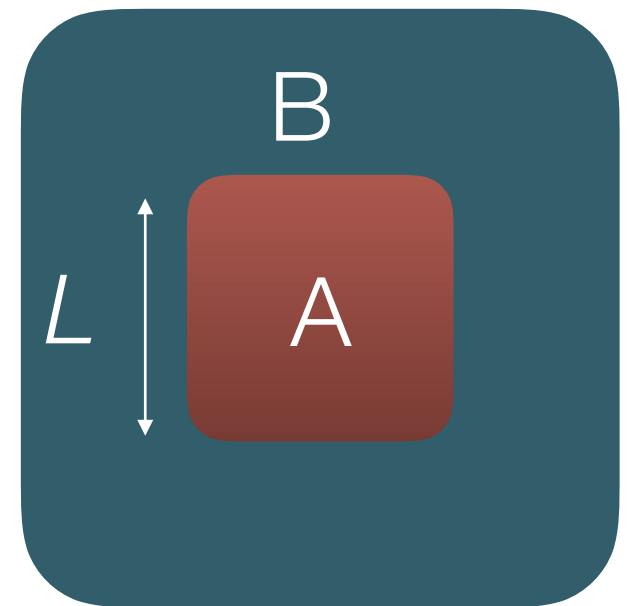
Ground state wave functions:

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

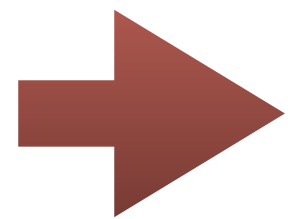
J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys, 277, **82** (2010)

Area low:

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



In $d=1$, MPS satisfies the area law.



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

A. It is Tensor Product State (TPS)!

Tensor Product State (TPS)

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

PEPS (Projected Entangled-Pair State)

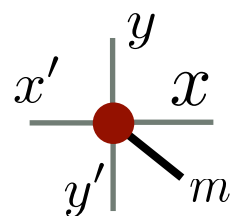
(F. Verstraete and J. Cirac, arXiv:cond-mat/0407066)

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

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

Tr: tensor network “contraction”

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



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

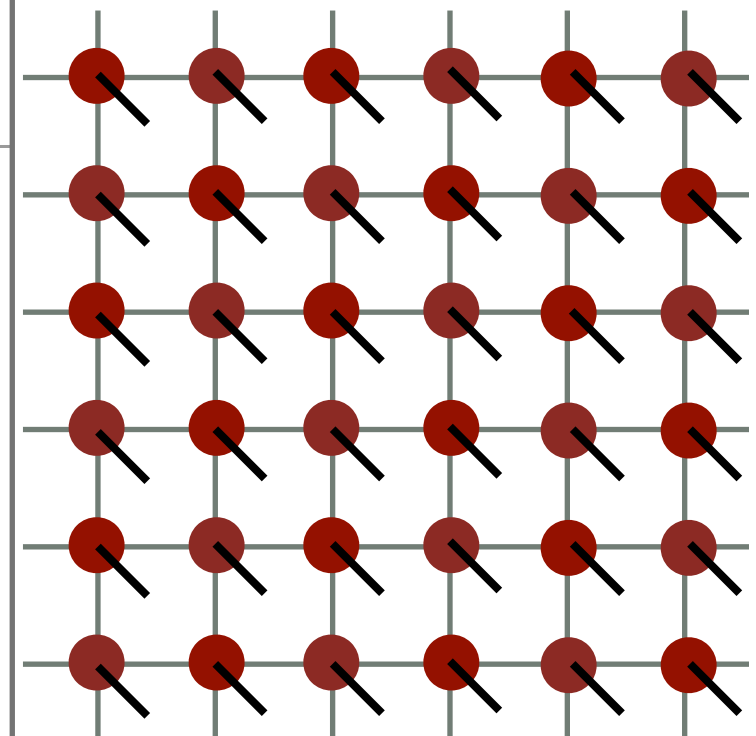
D = “bond dimension”

$m_i = 1, 2, \dots m$

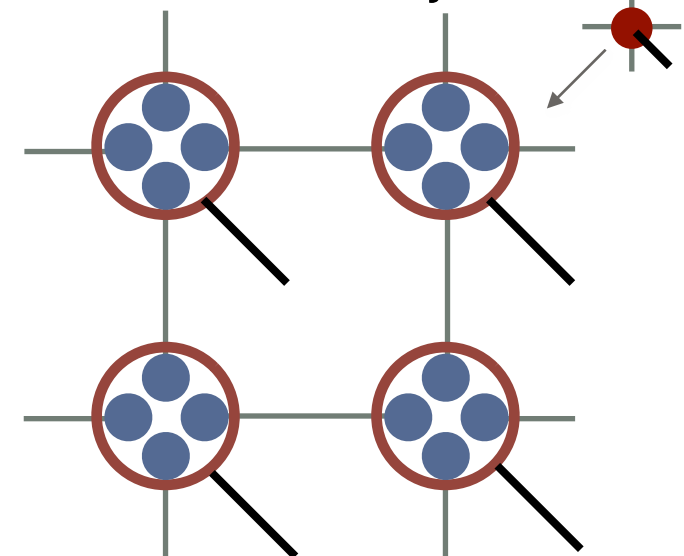
m = dimension of the local Hilbert space

* D can be larger than m . “Virtual state”

TPS on square lattice

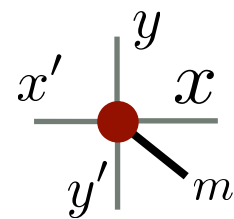
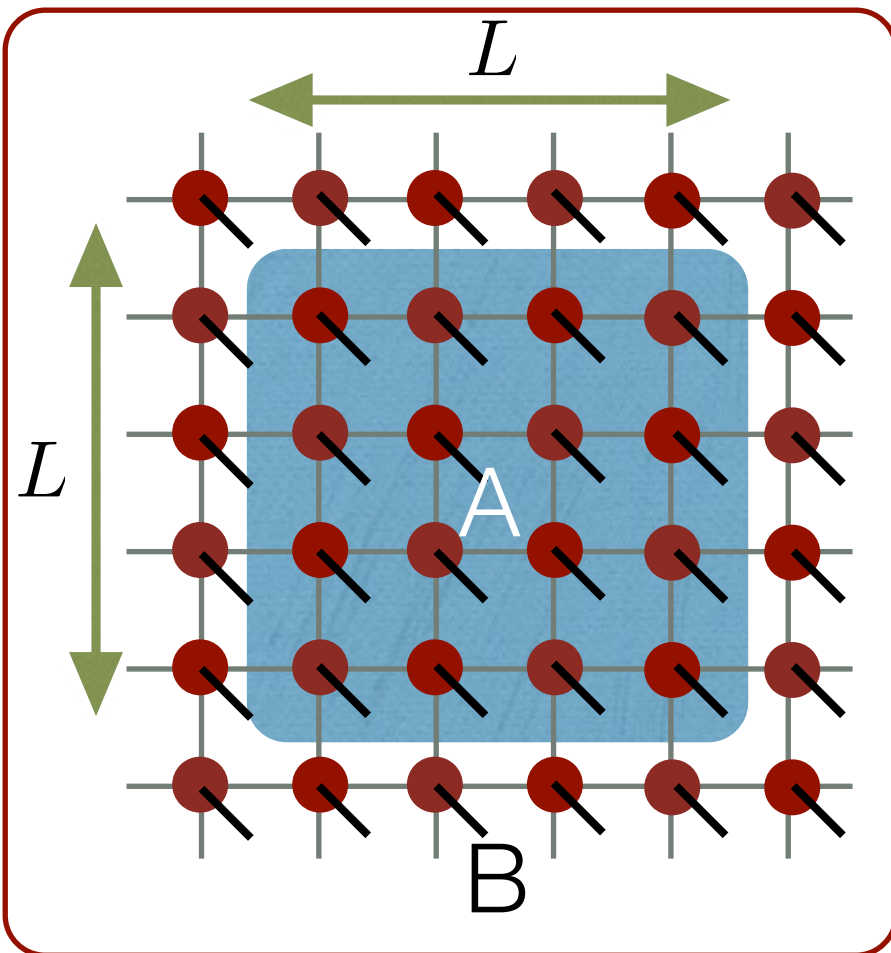


Tensor = Projector



Maximally entangled state
between D -state spins

Entanglement entropy of TPS (PEPS)



Bond dimension = D

of bonds connecting regions A and B

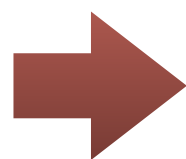
$$N_c(L) = 4L \quad (\text{square lattice})$$

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

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

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

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!

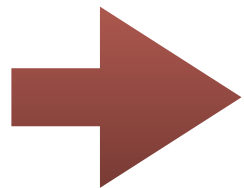
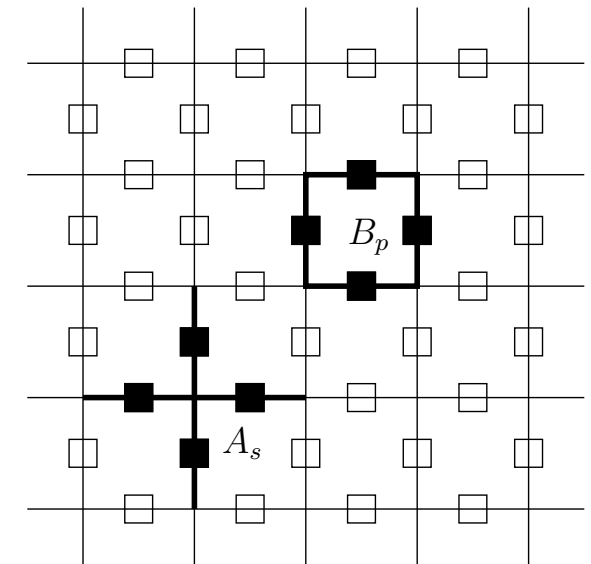
Example: Ground state represented by TPS

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 \mathbb{Z}_2 spin liquid state.

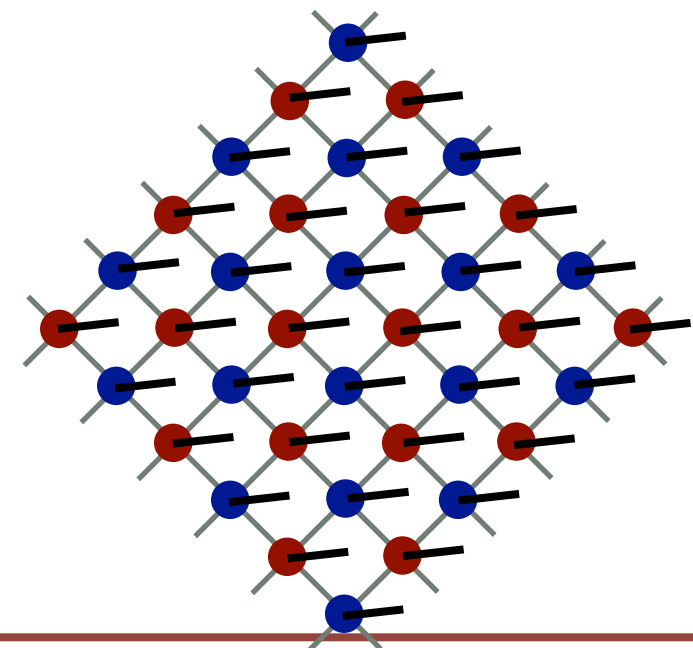
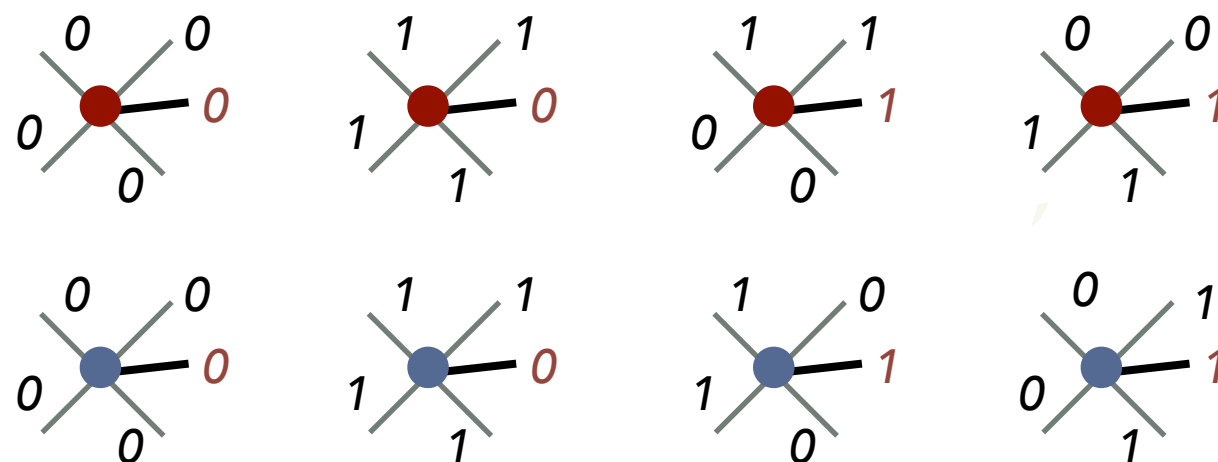
"Spin liquid" is a novel phase different from conventional magnetic orders.

It can be represented by D=2 TPS.

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

0,1: eigen state of σ_x

(Non-zero elements of tensor)



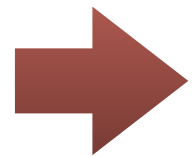
Difference between MPS and TPS

Cost of tensor network contraction:

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

MPS: $O(N)$

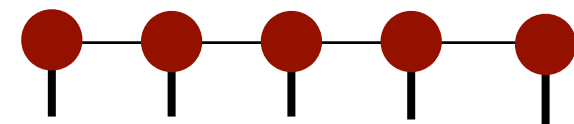
TPS: $O(e^{L^{d-1}})$



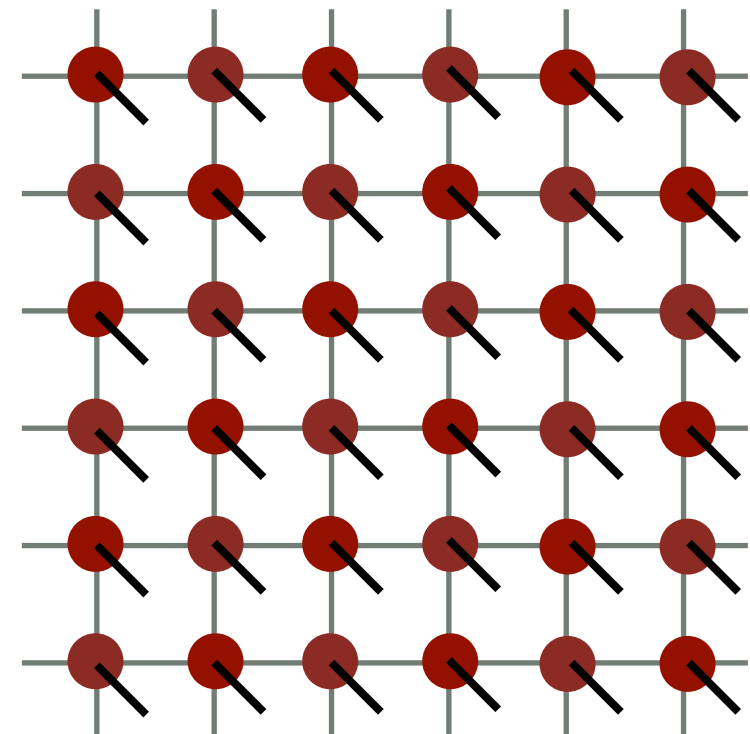
It is **impossible** to perform exact contraction even if we know local tensors in the case of TPS.

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

MPS



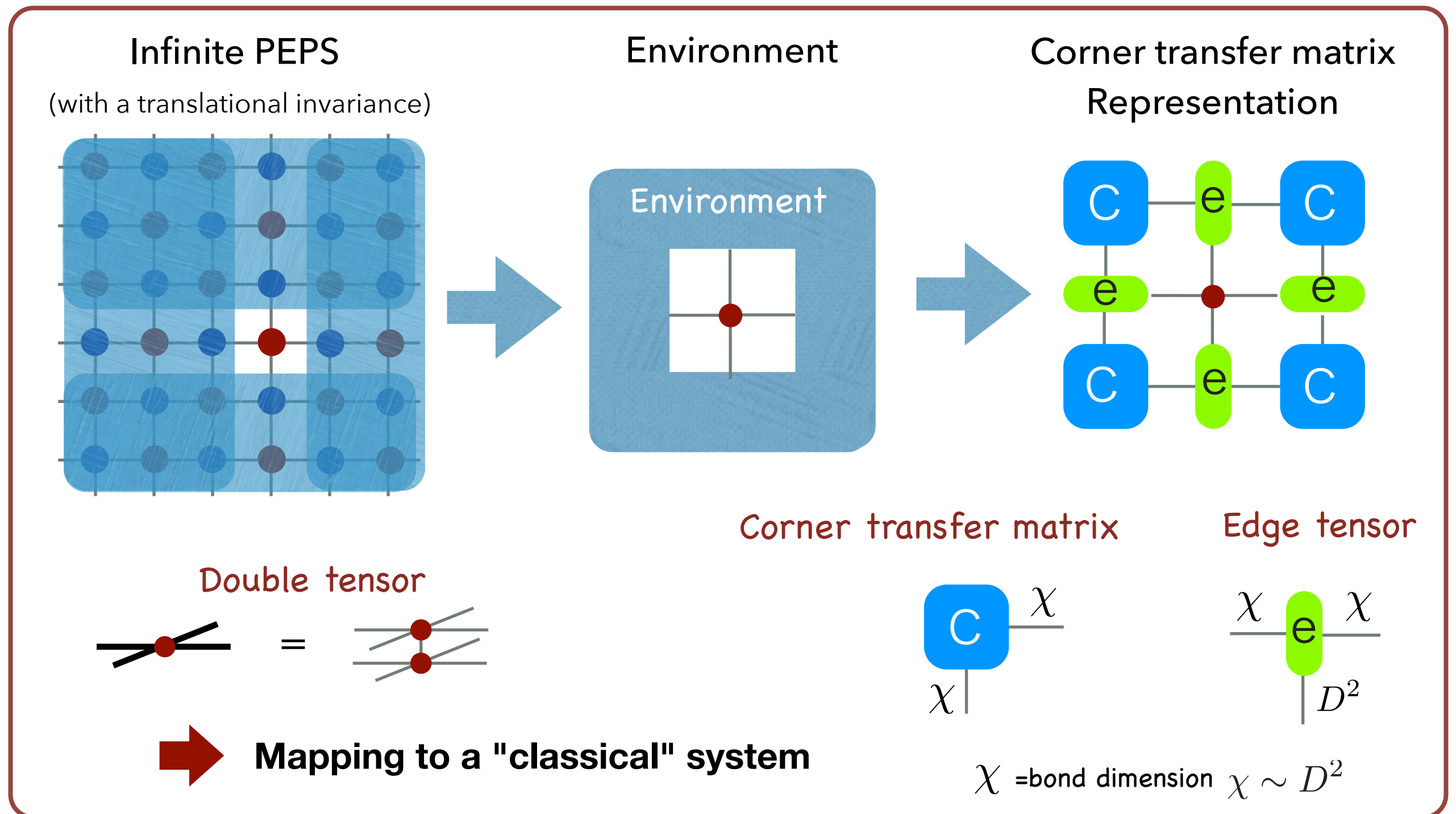
**TPS
(PEPS)**



Example of approximate contraction: CTM 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))



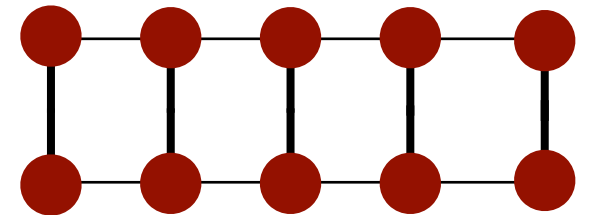
Cost of (approximate) contraction

MPS:

χ — — χ ($m \ll \chi$)

$$\text{Diagram 1} \times \text{Diagram 2} = \text{Diagram 3} \quad \boxed{O(\chi^3)}$$

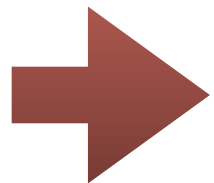
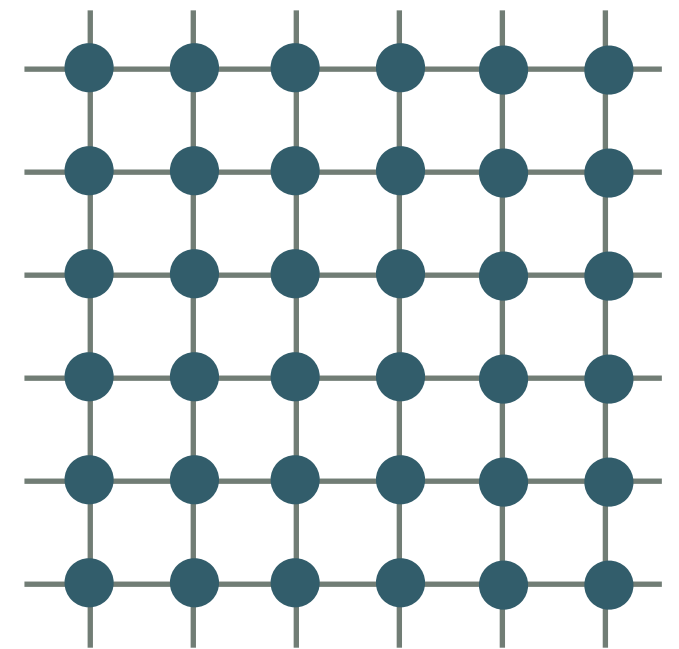
$$\langle \Psi | \Psi \rangle =$$



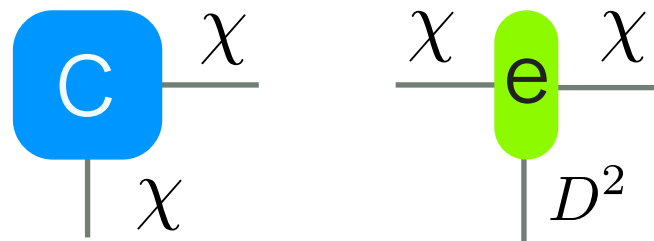
TPS:

A diagram of a vertex, represented by a red dot. Five half-edges extend from the vertex: one straight line to the top-left labeled D , one straight line to the top-right labeled D , one straight line to the left labeled D , one straight line to the bottom labeled D , and one diagonal line to the bottom-right labeled m .

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



When we use CTM environment in 2D,



$$O(\chi^2 D^6), O(\chi^3 D^4) \sim O(D^{10}) \quad (\chi \sim D^2)$$

We can treat very small bond dimensions in TPS!

The diagram shows an equality between two Feynman diagrams. On the left, two vertices (red circles) are connected by a vertical line. Each vertex has two external lines (gray) extending from it. On the right, a single vertex (blue circle) is shown with four external lines (black) extending from it. The lines are labeled D^2 .

Application of TPS to eigenvalue problem

For calculation of minimum eigenvalues and its eigenvector,
we can use similar techniques to those in MPS

Variational method:

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

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

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

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 $\langle \Psi_{\text{GS}} | \Psi_0 \rangle \neq 0$

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

(J. Jordan *et al*, Phys. Rev. Lett. **101**, 250602 (2008))

Example of application: Honeycomb lattice Kitaev Model

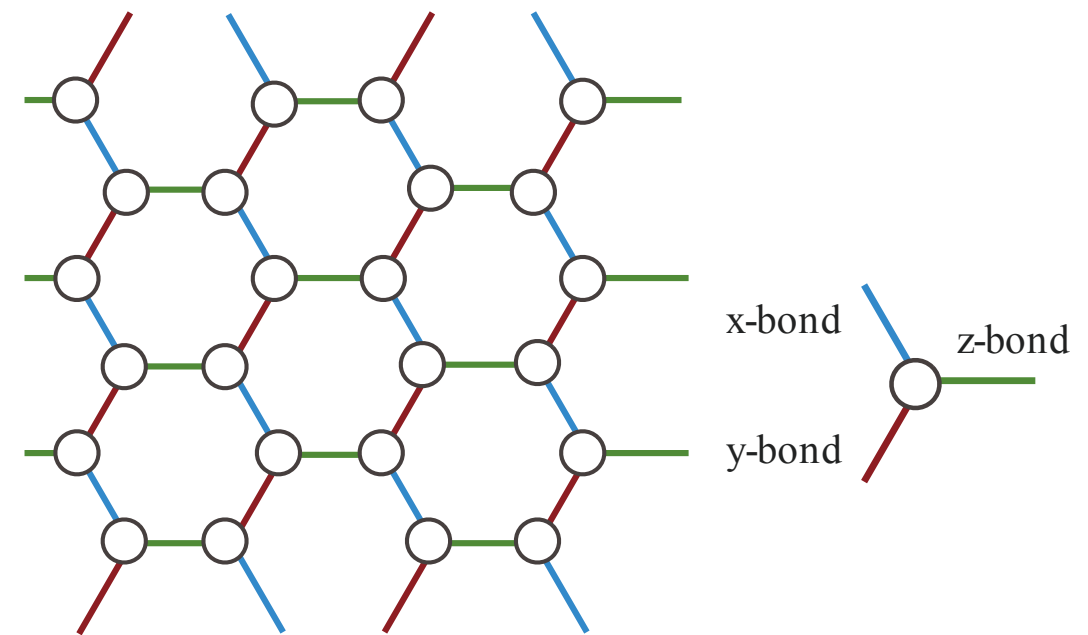
A. Kitaev, Annals of Physics 321, 2 (2006)

Kitaev model

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

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**

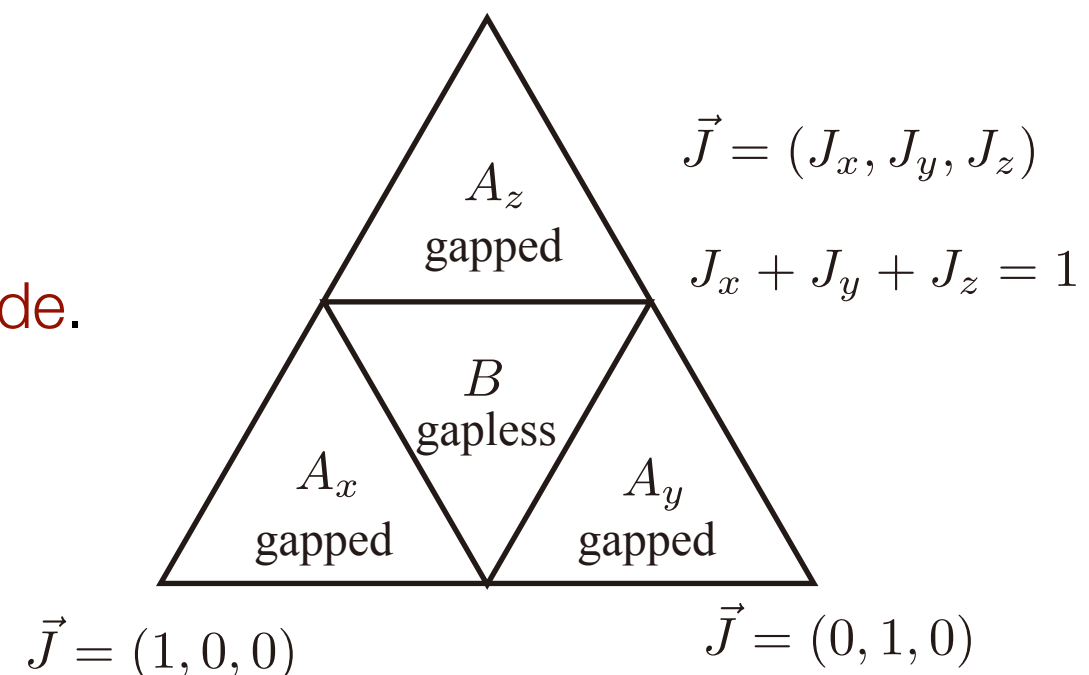
Anisotropic region (A) : gapped **spin liquid**

Cf. The anisotropic limit corresponds to the **Toric code**.

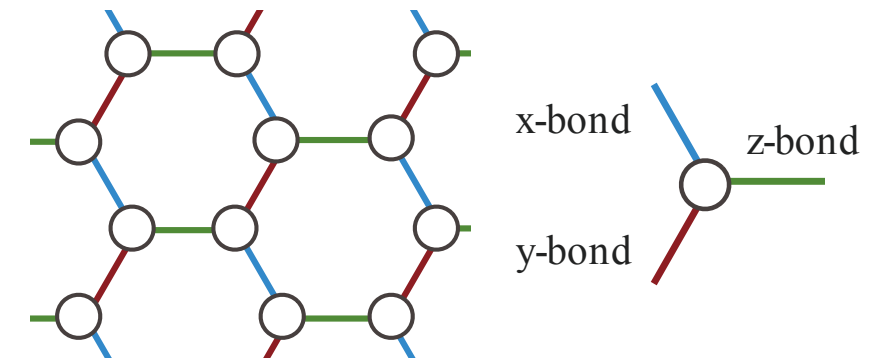
*Recently, researchers have realized that this type of models might appear in real materials.
Hot topic!

Phase diagram

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



Application : Kitaev spin liquid



Honeycomb lattice Kitaev model

At $J_x = J_y = J_z$, the ground state is
a gapless spin liquid.

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

$(\gamma = x, y, z)$

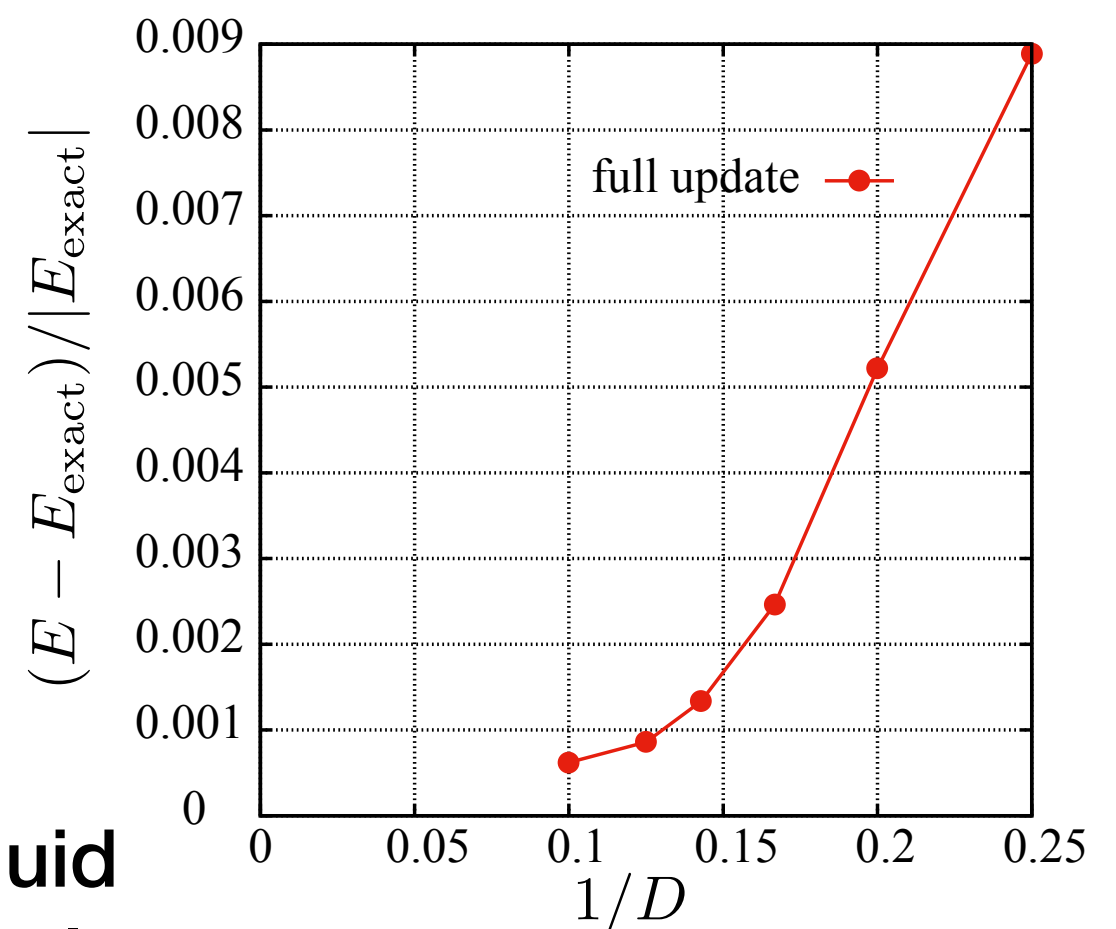
In the present (super)computers,
we can access around $D=10$ (maybe 16)
by using massively parallel code.

The error of the ground state
energy is **less than 10^{-3}**
for **infinite system!**

➔ **iTPS can represent Kitaev spin liquid
in the thermodynamic limit accurately.**

Energy error obtained by iTPS

(T. okubo et al, unpublished)



Interesting topics related to TPS

- Application to itinerant electron system, **which may break the area law**
(P. Corboz et al, Phys. Rev. B. **81**, 165104 (2010))
(P. Corboz, Phys. Rev. B. **93**, 045116 (2016))
- Characterization of topologies in wave function
 - **Symmetric tensor network and modular matrix**
(J.-W. Mei et al, Phys. Rev. B. **95**, 235107 (2017))
- Application to three dimensions
 - So far, there is no practical calculations for non-trivial models.
 - Mainly, due to the scaling: $O(D^{18})$?

Next week

- 第 1 回： 現代物理学における巨大なデータ
- 第 2 回： 現代物理学と情報圧縮
- 第 3 回： 情報圧縮の数理 1 (線形代数の復習)
- 第 4 回： 情報圧縮の数理 2 (特異値分解と低ランク近似)
- 第 5 回： 情報圧縮の数理 3 (スパース・モデリングの基礎)
- 第 6 回： 情報圧縮の数理 4 (クリロフ部分空間法の基礎)
- 第 7 回： 物質科学における情報圧縮
- 第 8 回： データ解析の高速化：スパース・モデリングの物質科学への応用
- 第 9 回： データ空間の圧縮：クリロフ部分空間法の物質科学への応用
- 第 10 回： 高度なデータ圧縮：情報のエンタングルメントと行列積表現
- 第 11 回： 行列積表現の固有値問題への応用
- 第 12 回： テンソルネットワーク表現への発展
- 第 13 回： テンソルネットワーク繰り込みによる情報圧縮**

Information compression by tensor network renormalization